

Simon A. Mathias

Hydraulics, Hydrology and Environmental Engineering



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Preface

This textbook has been developed from lecture notes used to teach M.Eng. and M.Sc. engineering students at Durham University. The book is split up into three parts containing ten chapters each. Part I is based on a taught module concerning civil engineering hydraulics. Part II is based on a taught module concerning hydrology and water resources. Part III is based on a taught module concerning environmental engineering.

The first five chapters of Part I cover a range of classical hydraulic topics including hydrostatics, Bernoulli equation, pipe flow, open channel flow and Airy waves. The remaining chapters include derivations of the shallow-water equations, method of characteristics solutions for the kinematic wave equation, Laplace transform solutions for the diffusion wave equation and numerical solutions obtained by the finite difference method. It is also shown how the advection-dispersion equation (analogous to the diffusion wave equation) can be used to describe chemical transport and heat transport in porous media.

Part II includes a comprehensive set of hydrological topics, with a focus on mathematical model formulation and derivation of analytical solutions. The first chapter looks at flood frequency analysis. The next four chapters look at groundwater flow, covering topics including Darcy's law, the Forchheimer equation, method of images, the specific storage coefficient, specific yield and pumping test analysis. The remaining chapters look at unsaturated flow processes, humidity measurement, potential evapotranspiration, solar radiation and rainfall runoff modelling.

Part III contains three chapters about environmental economics, three chapters about air pollution, three chapters about water quality and a final chapter about environmental impact assessment and uncertainty management. The objective of the environmental economics chapters is to help engineering students better ascribe value to environmental improvement. Economics topics covered include tragedy of the commons, cash flow analysis, supply and demand modelling, ecosystem services and cost of pollution on health. Air pollution topics covered include air quality control technologies, carbon capture and storage and atmospheric dispersion modelling. Water quality topics include water pollution, water treatment and wastewater treatment.

Readers are invited to actively engage with derivations of analytical solutions through a vast set of challenges, specified throughout the book. Each chapter also includes a problem sheet with worked solutions, comprising relevant and practical applications of the theoretical equations derived. Many of the problem sheets involve writing small MATLAB programmes aimed to help the reader gain deeper insight into parameter sensitivity and process understanding.

This book builds on a large body of referenced literature. Nevertheless, it is worth to point out that the writing style and format of this book has been particularly influenced by Massey and Ward-Smith [1], Stroud and Booth [2], Chapra and Canale [3], Cooper and Alley [4], Crittenden et al. [5] and Frazer and Jewkes [6]. The written material also builds heavily on my experience as a student under the instruction of Tony Grass and James Croll at University College London, Andrew Spink at the University of Birmingham as well as Adrian Butler, Howard Wheater, Neil McIntyre and Geoffrey Stephenson at Imperial College London. I am also grateful for important advice and guidance provided by my wife, Jinhua Mathias, and colleagues, including Jeroen van Hunen, Andy Aplin, Stefan Nielsen, Neil Goulty, Riccardo Scarpa, Stefano Giani and Mohammed Seaid at Durham University, Chris MacMinn at Oxford University, Graham Sander at Loughborough University, Andrew Ireson at the University of Saskatchewan and Gianni Vesuviano at the Centre for Ecology and Hydrology.

Durham, UK
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Simon A. Mathias

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Part I

Civil Engineering Hydraulics

Basic Principles of Fluid Mechanics

1

Abstract

This chapter introduces some basic principles of fluid mechanics. Equations are derived to describe hydrostatic forces on inclined plates. The concept of Archimedes' principle is explained and an analytical solution for assessing the stability of floating of objects is developed. The continuity, momentum and Bernoulli equations are derived using a control-volume within a streamtube, located within a moving incompressible and inviscid fluid. The Bernoulli equation is used to derive the Torricelli equation and equations describing flow over sharp crested weirs. Practical applications are presented through a problem sheet with worked solutions.

Notation

a	Acceleration [LT^{-2}].
a_1	Depth of low density fluid in a u-tube manometer [L].
a_2	Elevation difference between fluid interfaces in a u-tube manometer [L].
A	Area [L^2].
$\hat{A}$	Mean cross-sectional area [L^2].
B	Breadth [L].
E	Total head [L].
F	Force [MLT^{-2}].
F_b	Buoyant force [MLT^{-2}].
F_g	Gravitational force [MLT^{-2}].
g	Gravitational acceleration [LT^{-2}].
h	Hydraulic head [L].
h_v	Velocity head [L].
H	Depth [L].

H_F	Depth of a hydrostatic force [L].
I_{yy}	Second moment of area about a centroid in the y -direction [L^4].
L	Length [L].
L_{BG}	Distance between the centre of buoyancy and the centre of gravity [L].
L_{BM}	Distance between the centre of buoyancy and the metacentre [L].
M	Mass [M].
p	Fluid pressure [$ML^{-1}T^{-2}$].
p_0	Atmospheric pressure [$ML^{-1}T^{-2}$].
p_a	Absolute pressure [$ML^{-1}T^{-2}$].
Q	Flow rate [L^3T^{-1}].
s	Distance along a streamtube [L].
t	Time [T].
U	Moment [ML^2T^{-2}].
U_b	Moment due to a buoyancy force [ML^2T^{-2}].
U'_b	Moment due to a buoyancy force following a rotation [ML^2T^{-2}].
V_I	Immersed volume [L^3].
v	Fluid velocity [LT^{-1}].
y	Distance from a liquid surface in the plane of a submerged and inclined plate [L].
y_F	Distance from a liquid surface to the location where a hydrostatic force applies, in the plane of a submerged and inclined plate [L].
y_c	Distance to a centroid from a datum [L].
y'_c	Distance to a centroid from a datum following a rotation [L].
z	Elevation [L].
θ	Inclination angle [—].
ρ	Mass density of a fluid [ML^{-3}].
ρ_s	Mass density of a solid object [ML^{-3}].
ψ	Pressure head [L].
CoB	Centre of buoyancy.
CoG	Centre of gravity.

1.1 Introduction

This chapter provides a brief introduction to some basic principles of fluid mechanics. The first section focuses on hydrostatics. The second section focuses on moving fluids in the absence of frictional forces. All the results derived in this chapter are classic. Similar results with different derivations can be found in many existing textbooks concerning the mechanics of fluids. The reader is directed to [1] for alternative and sometimes more detailed explanations.

1.2 Hydrostatics

The study of forces in static fluid is referred to as hydrostatics. In this section we will develop the concept of hydrostatic pressure and use it to derive methods for measuring pressure, determining hydrostatic forces on inclined plates and assessing the stability of floating objects.

1.2.1 Hydrostatic Pressure

Consider a tank of static liquid with a free upper surface open to the atmosphere (Fig. 1.1). Let A [L^2] be the plan area of the tank, H [L] be the depth of the liquid within the tank, p_0 [$ML^{-1}T^{-2}$] be the atmospheric pressure, ρ [ML^{-3}] be the mass density of the liquid and g [LT^{-2}] be gravitational acceleration. The downward force applied to the base of the tank will be $A(p_0 + \rho g H)$. The absolute pressure, p_a [$ML^{-1}T^{-2}$], applied to the base of the tank is therefore $p_0 + \rho g H$.

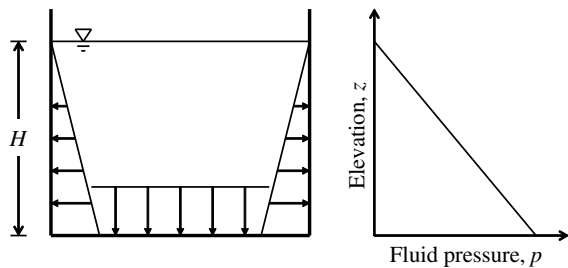
In hydraulics, we are more concerned with a relative pressure, which represents the difference between absolute pressure and atmospheric pressure. Hereafter, the term fluid pressure, p [$ML^{-1}T^{-2}$], is taken to mean the relative pressure of a fluid, $p \equiv p_a - p_0$ [$ML^{-1}T^{-2}$].

Referring back to the tank of liquid in Fig. 1.1, $p = 0$, at the liquid surface and $p = \rho g H$ at the base of the tank. Furthermore, if z [L] represents elevation above the base of the tank

$$p = \rho g(H - z) \quad (1.1)$$

Equation (1.1) is often referred to as a hydrostatic pressure profile. Interestingly, it will apply irrespective of the geometry of the tank of concern. Furthermore, pressure is isotropic, which means that its magnitude is independent of direction. This implies that the liquid applies a uniform force distribution to the base of the tank and a linear force distribution to the side walls of the tank (as indicated by the arrows in the tank shown in Fig. 1.1).

Fig. 1.1 Hydrostatic fluid pressure in a tank of liquid



1.2.2 Measuring Pressure

Note that hydrostatic pressure is independent of the quantity of fluid present. Instead, it is dependent on the elevation of the hydraulically connected free surface exposed to the atmosphere. For example, consider Fig. 1.2. The fluid pressure at the base of each of the first three devices (Fig. 1.2 a, b and c) should be the same because the elevation of the exposed free surface, in each device, is the same distance above the base of the underlying tanks.

The device shown in Fig. 1.2b is in fact a measuring device referred to as a piezometer. The fluid pressure at the top of the tank can be measured by multiplying the elevation difference between the top of the tank and the free surface in the piezometer by ρg .

The device shown in Fig. 1.2c is an alternative measuring device referred to as a u-tube manometer. The fluid pressure at the top of the tank can be measured by multiplying the elevation difference between the top of the tank and the free surface in the manometer by ρg . The advantage of the u-tube manometer, over the piezometer, is that fluids with different densities to that being measured can be used to either provide more or less sensitivity. Furthermore, it is possible to measure absolute pressures, which are less than atmospheric pressure.

Figure 1.2d shows a tank with the same pressure as that in Fig. 1.2c but with a u-tube manometer containing a less dense fluid (the lighter shade). Consequently, the free surface exposed to the atmosphere is higher in Fig. 1.2d as compared to in Fig. 1.2c. Small changes in pressure will lead to larger changes in fluid level when using a less dense fluid, hence it is more sensitive (as compared to when using a common fluid).

Figure 1.2e shows a tank with the same pressure as that in Fig. 1.2c but with a u-tube manometer containing a more dense fluid (the darker shade). Consequently, the free surface exposed to the atmosphere is lower in Fig. 1.2e as compared to in Fig. 1.2c. Large pressures lead to smaller fluid levels when using a more dense fluid, hence a smaller u-tube can be used (as compared to when using a common fluid).

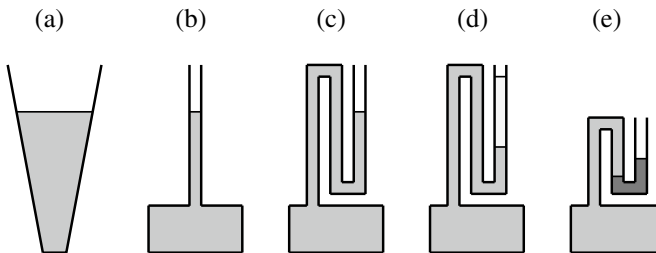


Fig. 1.2 Examples of different vessels that have the same fluid pressure at the base. **a** Inverted conical vase. **b** Tank with a piezometer. **c** Tank with a u-tube manometer containing common fluid. **d** Tank with a u-tube manometer containing less dense fluid (the lighter shade). **e** Tank with a u-tube manometer containing more dense fluid (the darker shade)

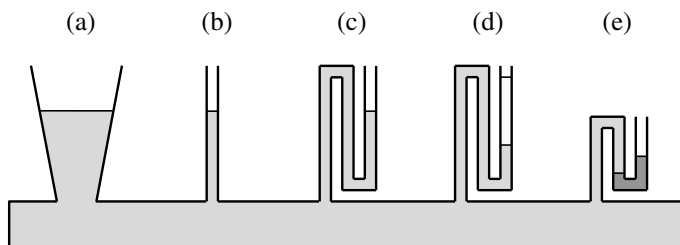


Fig. 1.3 Examples of different fluid pressure measuring devices in a common tank of liquid. **a** Inverted conical vase. **b** Piezometer. **c** U-tube manometer containing common fluid. **d** U-tube manometer containing less dense fluid (the lighter shade). **e** U-tube manometer containing more dense fluid (the darker shade)

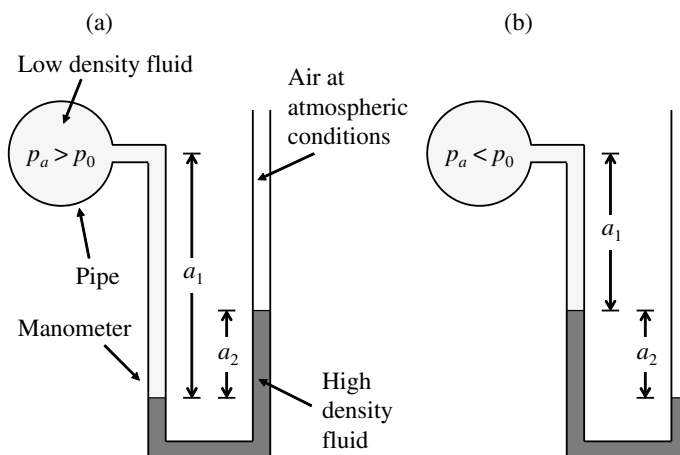


Fig. 1.4 High density fluid u-tube manometers connected to a pipe. The circles represent a cross-section through the pipe. **a** Measurement of an absolute fluid pressure greater than atmospheric pressure. **b** Measurement of an absolute fluid pressure greater than atmospheric

Note that given all five vessels in Fig. 1.2 are hydrostatic, exactly the same fluid levels would be observed if they were each linked to the same tank, such as shown in Fig. 1.3.

Figure 1.4a shows a u-tube manometer measuring the absolute pressure, p_a , of a fluid flowing in a pipe, where the absolute pressure is greater than atmospheric pressure, p_0 . The mass density of the low density fluid in the pipe is ρ_1 [ML⁻³] and the mass density of the high density fluid in the u-tube is ρ_2 [ML⁻³].

Challenge 1.1 Use the concept of hydrostatic pressure to determine an expression for the absolute pressure in the pipe shown in Fig. 1.4a.

The absolute pressure in the pipe, shown in Fig. 1.4a, can be obtained by equating two expressions for the absolute pressure at the interface between the low and high density fluids in the u-tube.

The hydrostatic pressure contribution due to the low density fluid is $\rho_1 a_1 g$. There is also the absolute pressure in the pipe, p_a . The absolute pressure at the interface between low density and high density fluids in the u-tube manometer is therefore $p_a + \rho_1 a_1 g$.

On the other hand, the hydrostatic pressure contribution due to the high density fluid is $\rho_2 a_2 g$. There is also the atmospheric pressure, p_0 . It can therefore also be said that the absolute pressure at the interface between low density and high density fluids in the u-tube manometer is $p_0 + \rho_2 a_2 g$.

Equating the two expressions above and solving for p_a gives us

$$p_a = p_0 + \rho_2 a_2 g - \rho_1 a_1 g \quad (1.2)$$

Figure 1.4b shows a u-tube manometer measuring the absolute pressure, p_a , of a fluid flowing in a pipe where the absolute pressure is less than atmospheric pressure, p_0 . Again, ρ_1 [ML⁻³] is the mass density of the low density fluid in the pipe and ρ_2 [ML⁻³] is the mass density of the high density fluid in the u-tube.

Challenge 1.2 Use the concept of hydrostatic pressure to determine an expression for the absolute pressure in the pipe shown in Fig. 1.4b.

The absolute pressure in the pipe, shown in Fig. 1.4b, can be obtained by determining an expression for the absolute pressure at the high density fluid free surface and equating this with the atmospheric pressure.

The hydrostatic pressure contribution due to the low density fluid is $\rho_1 a_1 g$. The hydrostatic pressure contribution due to the high density fluid is $\rho_2 a_2 g$. There is also the absolute pressure in the pipe, p_a . The absolute pressure at the high density fluid free surface is therefore $p_a + \rho_1 a_1 g + \rho_2 a_2 g$. Equating this with the atmospheric pressure, p_0 , and solving for p_a gives us

$$p_a = p_0 - \rho_2 a_2 g - \rho_1 a_1 g \quad (1.3)$$

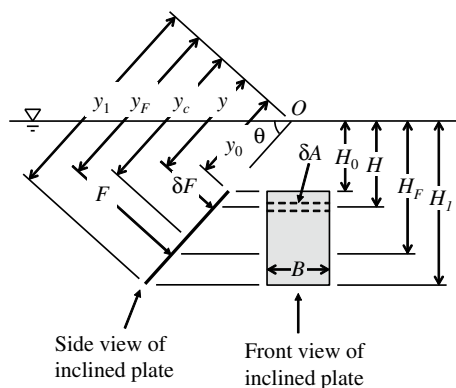
1.2.3 Hydrostatic Forces on Inclined Plates

Here we will derive expressions for the total force applied to a submerged inclined plate due to hydrostatic pressure. We will then use moment matching to determine the depth at which the force applies. To begin with, we will focus on a rectangular plate. The same theory will then be extended to account for plates of arbitrary geometries.

1.2.3.1 Rectangular Plate

Consider an immersed rectangular plate of breadth, B [L], and length, L [L], inclined at an angle, θ [–], to the horizontal axis (see Fig. 1.5). The depth of

Fig. 1.5 Hydrostatic pressure on an inclined rectangular plate



fluid above the top and bottom of the plate are denoted H_0 [L] and H_1 [L], respectively. Let y [L] be a distance from the liquid surface in the plane of the plate. The origin of the y -axis at the liquid surface is denoted O . The distance, along the y -axis, from O to the top and bottom of the plate are denoted y_0 [L] and y_1 [L], respectively. Note that $L = y_1 - y_0$, $H_0 = y_0 \sin \theta$ and $H_1 = y_1 \sin \theta$.

Challenge 1.3 Determine an expression for the force, δF [MLT^{-2}], applied to a thin strip of area, δA [L^2], located at a distance, y , along the y -axis due to hydrostatic pressure. Your final expression should be in terms of ρ , g , θ , y and δA .

Consider a thin strip of area, δA [L^2], located at a distance, y , along the y -axis. The fluid depth at this location is $y \sin \theta$. Therefore the hydrostatic pressure at this point is $\rho g y \sin \theta$. It follows that the force applied to the strip, δF [MLT^{-2}], due to hydrostatic pressure is found from

$$\delta F = \rho g y \sin \theta \delta A \quad (1.4)$$

Challenge 1.4 Determine an expression for the total force, F [MLT^{-2}], applied to the inclined plate due to hydrostatic pressure. Your final expression should be in terms of ρ , g , B , L , H_0 and H_1 .

The total force, F [MLT^{-2}], applied to the inclined plate is found by integrating Eq. (1.4)

$$F = \rho g \sin \theta \int y dA \quad (1.5)$$

Noting that the plate exists for $y \in [y_0, y_1]$ and $\frac{dA}{dy} = B$, it follows that

$$\begin{aligned} F &= \rho g B \sin \theta \int_{y_0}^{y_1} y dy \\ &= \rho g B \sin \theta \left(\frac{y_1^2 - y_0^2}{2} \right) \end{aligned}$$

Given that $L = y_1 - y_0$, $H_0 = y_0 \sin \theta$ and $H_1 = y_1 \sin \theta$, it can be further stated that

$$F = \rho g B L \left(\frac{H_0 + H_1}{2} \right) \quad (1.6)$$

Challenge 1.5 Determine an expression for the moment about O , δU [ML^2T^{-2}], applied to a thin strip of area, δA [L^2], located at a distance, y , along the y -axis, due to hydrostatic pressure. Your final expression should be in terms of ρ , g , θ , y and δA .

The hydrostatic force applied to a thin strip, gives rise to a moment about O , $\delta U = \delta F y$, where δF is given by Eq. (1.4). It follows that

$$\delta U = \rho g y^2 \sin \theta \delta A \quad (1.7)$$

Challenge 1.6 Determine an expression for the total moment about O , U [ML^2T^{-2}], applied to the inclined plate due to hydrostatic pressure.

The total moment about O , U [ML^2T^{-2}], applied to the inclined plate due to hydrostatic pressure is found by integrating Eq. (1.7)

$$U = \rho g \sin \theta \int y^2 dA \quad (1.8)$$

Noting again that the plate exists for $y \in [y_0, y_1]$ and $\frac{dA}{dy} = B$, it follows that

$$\begin{aligned} U &= \rho g B \sin \theta \int_{y_0}^{y_1} y^2 dy \\ &= \rho g B \sin \theta \left(\frac{y_1^3 - y_0^3}{3} \right) \\ &= \rho g B \sin \theta (y_1 - y_0) \left(\frac{y_0^2 + y_0 y_1 + y_1^2}{3} \right) \\ &= \rho g B L \csc \theta \left(\frac{H_0^2 + H_0 H_1 + H_1^2}{3} \right) \end{aligned} \quad (1.9)$$

Challenge 1.7 Use moment matching to determine the depth, H_F [L], at which the total force, F , applies.

Let H_F [L] be the depth at which the total force, F , applies. The location at which the total force acts on the y -axis, $y_F = H_F \csc \theta$. Consequently, it can also be stated that

$$U = F H_F \csc \theta \quad (1.10)$$

Substituting Eqs. (1.6) and (1.9) into Eq. (1.10) and solving for H_F leads to

$$H_F = \frac{2}{3} \left(\frac{H_0^2 + H_0 H_1 + H_1^2}{H_0 + H_1} \right) \quad (1.11)$$

Note that

$$\lim_{H_0 \rightarrow 0} H_F = \frac{2H_1}{3} \quad (1.12)$$

1.2.3.2 Plates with Arbitrary Geometries

Note that Eqs. (1.5) and (1.8) also apply to inclined plates with arbitrary geometries (see Fig. 1.6).

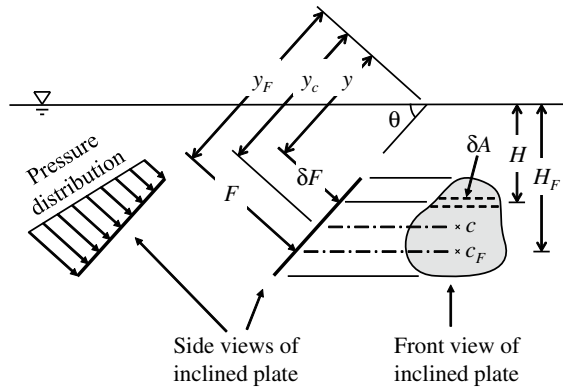
Let y_c [L] be the location (along the y -axis) of the centroid (analogous to the centre of gravity or centre of mass) for the plate of concern, defined by

$$y_c A = \int y dA \quad (1.13)$$

Substituting Eq. (1.13) into Eq. (1.5) leads to

$$F = \rho g y_c A \sin \theta \quad (1.14)$$

Fig. 1.6 Hydrostatic pressure on an inclined plate with arbitrary geometry



Let I_{yy} [L^4] be the second moment of area in the y -direction, about the centroid, for the plate of concern, defined by

$$I_{yy} = \int y(y - y_c) dA \quad (1.15)$$

Expanding the brackets in Eq. (1.15), substituting Eq. (1.13) and rearranging leads to

$$\int y^2 dA = I_{yy} + y_c^2 A \quad (1.16)$$

which is often referred to as the parallel axis theorem [2, p. 90].

Substituting Eq. (1.16) into Eq. (1.8) leads to

$$U = \rho g (I_{yy} + y_c^2 A) \sin \theta \quad (1.17)$$

Substituting Eqs. (1.14) and (1.17) into Eq. (1.10) and solving for H_F then gives us [1, p. 62]

$$H_F = \left(\frac{I_{yy}}{y_c A} + y_c \right) \sin \theta \quad (1.18)$$

For the aforementioned inclined rectangular plate, $A = BL$, $y_c = \left(\frac{H_0 + H_1}{2} \right) \csc \theta$ and $I_{yy} = \frac{BL^3}{12}$ [2, p. 97], which on substitution into Eqs. (1.14) and (1.18) leads to Eqs. (1.6) and (1.11), respectively. Expressions for A , y_c and I_{yy} are available (e.g. [3]) or can be determined for any alternative geometry.

1.2.4 Buoyancy

Consider a vertically prismatic solid object of length, L [L], and cross-sectional area, A [L^2]. The solid object is fully immersed within a hydrostatic fluid of mass density, ρ [ML^{-3}]. The depth of fluid above the base of the object is H [L].

Challenge 1.8 Determine the net upward force exerted by the hydrostatic liquid on the solid object.

The hydrostatic fluid exerts a downward force on the object of $F_1 = \rho g (H - L)A$ and an upward force on the object of $F_2 = \rho g HA$. The net upward force, F_b [MLT^{-2}], exerted by the hydrostatic liquid is therefore

$$F_b = F_2 - F_1 = \rho g LA \quad (1.19)$$

This net-upward force, F_b , is commonly referred to as the buoyant force. Providing the weight of a solid object, F_g [MLT^{-2}], is less than its associated buoyant force, the object will float at the surface of a liquid. Furthermore, the depth of immersion, H [L], can be determined by recognising that, for floating objects, $F_g = F_b$.

Challenge 1.9 Determine the depth of immersion, H [L], for the previously mentioned vertically prismatic object, assuming it has a mass density of ρ_s [ML⁻³] where $\rho_s < \rho$.

Suppose the previously mentioned vertically prismatic object has a mass density of ρ_s [ML⁻³], where $\rho_s < \rho$. In this case we would expect the object to float at the liquid surface. Let H [L] represent the depth of liquid above the base of the object (i.e., the depth of immersion). Given that the object is floating, the top surface of the object is not exposed to the fluid. Therefore the downward force acting on the object due to the hydrostatic fluid, $F_1 = 0$. The upward force acting on the object due to the hydrostatic fluid, $F_2 = \rho g H A$. It follows that the buoyant force, $F_b = F_2 - F_1 = \rho g H A$. The weight of the object, $F_g = \rho_s g L A$. Setting $F_g = F_b$ and solving for H then leads to

$$H = \frac{\rho_s L}{\rho} \quad (1.20)$$

1.2.4.1 Archimedes' Principle

Archimedes' principle states more generally that the buoyant force, F_b , acting on a fully or partially immersed object is equal to the weight of fluid displaced by the immersed volume V_I [L³], for the object of concern, i.e.,

$$F_b = \rho g V_I \quad (1.21)$$

In the case of the fully immersed vertically prismatic object (recall Eq. (1.19)) $V_I = LA$. In the case of the partially immersed vertically prismatic object (recall Eq. (1.20)) $V_I = HA$. Archimedes' principle can also be shown to apply to solid objectives of any arbitrary and irregular geometry.

Figure 1.7a shows a vertical section through a fully immersed irregular solid object. The fluid pressure acting downwards on the upper surface of the object is linearly proportional to the depth of water above the upper surface (see Fig. 1.7b). The fluid

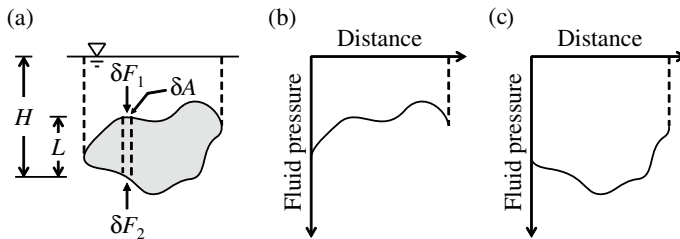


Fig. 1.7 **a** Vertical hydrostatic forces applied to a prismatic element within an immersed solid object (the shaded region). **b** Hydrostatic pressure distribution applied downwards on the upper surface of the immersed solid object. **c** Hydrostatic pressure distribution applied upwards on the lower surface of the immersed solid object

pressure acting upwards on the lower surface of the object is linearly proportional to the depth of water above the lower surface (see Fig. 1.7c).

Consider a vertically prismatic element, within the solid object, of plan view area, δA [L^2], and thickness, L [L]. The depth of water above the base of the element is H [L]. The downward force due to hydrostatic pressure acting on the top of the element is

$$\delta F_1 = \rho g(H - L)\delta A$$

The upward force due to hydrostatic pressure acting on the base of the element is

$$\delta F_2 = \rho g H \delta A$$

The buoyant force acting on the element is

$$\delta F_b = \delta F_2 - \delta F_1 = \rho g L \delta A$$

Noting that L is spatially variable due to the irregularity of the object, the total buoyant force acting on the object is found from

$$F_b = \rho g \int L dA$$

But of course, in this case, $\int L dA = V_I$ and so Eq. (1.21) applies.

1.2.4.2 Stability of Floating Objects

Whether or not a floating object is stable depends on the locations of both its centre of gravity (CoG) and centre of buoyancy (CoB). Consider the vertical section through a floating object shown in Fig. 1.8a. The CoG represents the location at which the weight of the object, F_g [MLT^{-2}], acts. The CoB represents the location at which the associated buoyant force, F_b [MLT^{-2}], acts.

If the CoG is below the CoB, the object will be unconditionally stable. However, it is commonly the case that the CoG is above the CoB. Providing the CoG is directly above the CoB, the object will remain upright in the liquid. However, a minor rotation of the object of concern will lead to both the CoG and CoB to form a turning moment, causing the object to rotate until the CoG and the CoB reside in the same vertical plane again. This may lead to the object returning to its upright position. Alternatively, the object may continue to rotate in the direction of the perturbation, causing it to capsize.

Consider Fig. 1.8a and b. When the object is upright, F_g and F_b act in the same vertical plane and therefore do not form a turning moment (Fig. 1.8a). However, tilting the object clockwise, by a small angle, θ [$-$], leads to the submerged portion of the object being predominantly on the right-hand-side. This in turn leads to the CoB moving to the right. In contrast, providing the load within the object is not redistributed (which is reasonable assumption, given that θ is small), the location of the CoG, relative to the object, remains unchanged. But importantly, the two loads, F_g and F_b , no longer act in the same vertical plane and therefore form a counter-clockwise turning moment. However, the effect of this turning moment is to return the object back to the original upright position. In this case, the object can be described as being buoyantly stable.

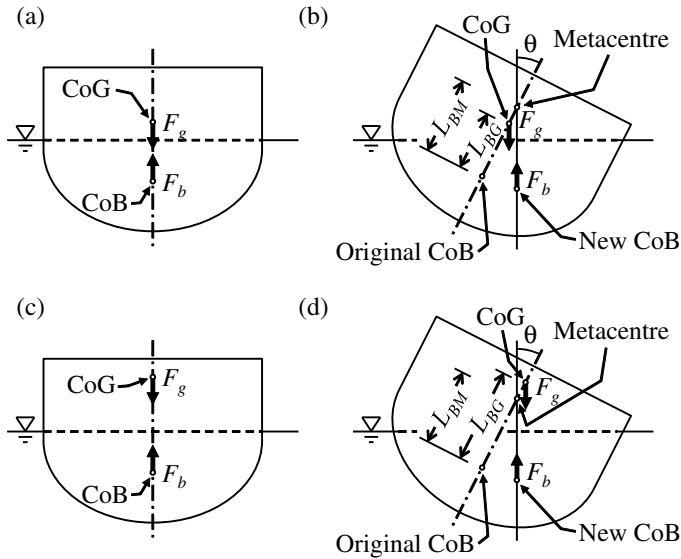


Fig. 1.8 Schematic diagrams showing locations of the centre of gravity (CoG), centre of buoyancy (CoB) and metacentre for a floating object that is tilted clockwise from an upright position. **a** and **b** represent an object that is buoyantly stable. **c** and **d** represent an object that is buoyantly unstable

Consider Fig. 1.8c and d. The only difference between the objects in Fig. 1.8a and c is that the CoG for the object is higher in Fig. 1.8c. Consequently, when the object is tilted clockwise, the new CoB is to the left of the CoG (see Fig. 1.8d) such that the two associated forces form a clockwise turning moment, which will not return the boat back to the original upright position. Instead, this clockwise turning moment will cause the boat to carry on rotating clockwise such that it will capsize. In this case, the object can be described as being buoyantly unstable.

Whether or not an object is buoyantly stable is of particular interest to the maritime community. Interestingly, it is possible to derive an expression that predicts the buoyant stability of an objective, which can be written purely in terms of its geometrical properties. The starting point is to consider a vertical line that crosses the new CoB due to rotation and intersects the line connecting the original CoB and the CoG of the object of concern. This intersection point is referred to as the metacentre (see Fig. 1.8b and d).

If the metacentre is to the right of the CoG, then the rotated CoB is also to the right of the CoG and the object is buoyantly stable (as in Fig. 1.8b). In this case, the distance between original CoB and the CoG, L_{BG} [L], is less than the distance between the original CoB and the metacentre, L_{BM} [L].

If the metacentre is to the left of the CoG, then the rotated CoB is also to the left of the CoG and the object is buoyantly unstable (as in Fig. 1.8d). In this case, the distance between original CoB and the CoG, L_{BG} [L], is greater than the distance between the original CoB and the metacentre, L_{BM} [L].

To summarise:

- $L_{BG} < L_{BM}$ means buoyantly stable.
- $L_{BG} > L_{BM}$ means buoyantly unstable.

The challenge is therefore to derive an expression for L_{BM} .

1.2.4.3 Distance Between Centre of Buoyancy and Metacentre

Figure 1.9 shows a more detailed annotation of Fig. 1.8b, which will aid in the determination of an expression for the distance, L_{BM} [L], between the original CoB and the metacentre.

Let y [L] be a horizontal distance from an arbitrary point to the left of the floating object. Consider a prismatic element of plan area, δA [L²], located at a distance, y , along the y -axis. Let $H(x, y)$ [L] be the depth of liquid above the base of the element. The buoyant force associated with this prismatic element is found from $\delta F_b = \rho g H \delta A$ [MLT⁻²]. This buoyant force gives rise to a moment about the origin of the y -axis, of $\delta U_b = \delta F_b y$ [ML²T⁻²]. The moment, U_b [ML²T⁻²], due to the total buoyant force of the object, is therefore found from

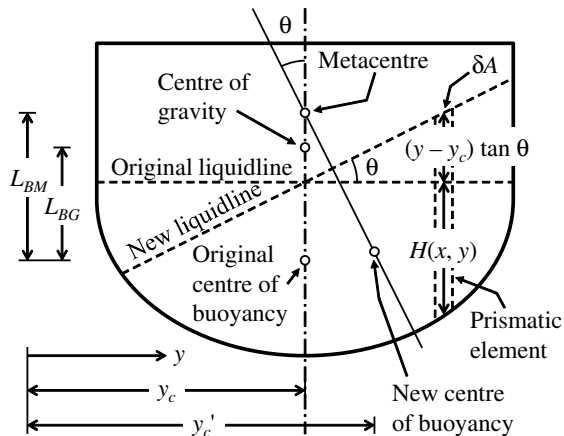
$$U_b = \rho g \int y H dA \quad (1.22)$$

Let y_c [L] denote the location of the CoB (prior to rotation) on the y -axis. It also therefore follows that

$$U_b = F_b y_c \quad (1.23)$$

where F_b is the total buoyant force defined by Archimedes' principle (Eq. (1.21)).

Fig. 1.9 Detailed annotation of Fig. 1.8b



Substituting Eqs. (1.21) and (1.22) into Eq. (1.23) and solving for y_c gives us

$$y_c = \frac{\int y H dA}{V_I} \quad (1.24)$$

where V_I [L^3] is the total immersed volume of the object.

Consider the aforementioned prismatic element following a small clockwise rotation of θ [–]. The depth of liquid above the base of the element is now $H + (y - y_c) \tan \theta$ (see Fig. 1.9). Considering Eq. (1.22), the moment, U'_b [ML^2T^{-2}], due to the total buoyant force of the object after rotation, is found from

$$U'_b = \rho g \int y [H + (y - y_c) \tan \theta] dA \quad (1.25)$$

Let y'_c [L] denote the new location of the CoB (after rotation) on the y -axis. It also therefore follows that

$$U'_b = F_b y'_c \quad (1.26)$$

where again, F_b is the total buoyant force defined by Archimedes' principle (Eq. (1.21)).

Substituting Eqs. (1.21) and (1.25) into Eq. (1.26) and solving for y'_c gives us

$$y'_c = \frac{\int y [H + (y - y_c) \tan \theta] dA}{V_I} \quad (1.27)$$

Furthermore, substituting Eqs. (1.15) and (1.24) into Eq. (1.27) leads to

$$y'_c - y_c = \frac{I_{yy} \tan \theta}{V_I} \quad (1.28)$$

where I_{yy} [L^4] is the second moment of area.

Moreover, it can be said that (see Fig. 1.9)

$$y'_c - y_c = L_{BM} \tan \theta + O(\theta) \quad (1.29)$$

Equating Eqs. (1.28) and (1.29) and imposing that $\theta \ll 1$ therefore gives us [1, p. 75]

$$L_{BM} = \frac{I_{yy}}{V_I} \quad (1.30)$$

So it can be said that a floating object should be buoyantly stable providing

$$L_{BG} < \frac{I_{yy}}{V_I} \quad (1.31)$$

1.3 Moving Fluids

Fluid movement is a three-dimensional process with fluid particles moving along complicated and varying fluid pathways. A simple method for reducing a three-dimensional system to a one-dimensional problem is to focus on individual fluid pathways. Each pathway can be thought of as a streamtube. The rule about streamtubes is that fluid particles can only travel along a streamtube and cannot travel across a streamtube. Consequently, we only need to consider a one-dimensional distance along a streamtube. Below we will use this important concept to derive three extensively used hydraulic equations to describe moving fluids:

1. The continuity equation.
2. The momentum equation.
3. The Bernoulli equation.

It will then be demonstrated how to use these concepts to measure fluid velocity with a Pitot tube, predict the rate at which a tank of liquid drains through an orifice and measure flow rate in an open channel using a sharp crested weir.

1.3.1 Control-Volume in a Streamtube

Consider steady-state, incompressible and inviscid flow through a streamtube (Fig. 1.10). Steady-state implies there are no changes in time. Incompressible flow implies that fluid density is constant. Inviscid flow implies that the fluid has no viscosity and frictional losses are negligible.

A control-volume (CV) is isolated from the streamtube for further analysis (Fig. 1.11). The length of the CV is δs [L] and s [L] is a directional distance along the streamtube in the direction of moving fluid. The cross-sectional areas of the streamtube inlet and outlet are denoted A [L²] and $A + \delta A$ [L²], respectively. The elevation above a reference datum of the inlet and outlet are denoted z [L] and $z + \delta z$ [L], respectively. The fluid pressure at the inlet and outlet are denoted p [ML⁻¹T⁻²] and $p + \delta p$ [ML⁻¹T⁻²], respectively. The cross-sectional mean fluid velocity at the inlet and outlet are denoted v [LT⁻¹] and $v + \delta v$ [LT⁻¹], respectively. The rate of

Fig. 1.10 Schematic diagram of a streamtube

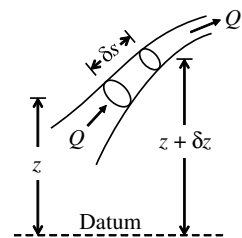
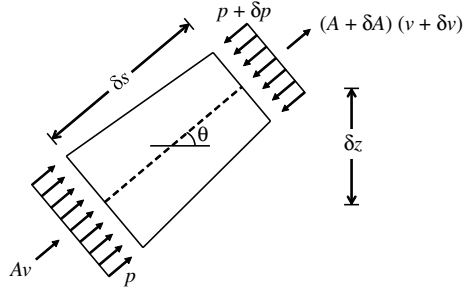


Fig. 1.11 Schematic diagram of a control-volume within a streamtube



fluid volume movement flowing through the streamtube is denoted Q [L^3T^{-1}]. The density of the fluid is denoted ρ [ML^{-3}].

1.3.2 The Continuity Equation

Challenge 1.10 Apply the principle of mass conservation to the CV described above and derive an expression relating v , δv , A , δA and Q .

Mass conservation dictates that the change in mass of fluid within a CV is equal to the mass of fluid entering a CV minus the mass of fluid leaving a CV. Under steady-state conditions there should be no change in mass. Therefore the mass of fluid entering a CV should be equal to the mass of fluid leaving a CV. For incompressible flows there is no change in density. It follows that for steady-state incompressible flow, the volume of fluid entering a CV should be equal to the volume of fluid leaving a CV such that [1, p. 91]

$$Av = (A + \delta A)(v + \delta v) = Q \quad (1.32)$$

which is widely referred to as the continuity equation.

1.3.3 The Momentum Equation

Challenge 1.11 Use Newton's second law to find an expression for the net-force acting on the CV in the s -direction in terms of ρ , Q and δv .

Newton's second law states that

$$F = Ma \quad (1.33)$$

where F [MLT^{-2}] is a force, M [M] is mass and a [LT^{-2}] is acceleration.

The acceleration, a , of fluid particles along the s -axis, is found from

$$a \equiv \frac{dv}{dt} = \frac{\partial v}{\partial t} + \frac{ds}{dt} \frac{\partial v}{\partial s}$$

where v [LT^{-1}] is the fluid velocity in the s -direction and t [T] is time.

It can also be said that

$$v = \frac{ds}{dt}$$

such that

$$a = \frac{\partial v}{\partial t} + v \frac{\partial v}{\partial s} \quad (1.34)$$

Furthermore, given that the flow is assumed to be steady-state, v is a constant with time and

$$a = v \frac{\partial v}{\partial s} \quad (1.35)$$

Recalling that $Q = Av$ it can be further stated that

$$a = \frac{Q}{A} \frac{\partial v}{\partial s}$$

and, assuming that a is constant across the CV,

$$a = \frac{Q}{\hat{A}} \frac{\delta v}{\delta s} \quad (1.36)$$

where $\hat{A}$ is the mean cross-sectional area of the CV.

The mass of fluid contained within the CV is found from

$$M = \hat{A} \delta s \rho \quad (1.37)$$

Substituting Eqs. (1.36) and (1.37) into Eq. (1.33) leads to [1, p. 136]

$$F = \rho Q \delta v \quad (1.38)$$

which is widely referred to as the momentum equation.

1.3.4 The Bernoulli Equation

Challenge 1.12 Apply the momentum equation to the CV and derive a relationship between p , v and z .

To bring pressure into the system we need to quantify the net-force acting on the CV in the s -direction. This can be found from

$$F = \sum_{i=1}^3 F_i$$

where F_1 is the force due to the fluid pressure, p , on the inlet of the CV, found from

$$F_1 = Ap$$

F_2 is the force due to the fluid pressure on the outlet of the CV, found from

$$F_2 = -(A + \delta A)(p + \delta p)$$

and F_3 is the force due to the self-weight of the fluid within the CV, found from (recall Eq. (1.37))

$$F_3 = -\hat{A}\delta s\rho g \sin \theta$$

where g [LT^{-2}] is gravitational acceleration and θ [–] is the angle of the s -axis to the horizontal axis.

Noting that $\sin \theta = \frac{\delta z}{\delta s}$, it also follows that

$$F_3 = -\hat{A}\rho g \delta z$$

and therefore

$$F = -\delta Ap - (A + \delta A)\delta p - \hat{A}\rho g \delta z \quad (1.39)$$

Equating Eqs. (1.38) and (1.39) then leads to

$$\rho Q \delta v = -\delta Ap - (A + \delta A)\delta p - \hat{A}\rho g \delta z$$

which can rearranged to get

$$\frac{p}{\hat{A}\rho g} \frac{\delta A}{\delta s} + \frac{(A + \delta A)}{\hat{A}\rho g} \frac{\delta p}{\delta s} + \frac{Q}{\hat{A}g} \frac{\delta v}{\delta s} + \frac{\delta z}{\delta s} = 0$$

If the CV is infinitesimally small (i.e., $\delta s \rightarrow 0$, $\delta A \rightarrow 0$ and $\hat{A} \rightarrow A$) it can be further stated that

$$\frac{p}{A\rho g} \frac{\partial A}{\partial s} + \frac{1}{\rho g} \frac{\partial p}{\partial s} + \frac{v}{g} \frac{\partial v}{\partial s} + \frac{\partial z}{\partial s} = 0$$

Furthermore, because a streamtube should be smoothly varying in cross-sectional area, $\frac{\partial A}{\partial s} \ll A$ and

$$\frac{1}{\rho g} \frac{\partial p}{\partial s} + \frac{v}{g} \frac{\partial v}{\partial s} + \frac{\partial z}{\partial s} = 0$$

Integrating both sides with respect to s then leads to [1, p. 94]

$$\frac{p}{\rho g} + \frac{v^2}{2g} + z = E \quad (1.40)$$

where E [L] is a term that is constant along the streamtube. Equation (1.40) is widely referred to as the Bernoulli equation.

The constant, E [L], in Eq. (1.40) is often referred to as the total head, which represents the total mechanical energy per unit weight of fluid. Total head can be split into the following separate quantities:

$$E = \psi + h_v + z = h + h_v$$

where ψ [L], h_v [L] and h [L] are referred to as the pressure head, velocity head and hydraulic head, respectively, found from:

$$\psi = \frac{p}{\rho g}, \quad h_v = \frac{v^2}{2g}, \quad h = \psi + z$$

The Bernoulli equation, Eq. (1.40), gives that, for steady-state, incompressible and inviscid flow, the sum of the hydraulic head and velocity head is constant along a streamtube.

1.3.5 Summary of Key Results

Challenge 1.13 Set $A = A_1$, $A + \delta A = A_2$, $v = v_1$, $v + \delta v = v_2$, $p = p_1$, $p + \delta p = p_2$, $z = z_1$ and $z + \delta z = z_2$ in Eqs. (1.32), (1.38) and (1.40).

The continuity equation: $A_1 v_1 = A_2 v_2$

The momentum equation: $F = \rho Q(v_2 - v_1)$

The Bernoulli equation: $E = \frac{p_1}{\rho g} + \frac{v_1^2}{2g} + z_1 = \frac{p_2}{\rho g} + \frac{v_2^2}{2g} + z_2$.

1.3.6 Measuring Fluid Velocity Using a Pitot Tube

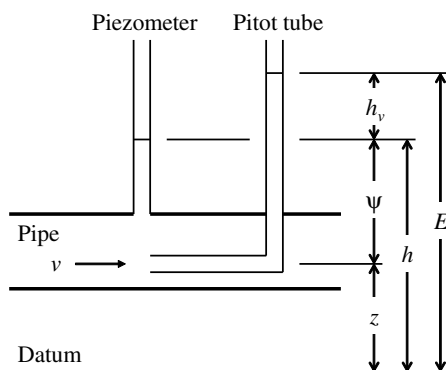
Whereas hydraulic head can be measured using a piezometer, the measurement of total head requires a modified device known as a Pitot tube (see Fig. 1.12).

A piezometer is a vertical tube which should have an opening orientated normal to the fluid flow direction and located at the wall of a given pipe. Consequently, fluid particles within a piezometer should be static such that the elevation (above a given datum) of a liquid surface within its tube represents the hydraulic head, h .

A pitot tube is very similar to a piezometer except its opening should be orientated parallel to the flow direction and located directly where a velocity measurement is required. Consequently, fluid particles within the opening of a pitot tube should possess a similar kinetic energy to those particles outside of the Pitot tube. It follows that the elevation (above a given datum) of a liquid surface within its tube should represent the total head, E . A measurement of fluid velocity can be determined from

$$v = \sqrt{2g(E - h)}$$

Fig. 1.12 Schematic diagram of a piezometer and Pitot tube



1.3.7 The Torricelli Equation

Consider a streamtube within a large tank containing liquid draining through a small orifice at some vertical distance, H [L], below the liquid surface (Fig. 1.13). If the tank is big enough and the orifice is small enough, the liquid level in the tank will remain virtually unchanged. Let v [LT^{-1}] be the fluid velocity at the orifice. The fluid velocity at the liquid surface can be assumed zero.

Challenge 1.14 Use the Bernoulli equation to determine a relationship between the fluid velocity at the orifice, v , and the depth of water above, H .

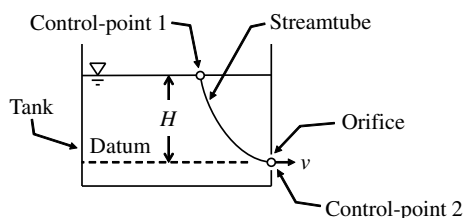
Consider two control-points along the streamtube. Control-point 1 is located at the liquid surface. Control-point 2 is located at the orifice. The Bernoulli equation states that

$$\frac{p_1}{\rho g} + \frac{v_1^2}{2g} + z_1 = \frac{p_2}{\rho g} + \frac{v_2^2}{2g} + z_2$$

In this context p_1 , v_1 and z_1 are the pressure, fluid velocity and elevation above a datum, respectively, for Control-point 1 whereas p_2 , v_2 and z_2 are the pressure, fluid velocity and elevation above a datum, respectively, for Control-point 2.

Both the liquid surface and the orifice are exposed to the atmosphere. Therefore $p_1 = p_2 = 0$. Given that the fluid velocity is zero at the liquid surface and v at the

Fig. 1.13 Schematic diagram of a tank of liquid draining through an orifice



orifice, $v_1 = 0$ and $v_2 = v$. Taking the datum to be at the elevation of the orifice, $z_1 = H$ and $z_2 = 0$. Substituting the above information into the Bernoulli equation and solving for v leads to [1, p. 114]

$$v = \sqrt{2gH} \quad (1.41)$$

which is commonly referred to as the Torricelli equation.

1.3.8 Flow over a Sharp Crested Weir

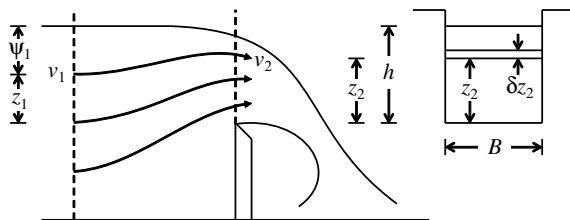
Sharp crested weirs (SCW) are often used to measure flow of liquid in open channels. An SCW typically comprises an obstruction with a sharp-edged opening, over which upstream liquid is forced to flow. Typically, the opening is of rectangular, triangular or trapezoidal section. The sharp edge is necessary to minimize energy losses as the liquid flows over the top. The sheet of liquid that flows out of the opening is referred to as the nappe. The underside of the nappe should be clear of an underlying solid bounding surface such that the nappe is close to atmospheric pressure throughout. For analysis the following assumptions are made:

1. Pressure throughout the nappe is at atmospheric pressure.
2. The upstream liquid surface is horizontal right up to the edge of the SCW.
3. Fluid pressure upstream of the SCW is hydrostatic.
4. Kinetic energy of the liquid upstream of the SCW is negligibly small compared to pressure energy and gravitational potential energy.

Challenge 1.15 Develop an expression for the flow rate, Q [L^3T^{-1}], through a rectangular SCW, of breadth B [L], in terms of g , B and the elevation of the liquid surface above the base of the SCW opening, denoted h [L] (Fig. 1.14).

Consider a rectangular SCW of breadth B . Liquid flows over the weir with a liquid depth of h (see Fig. 1.14). Let z be the elevation of a point above the base of the SCW opening. Now consider a control-point (CP) within a streamtube upstream

Fig. 1.14 Streamtubes across a sharp crested weir



of the SCW. Let p_1 , v_1 and z_1 be the pressure, fluid velocity and elevation at the CP, respectively. Similarly, let p_2 , v_2 and z_2 be the pressure, fluid velocity and elevation in the same streamtube but immediately above the SCW, respectively (Fig. 1.14). From Eq. (1.40) we have that

$$\frac{p_1}{\rho g} + \frac{v_1^2}{2g} + z_1 = \frac{p_2}{\rho g} + \frac{v_2^2}{2g} + z_2$$

Because of Assumption 1, $p_2 = 0$. Because of Assumptions 2 and 3, $\frac{p_1}{\rho g} + z_1 = h$. Because of Assumption 4, $v_1 = 0$. It follows that

$$v_2 = \sqrt{2g(h - z_2)} \quad (1.42)$$

from which it can be seen that the velocity varies with elevation within the SCW.

The total flow rate through the SCW is found from [1, p. 128]

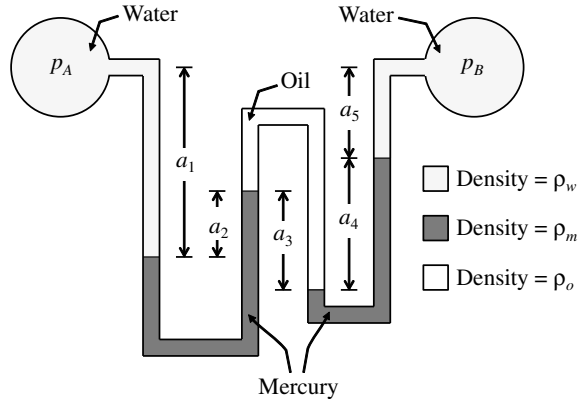
$$\begin{aligned} Q &= \int v_2 dA \\ &= B \int_0^h v_2 dz_2 \\ &= B\sqrt{2g} \int_0^h (h - z_2)^{1/2} dz_2 \\ &= B\sqrt{2g} \left[-\frac{2}{3}(h - z_2)^{3/2} \right]_0^h \\ &= \frac{2B}{3} \sqrt{2gh^3} \end{aligned} \quad (1.43)$$

1.4 Problem Sheet

Problem 1.1 (see Worked Solution 1.1)

A multi-fluid manometer is used to measure the pressure difference between two points in a water pipe network (see Fig. 1.15). Use hydrostatics to determine an expression for the pressure difference, $p_A - p_B$, in terms of the three fluid densities (ρ_w , ρ_m and ρ_o) and the five measured fluid depths (a_1 , a_2 , a_3 , a_4 and a_5).

Fig. 1.15 Two points in a water pipe network connected to a multi-fluid manometer



Problem 1.2 (see Worked Solution 1.2)

A prismatic trough of isosceles triangular cross-section is filled with water with a density of 1000 kg m^{-3} . The isosceles triangle is of width, 0.5 m, and height, 0.5 m. The length of the trough is 3 m.

- Determine the magnitude and depth of the hydrostatic force on each of the inclined rectangular side walls.
- Determine the magnitude and depth of the hydrostatic force on each of the vertical triangular end walls.

Problem 1.3 (see Worked Solution 1.3)

A cylindrical buoy of 1 m diameter and 1.25 m height has a mass of 70 kg.

- Determine the depth of immersion when the buoy is floating in water with a density of 1000 kg m^{-3} .
- Check whether the buoy is buoyantly stable. Hint: The second moment of area of a circular section is $\frac{\pi D^4}{64}$ where D [L] is the diameter [2, p. 97].
- It is planned to place a flashing light on the top of the buoy. The mass of the light is 12 kg. Check whether the buoy will remain buoyantly stable.
- Determine the maximum mass of flashing light that can be held in place whilst ensuring the buoy remains buoyantly stable.

Problem 1.4 (see Worked Solution 1.4)

A water pipe, of varying cross-sectional area, tapers from 0.3 m^2 at point A to 0.2 m^2 at point B. Point B is 5 m above point A. The velocity and pressure of the water at point A is 2.2 m s^{-1} and 120 kPa, respectively. Use the Bernoulli equation to determine the fluid pressure at point B.

Problem 1.5 (see Worked Solution 1.5)

A long bridge crosses a river and is supported by 1.4 m wide piers, each equally spaced by 7 m from centre to centre. The water depth upstream of the bridge is 1.8 m. The water depth between the piers is 1.55 m. Assuming the river bed is horizontal, use the Bernoulli equation to determine the volumetric flow rate under one arch.

Problem 1.6 (see Worked Solution 1.6)

A tapered pipe-bend of circular section has a 300 mm diameter inlet and 150 mm diameter outlet. The pipe-axis at the inlet is horizontal. The centre of outlet section is 1.4 m above the centre of the inlet section. The total volume of fluid contained within the bend is 0.085 m^3 . Furthermore, the pipe-axis at the outlet is inclined at an angle of 60° to the horizontal axis. Determine the magnitude and direction of the net-force exerted on the pipe-bend by water flowing through it at $0.23 \text{ m}^3 \text{ s}^{-1}$ when the inlet gauge pressure is 140 kPa.

Problem 1.7 (see Worked Solution 1.7)

Consider a sharp crested weir (SCW) of symmetric trapezoidal section. The depth of the opening is 280 mm. The base of the opening is 100 mm wide and the top of the opening is 400 mm wide. Develop a relationship between the SCW discharge rate and the water depth upstream of the SCW and determine the discharge when the upstream liquid surface is 236 mm above the base of the SCW opening.

1.5 Worked Solutions

Worked Solution 1.1 (see Problem 1.1)

The best way to approach this is to first develop expressions for p_A and p_B in terms of an intermediate pressure p_C , which represents the pressure at the mercury-oil

interface in the left-hand-side set of manometer tubes (see Fig. 1.15). Note that this pressure also applies at an elevation of a_3 above the mercury-oil interface in the right-hand-side set of manometer tubes.

Considering the pressure at the mercury-water interface in the left-hand-set of manometer tubes we can say $p_A + \rho_w g a_1 = p_C + \rho_m g a_2$

where ρ_w is the mass density of water and ρ_m is the mass density of mercury.

Solving for p_A gives us

$$p_A = p_C + \rho_m g a_2 - \rho_w g a_1 \quad (1.44)$$

Considering the pressure at the mercury-oil interface in the right-hand-set of manometer tubes we can say

$$p_C + \rho_o g a_3 = p_B + \rho_w g a_5 + \rho_m g a_4$$

where ρ_o is the mass density of the oil.

Solving for p_B gives us

$$p_B = p_C + \rho_o g a_3 - \rho_m g a_4 - \rho_w g a_5 \quad (1.45)$$

Subtracting Eq. (1.45) from Eq. (1.44) then leads to

$$p_A - p_B = \rho_m g (a_2 + a_4) - \rho_w g (a_1 - a_5) - \rho_o g a_3 \quad (1.46)$$

Worked Solution 1.2 (see Problem 1.2)

(a) The side-walls of the trough are analogous to inclined rectangular plates. The hydrostatic force, F , on an inclined rectangular plate is found from Eq. (1.6). In this case, $\rho = 1000 \text{ kg m}^{-3}$, $g = 9.81 \text{ m s}^{-2}$, $B = 3 \text{ m}$, $H_0 = 0 \text{ m}$, $H_1 = 0.5 \text{ m}$ and $L = \sqrt{\frac{W^2}{4} + H_1^2}$ where $W = 0.5 \text{ m}$. It follows that the hydrostatic force acting on each side wall, $F = 4110 \text{ N}$.

The depth of the hydrostatic force, H_F , in this case, is found from Eq. (1.12). It follows that $H_F = 0.333 \text{ m}$.

(b) The hydrostatic force, F , acting on the end walls can be found from Eq. (1.14) where y_c is found from Eq. (1.13). The area of a triangular end-wall is found from

$$A = \frac{W H_1}{2} \quad (1.47)$$

The area, δA , of a horizontal and elemental strip of thickness, δy , at a depth, y , is found from

$$\delta A = W \left(1 - \frac{y}{H_1} \right) \delta y \quad (1.48)$$

Substituting Eqs. (1.47) and (1.48) into Eq. (1.13) leads to

$$y_c = \frac{2}{W H_1} \int_0^{H_1} W \left(y - \frac{y^2}{H_1} \right) dy$$

$$\begin{aligned}
 &= \frac{2}{H_1} \left[\frac{y^2}{2} - \frac{y^3}{3H_1} \right]_0^{H_1} \\
 &= \frac{H_1}{3}
 \end{aligned} \tag{1.49}$$

Substituting Eqs. (1.47) and (1.49) into Eq. (1.14) leads to

$$F = \frac{\rho g W H_1^2 \sin \theta}{6} \tag{1.50}$$

Because the end wall is vertical, $\sin \theta = 1$. Letting $\rho = 1000 \text{ kg m}^{-3}$, $g = 9.81 \text{ m s}^{-2}$, $B = 3 \text{ m}$, $H_1 = 0.5 \text{ m}$ and $W = 0.5$, it follows that the hydrostatic force on each end wall, $F = 204 \text{ N}$.

The depth of the hydrostatic force, H_F , is found from Eq. (1.18) where I_{yy} is found from Eq. (1.15). Substituting Eqs. (1.48) and (1.49) into Eq. (1.15) leads to [2, p. 94]

$$\begin{aligned}
 I_{yy} &= \int_0^{H_1} W \left(y - \frac{H_1}{3} \right) \left(y - \frac{y^2}{H_1} \right) dy \\
 &= \int_0^{H_1} W \left(\frac{4y^2}{3} - \frac{y^3}{H_1} - \frac{H_1 y}{3} \right) dy \\
 &= W \left[\frac{4y^3}{9} - \frac{y^4}{4H_1} - \frac{H_1 y^2}{6} \right]_0^{H_1} dy \\
 &= \frac{W H_1^3}{36}
 \end{aligned} \tag{1.51}$$

Substituting Eqs. (1.47), (1.49) and (1.51) into Eq. (1.18) leads to

$$H_F = \frac{H_1}{2} \sin \theta \tag{1.52}$$

Given that $H_1 = 0.5 \text{ m}$ and $\sin \theta = 1$ it follows that the hydrostatic force on each end wall is located at a depth, $H_F = 0.25 \text{ m}$.

Worked Solution 1.3 (see Problem 1.3)

(a) For a floating object, the buoyant force is equal to the weight of the object of concern. Given Eq. (1.21), it can therefore be said that

$$M_1 g = \rho g V_I \tag{1.53}$$

where M_1 [M] is the mass of the buoy, g [LT^{-2}] is gravitational acceleration, ρ [ML^{-3}] is the fluid density and V_I [L^3] is the immersed volume of the buoy. It follows that

$$V_I = \frac{M_1}{\rho} \tag{1.54}$$

Given that the buoy is cylindrical

$$V_I = \frac{\pi D^2 H}{4} \quad (1.55)$$

where H [L] is the depth of immersion.

Equating Eqs. (1.54) and (1.55) and solving for H leads to

$$H = \frac{4M_1}{\pi D^2 \rho} \quad (1.56)$$

Letting $M_1 = 70$ kg, $D = 1$ m and $\rho = 1000$ kg m⁻³ it therefore follows that $H = 0.0891$ m.

(b) To determine whether the buoy is buoyantly stable we need to check that (recall Eq. (1.31))

$$L_{BM} - L_{BG} > 0$$

where L_{BG} [L] is the distance from the centre of buoyancy (CoB) to the centre of gravity (CoG) and L_{BM} [L] is the distance from the CoB to the metacentre.

For a circular section, the second moment of area, I_{yy} [L⁴], is found from

$$I_{yy} = \frac{\pi D^4}{64} \quad (1.57)$$

Substituting Eqs. (1.54) and (1.57) into Eq. (1.30) leads to

$$L_{BM} = \frac{\pi D^4 \rho}{64M_1} \quad (1.58)$$

Let L_{OB} and L_{OG} be the elevations of the CoB and CoG above the base of the buoy, respectively. It can therefore be said that $L_{BG} = L_{OG} - L_{OB}$. Given the simple geometrical nature of the cylindrical buoy it can be understood that (recall Eq. (1.56))

$$L_{OB} = \frac{H}{2} = \frac{2M_1}{\pi D^2 \rho} \quad (1.59)$$

$$L_{OG} = \frac{L}{2} \quad (1.60)$$

where L [L] is the height of the buoy. Consequently

$$L_{BM} - L_{BG} = \frac{\pi D^4 \rho}{64M_1} - \frac{L}{2} + \frac{2M_1}{\pi D^2 \rho}$$

Letting $L = 1.25$ m, $L_{BM} - L_{BG} = 0.121$ m, which is > 0 so the buoy is buoyantly stable.

(c) In this case (compare with Eq. (1.61)),

$$V_I = \frac{M_1 + M_2}{\rho} \quad (1.61)$$

where M_2 [M] is the mass of light attached to the top of the buoy.

Substituting Eqs. (1.61) and (1.57) into Eq. (1.30) leads to

$$L_{BM} = \frac{\pi D^4 \rho}{64(M_1 + M_2)} \quad (1.62)$$

Given Eq. (1.59), it further follows that, in this case,

$$L_{OB} = \frac{2(M_1 + M_2)}{\pi D^2 \rho} \quad (1.63)$$

The elevation of the CoG for the combined buoy and light system is obtained from

$$(M_1 + M_2)L_{OG} = \frac{M_1 L}{2} + M_2 L$$

which recognises that the CoG of buoy is half-way up the buoy and the CoG of the light is at the top of the buoy. It therefore follows that

$$L_{OG} = \left(\frac{M_1 + 2M_2}{M_1 + M_2} \right) \frac{L}{2} \quad (1.64)$$

So in the presence of the light attached to the top of the buoy

$$L_{BM} - L_{BG} = \frac{\pi D^4 \rho}{64(M_1 + M_2)} - \left(\frac{M_1 + 2M_2}{M_1 + M_2} \right) \frac{L}{2} + \frac{2(M_1 + M_2)}{\pi D^2 \rho} \quad (1.65)$$

Letting $M_2 = 12$ kg, $L_{BM} - L_{BG} = -0.0656$ m, which is < 0 so the buoy is not buoyantly stable when the light is attached to it.

(d) The maximum mass of light that can be attached to the buoy can be determined by solving Eq. (1.65) for M_2 and setting $L_{BM} - L_{BG} = 0$.

Multiplying both sides of Eq. (1.65) by $(M_1 + M_2)$ leads to

$$(M_1 + M_2)(L_{BM} - L_{BG}) = \frac{\pi D^4 \rho}{64} - (M_1 + 2M_2) \frac{L}{2} + \frac{2(M_1 + M_2)^2}{\pi D^2 \rho}$$

Collecting terms of M_2 gives us

$$aM_2^2 + bM_2 + c = 0$$

where

$$a = \frac{2}{\pi D^2 \rho}$$

$$b = L_{BG} - L_{BM} - L + \frac{4M_1}{\pi D^2 \rho}$$

$$c = \frac{\pi D^4 \rho}{64} + \left(L_{BG} - L_{BM} - \frac{L}{2} \right) M_1 + \frac{2M_1^2}{\pi D^2 \rho}$$

Solving for M_2 then leads to

$$M_2 = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad (1.66)$$

Setting $L_{BM} - L_{BG} = 0$ then leads to $M_2 = 1820$ kg or 7.31 kg. The latter is obviously the relevant answer. So the maximum sized light for the buoy to remain buoyantly stable is 7.31 kg.

Worked Solution 1.4 (see Problem 1.4)

Using the Bernoulli equation we can say that

$$p_2 = p_1 + \rho \left[\frac{v_1^2 - v_2^2}{2} + g(z_1 - z_2) \right]$$

From the information provided we have that $A_1 = 0.3 \text{ m}^2$, $A_2 = 0.2 \text{ m}^2$, $z_1 = 0 \text{ m}$, $z_2 = 5 \text{ m}$, $v_1 = 2.2 \text{ m s}^{-1}$ and $p_1 = 120,000 \text{ Pa}$. It is also assumed that the density of water, $\rho = 1000 \text{ kg m}^{-3}$.

From the continuity equation we have that

$$v_2 = \frac{A_1}{A_2} v_1$$

therefore

$$p_2 = p_1 + \rho \left[\frac{v_1^2}{2A_2^2} (A_2^2 - A_1^2) + g(z_1 - z_2) \right]$$

So the pressure at point B is 67.9 kPa.

Worked Solution 1.5 (see Problem 1.5)

Consider a streamtube on the water surface. The pressure within the streamtube, both upstream of the bridge and under the arch, will be atmospheric. It follows from the Bernoulli equation that

$$v_2^2 - v_1^2 = 2g(z_1 - z_2)$$

where in this case $z_1 = 1.8 \text{ m}$ and $z_2 = 1.55 \text{ m}$.

From the continuity equation we have that

$$v_1 = \frac{Q}{B_1 z_1} \quad \text{and} \quad v_2 = \frac{Q}{B_2 z_2}$$

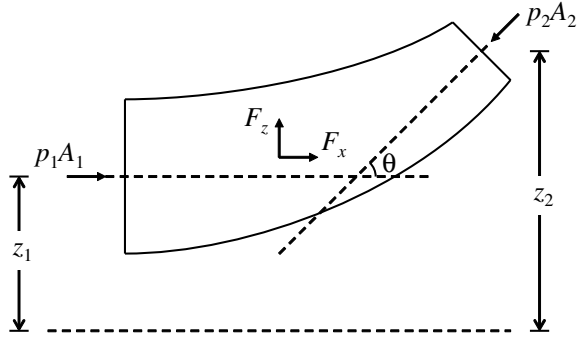
where $B_1 = 7 \text{ m}$ and $B_2 = 7 - 1.4 = 5.6 \text{ m}$.

Substituting the above equations into our rearranged form of the Bernoulli equation leads to

$$Q = \sqrt{2g(z_1 - z_2) \left[\frac{1}{(B_2 z_2)^2} - \frac{1}{(B_1 z_1)^2} \right]^{-1}}$$

Substituting the above values then leads to a flow rate of $26.5 \text{ m}^3 \text{ s}^{-1}$.

Fig. 1.16 Schematic diagram of tapered pipe-bend



Worked Solution 1.6 (see Problem 1.6)

Given the information provided, it can be said that $\theta = 60^\circ$, $D_1 = 0.3$ m, $D_2 = 0.15$ m, $p_1 = 140,000$ Pa, $Q = 0.23$ m³s⁻¹, $z_1 = 0$ m, $z_2 = 1.4$ m and $V = 0.085$ m³ (see Fig. 1.16). It is also assumed that the density of water, $\rho = 1000$ kg m⁻³.

Applying the momentum equation in x and z directions leads to

$$F_x + A_1 p_1 - A_2 p_2 \cos \theta = \rho Q (v_2 \cos \theta - v_1)$$

and

$$F_z - A_2 p_2 \sin \theta - \rho g V = \rho Q v_2 \sin \theta$$

where F_x and F_z are the net-forces exerted by the pipe-bend on the fluid in the x and z directions, respectively, with

$$A_1 = \frac{\pi D_1^2}{4} \quad \text{and} \quad A_2 = \frac{\pi D_2^2}{4}$$

From the continuity equation we have that

$$v_1 = \frac{4Q}{\pi D_1^2} \quad \text{and} \quad v_2 = \frac{4Q}{\pi D_2^2}$$

From the Bernoulli equation we then have that

$$p_2 = p_1 + \frac{8\rho Q^2}{\pi^2} \left(\frac{1}{D_1^4} - \frac{1}{D_2^4} \right) + \rho g (z_1 - z_2) = 46,860 \text{ Pa}$$

It follows from the momentum equations that

$$F_x = \frac{4\rho Q^2}{\pi} \left(\frac{\cos \theta}{D_2^2} - \frac{1}{D_1^2} \right) - \frac{\pi}{4} (D_1^2 p_1 - D_2^2 p_2 \cos \theta) = -8,734 \text{ N}$$

and

$$F_z = \left(\frac{4\rho Q^2}{\pi D_2^2} + \frac{\pi D_2^2 p_2}{4} \right) \sin \theta + \rho g V = 4144 \text{ N}$$

The resultant force and angle are then found from

$$F = \sqrt{F_x^2 + F_z^2} = 9,667 \text{ N}$$

and

$$\beta = \arctan(F_z/F_x) = -25.38^\circ$$

So the net-force acting on the pipe-bend is 9.67 kN acting downwards, away from the inlet, at an angle of 25.4° to the horizontal axis.

Worked Solution 1.7 (see Problem 1.7)

The discharge rate, Q , can be found from

$$Q = \int v dA = \int_0^h v \frac{dA}{dz} dz$$

where, from Eq. (1.42),

$$v = \sqrt{2g(h - z)}$$

with h [L] being the depth of water above the base of SCW opening, z [L] being elevation above the base of the SCW opening and A [L²] being the cross-sectional area of the opening below z .

Considering the trapezoidal geometry of the opening, let $B_1 = 0.1$ m, $B_2 = 0.4$ m and $H = 0.28$ m such that (see Fig. 1.17)

$$A(z) = B_1 z + \left(\frac{B_2 - B_1}{H} \right) \frac{z^2}{2}$$

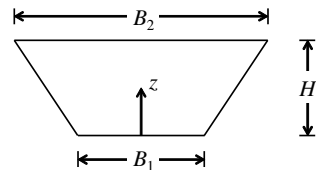
and

$$\frac{dA}{dz} = B_1 + \left(\frac{B_2 - B_1}{H} \right) z$$

It follows that

$$Q = \sqrt{2g} \int_0^h B_1 (h - z)^{1/2} + \left(\frac{B_2 - B_1}{H} \right) z (h - z)^{1/2} dz$$

Fig. 1.17 Schematic diagram of sharp crested weir of symmetric trapezoidal section



To aid integration, let $\xi = h - z$ such that

$$\begin{aligned}
 Q &= \sqrt{2g} \int_0^h B_1 \xi^{1/2} + \left(\frac{B_2 - B_1}{H} \right) (h - \xi) \xi^{1/2} d\xi \\
 &= \sqrt{2g} \int_0^h \left[B_1 + (B_2 - B_1) \frac{h}{H} \right] \xi^{1/2} - \left(\frac{B_2 - B_1}{H} \right) \xi^{3/2} d\xi \\
 &= \sqrt{2g} \left[\frac{2}{3} \left(B_1 + (B_2 - B_1) \frac{h}{H} \right) \xi^{3/2} - \frac{2}{5} \left(\frac{B_2 - B_1}{H} \right) \xi^{5/2} \right]_0^h \\
 &= \sqrt{2g} \left[\frac{2B_1 h^{3/2}}{3} + \frac{4}{15} \left(\frac{B_2 - B_1}{H} \right) h^{5/2} \right] \\
 &= \frac{2}{3} \sqrt{2gh^3} \left[B_1 + \frac{2}{5} (B_2 - B_1) \frac{h}{H} \right]
 \end{aligned}$$

For $h = 0.236$ m, it follows that $Q = 0.0681 \text{ m}^3 \text{s}^{-1}$.

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Flow in Pipes and Normal Flow in Open Channels

2

Abstract

This chapter develops theoretical equations to describe steady-state flow in pipes and normal flow in open channels. First we look at steady laminar flow between two parallel plates and Poiseuille's equation for steady laminar flow through cylindrical pipes. A skin friction model is used to derive the Darcy-Weisbach equation for steady turbulent flow in non-prismatic and non-cylindrical pipes. Darcy-Weisbach friction factors are derived for steady laminar flow between parallel plates and steady laminar flow through cylindrical pipes. The empirical Chezy and Manning equations for open channel flow are presented and related back to the Darcy-Weisbach equation, by deriving associated relationships for the Darcy-Weisbach friction factor. The normal flow assumption, for open channel flow, is explained and defined. Practical applications are presented through a problem sheet with worked solutions.

Notation

a	Acceleration [LT^{-2}].
A	Area [L^2].
A_n	Normal area [L^2].
$\hat{A}$	Mean cross-sectional area [L^2].
b	Separation distance [L].
B	Breadth [L].
c_0	Geometrical factor [—].
C	Chezy coefficient [$\text{L}^{\frac{1}{2}}\text{T}^{-1}$].
D	Diameter [L].
E	Total head [L].
f	Friction factor [—].
f_n	Normal friction factor [—].
F	Force [MLT^{-2}].

g	Gravitational acceleration [LT^{-2}].
h	Hydraulic head [L].
h_v	Velocity head [L].
H	Depth [L].
H_n	Normal depth [L].
L	Length [L].
m	Hydraulic radius [L].
m_n	Normal hydraulic radius [L].
n	Manning coefficient [$\text{L}^{-\frac{1}{3}}\text{T}$].
M	Mass [M].
p	Fluid pressure [$\text{ML}^{-1}\text{T}^{-2}$].
p_n	Normal stress [$\text{ML}^{-1}\text{T}^{-2}$].
p_s	Static pressure [$\text{ML}^{-1}\text{T}^{-2}$].
p_v	Velocity pressure [$\text{ML}^{-1}\text{T}^{-2}$].
P	Wetted perimeter [L].
P_n	Normal wetted perimeter [L].
$\hat{P}$	Mean wetted perimeter [L].
Q	Flow rate [L^3T^{-1}].
r	Radial distance [L].
Re	Reynolds number [-].
s	Distance along a streamtube [L].
S_0	Bed slope [-].
S_f	Friction slope [-].
t	Time [T].
v	Fluid velocity [LT^{-1}].
v_n	Normal velocity [LT^{-1}].
$\hat{v}$	Mean fluid velocity [LT^{-1}].
z	Elevation [L].
θ	Inclination angle [-].
κ	Surface roughness [L].
μ	Dynamic viscosity [$\text{ML}^{-1}\text{T}^{-1}$].
ξ	Distance [L].
ρ	Mass density of a fluid [ML^{-3}].
ψ	Pressure head [L].
τ	Shear stress [$\text{ML}^{-1}\text{T}^{-2}$].
τ_0	Wall shear stress [$\text{ML}^{-1}\text{T}^{-2}$].

2.1 Introduction

Total head represents the mechanical energy per unit weight of fluid. For steady-state, incompressible and inviscid flow, the Bernoulli equation gives that total head is constant along a streamtube (see Sect. 1.3.4). Inviscid flow implies that the fluid of concern has no viscosity and frictional losses are negligible. However, frictional

forces are often important and total head is lost along a streamtube. The rate at which total head is lost with distance is referred to as the friction slope. In this chapter we will derive a set of equations relating friction slope to fluid velocity for a range of different steady-state scenarios of interest.

The momentum equation is used to derive equations describing steady laminar flow between two parallel plates and through cylindrical pipes. A uniform flow assumption is imposed to derive the Darcy–Weisbach equation for turbulent flow in non-cylindrical pipes. Two empirical laws, the Chezy equation and the Manning equation, are presented for describing flow in open channels. The concept of normal flow in open channels is introduced.

2.2 Friction Slope

Recall the definition of total head, E [L], (Eq. (1.40))

$$E = \frac{p}{\rho g} + \frac{v^2}{2g} + z \quad (2.1)$$

where p [$\text{ML}^{-1}\text{T}^{-2}$] is fluid pressure, ρ [ML^{-3}] is fluid density, g [LT^{-2}] is gravitational acceleration and v [LT^{-1}] is fluid velocity.

The friction slope, S_f [–], is defined by

$$S_f = -\frac{\partial E}{\partial s} \quad (2.2)$$

where s [L] is distance along a streamtube.

2.3 Steady Laminar Flow

2.3.1 Viscosity

The presence of frictional forces gives rise to fluid particles tending to get stuck on solid surfaces. Consequently, fluid velocity, v [LT^{-1}], tends to be zero at solid boundaries and increases with distance, ξ [L], from such boundaries (Fig. 2.1a).

Fluid flowing slowly past a solid surface tends to move as a set of thin layers travelling at different velocities. These thin layers are commonly referred to as lamina and this mode of flow is commonly referred to as laminar flow. The difference in velocity between each fluid layer gives rise to a frictional shear stress, τ [$\text{ML}^{-1}\text{T}^{-2}$] (Fig. 2.1b).

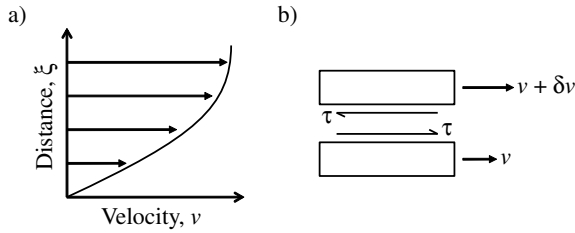


Fig. 2.1 **a** Velocity profile expected during laminar flow past a solid surface. **b** Shear stress (τ) development between two fluid laminae moving at different velocities (v)

Table 2.1 Density, ρ , and dynamic viscosity, μ , for selected fluids at 101 kPa and 20 °C (after [1, p. 27])

Fluid	ρ (kg m ⁻³)	μ (Pa s)
Hydrogen	0.084	9.0×10^{-6}
Air	1.20	1.8×10^{-5}
Petrol	680	2.9×10^{-4}
Water	1000	1.0×10^{-3}
Mercury	13,500	1.5×10^{-3}
SAE 30 engine oil	891	2.9×10^{-1}

It is often assumed that fluid shear stress is linearly proportional to velocity gradient. The coefficient of proportionality is referred to as the dynamic viscosity, μ [ML⁻¹T⁻¹], i.e.,

$$\tau = \mu \frac{\partial v}{\partial \xi} \quad (2.3)$$

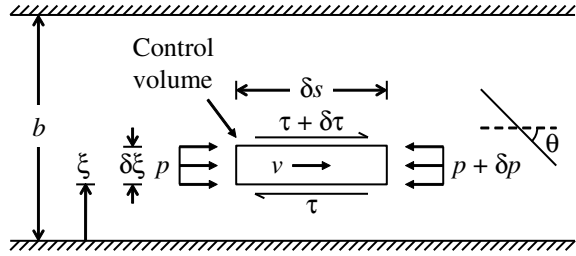
Fluids that conform to Eq. (2.3) are referred to as Newtonian fluids. Fluids conforming to alternative relationships are referred to as non-Newtonian fluids. Density and dynamic viscosity values for a selection of fluids are provided in Table 2.1. Gases tend to have very low viscosities. Thick liquids tend to have very high viscosities.

In what follows, we will use Eq. (2.3) to derive relationships between S_f and v for steady laminar flow between two parallel plates and steady laminar flow through a cylindrical pipe.

2.3.2 Flow Between Two Parallel Plates

An incompressible fluid, of mass density, ρ [ML⁻³], flows in between two semi-infinite parallel plates, separated by a distance, b [L], which is orientated at an angle, θ [–], to the horizontal. Consider fluid contained within a cuboid control-volume (CV), located at a distance, ξ , from the lower bounding surface, of thickness, $\delta \xi$, length, δs , and breadth (normal to the page), B (see Fig. 2.2). The fluid pressure

Fig. 2.2 A control volume (CV) located within fluid moving between two parallel plates



acting on the inlet of the CV is p whereas the pressure acting on the outlet is $p + \delta p$. Fluid moving along the underside of the CV moves slower than fluid within the CV giving rise to a shear stress, τ , acting in the opposite direction of the fluid flow. Fluid moving along the upper side of the CV moves faster than fluid within the CV giving rise to a shear stress, $\tau + \delta \tau$, acting in the direction of the fluid flow.

Challenge 2.1 Apply the momentum equation to the CV, shown in Fig. 2.2, to derive a relationship between the fluid shear stress, τ , and friction slope, S_f .

The volumetric flow rate of fluid through the CV is $B\delta\xi v$. The momentum equation (recall Eq. (1.38)) therefore gives that,

$$F = \rho B\delta\xi v \delta v \quad (2.4)$$

where F [MLT⁻²] is the net-force acting on the CV, in the flow direction, found from

$$F = \sum_{i=1}^5 F_i \quad (2.5)$$

F_1 is the force due to the fluid pressure, p , on the inlet of the CV, found from

$$F_1 = B\delta\xi p$$

F_2 is the force due to the fluid pressure on the outlet of the CV, found from

$$F_2 = -B\delta\xi(p + \delta p)$$

F_3 is the force due to the self-weight of the fluid within the CV, found from

$$F_3 = -B\delta\xi\delta s\rho g \sin \theta = B\delta\xi\rho g\delta z$$

F_4 is the shear force acting on the underside of the CV, found from

$$F_4 = -B\delta s\tau$$

and F_5 is the shear force acting on the topside of the CV, found from

$$F_5 = B\delta s(\tau + \delta \tau)$$

Recall that $\sin \theta = \frac{\delta z}{\delta s}$ where z is elevation.

Equating Eqs. (2.4) and (2.5) leads to

$$B\delta\xi p - B\delta\xi(p + \delta p) - B\delta\xi\rho g\delta z - B\delta s\tau + B\delta s(\tau + \delta\tau) = \rho B\delta\xi v\delta v$$

which can be simplified and rearranged to get

$$\frac{\delta\tau}{\delta\xi} = \rho g \left(\frac{1}{\rho g} \frac{\delta p}{\delta s} + \frac{v}{g} \frac{\delta v}{\delta s} + \frac{\delta z}{\delta s} \right)$$

For an infinitesimally small CV (i.e., $\delta\xi \rightarrow 0$ and $\delta s \rightarrow 0$) it can be further stated that

$$\frac{\partial\tau}{\partial\xi} = -\rho g S_f \quad (2.6)$$

where S_f [–] is the friction slope, define in Eq. (2.2).

Challenge 2.2 Equate Eqs. (2.3) and (2.6) and derive an expression relating v to S_f .

Equating Eqs. (2.3) and (2.6) and dividing both sides by μ leads to

$$\frac{\partial^2 v}{\partial\xi^2} = -\frac{\rho g S_f}{\mu}$$

Integrating both sides with respect to ξ twice then yields

$$v = -\frac{\rho g \xi^2 S_f}{2\mu} + A_1 \xi + A_2$$

where A_1 and A_2 are integration constants.

Recall that the fluid velocity at the bounding solid surfaces is zero, i.e.,

$$\begin{aligned} v &= 0, \xi = 0 \\ v &= 0, \xi = b \end{aligned}$$

It follows that $A_2 = 0$, $A_1 = \frac{\rho g b S_f}{2\mu}$ and [2, p. 201]

$$v = \frac{\rho g (b\xi - \xi^2) S_f}{2\mu} \quad (2.7)$$

Challenge 2.3 Determine an expression for the mean velocity of the fluid flowing between the parallel plates.

The mean fluid velocity between the parallel plates, $\hat{v}$, is obtained from [2, p. 201]

$$\begin{aligned}
 \hat{v} &= \frac{1}{b} \int_0^b v d\xi \\
 &= \frac{1}{b} \int_0^b \frac{\rho g (b\xi - \xi^2) S_f}{2\mu} d\xi \\
 &= \frac{\rho g S_f}{2\mu b} \left[\frac{b\xi^2}{2} - \frac{\xi^3}{3} \right]_0^b \\
 &= \frac{\rho g b^2 S_f}{12\mu}
 \end{aligned} \tag{2.8}$$

2.3.3 Flow Through a Cylindrical Pipe

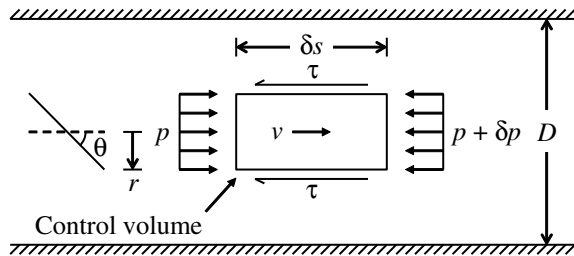
An incompressible fluid, of mass density, ρ [ML^{-3}], flows through a cylindrical pipe of diameter, D [L], which is orientated at an angle, θ [–], to the horizontal. Consider fluid contained within a cylindrical control-volume (CV), orientated along the central axis of the pipe, of radius, r [L], and length, δs [L] (see Fig. 2.3). The fluid pressure acting on the inlet of the CV is p [$\text{ML}^{-1}\text{T}^{-2}$] whereas the pressure acting on the outlet is $p + \delta p$ [$\text{ML}^{-1}\text{T}^{-2}$]. Fluid moving along the outside of the CV moves slower than fluid within the CV giving rise to a shear stress, τ , [$\text{ML}^{-1}\text{T}^{-2}$] acting in the opposite direction of the fluid flow.

Challenge 2.4 Apply the momentum equation to the CV, shown in Fig. 2.3, to derive a relationship between the fluid shear stress, τ , and friction slope, S_f .

In this case, the volumetric flow rate of fluid through the CV is $\pi r^2 v$. The momentum equation (recall Eq. (1.38)) therefore gives that

$$F = \rho \pi r^2 v \delta v \tag{2.9}$$

Fig. 2.3 A control volume located within fluid moving through a cylindrical pipe



where F [MLT^{-1}] is the net-force acting on the CV, in the flow direction, found from

$$F = \sum_{i=1}^4 F_i \quad (2.10)$$

F_1 is the force due to the fluid pressure, p , on the inlet of the CV, found from

$$F_1 = \pi r^2 p$$

F_2 is the force due to the fluid pressure on the outlet of the CV, found from

$$F_2 = -\pi r^2 (p + \delta p)$$

F_3 is the force due to the self-weight of the fluid within the CV, found from

$$F_3 = -\pi r^2 \delta s \rho g \sin \theta = -\pi r^2 \rho g \delta z$$

and F_4 is the force due to the fluid shear stress, τ , found from

$$F_4 = -2\pi r \delta s \tau$$

Recall again that $\sin \theta = \frac{\delta z}{\delta s}$.

Equating Eqs. (2.9) and (2.10) leads to

$$\pi r^2 p - \pi r^2 (p + \delta p) - \pi r^2 \rho g \delta z - 2\pi r \delta s \tau = \rho \pi r^2 v \delta v$$

which can be simplified and rearranged to get

$$\tau = -\frac{\rho g r}{2} \left(\frac{1}{\rho g} \frac{\delta p}{\delta s} + \frac{v}{g} \frac{\delta v}{\delta s} + \frac{\delta z}{\delta s} \right)$$

For an infinitesimally small CV (i.e., $\delta s \rightarrow 0$) it can be further stated that

$$\tau = \frac{\rho g r S_f}{2} \quad (2.11)$$

where S_f [–] is the friction slope defined in Eq. (2.2).

Challenge 2.5 Equate Eqs. (2.3) and (2.11) and derive an expression relating v to S_f .

Consider again Eq. (2.3). Given that r is the distance from the centre of the pipe, whereas ξ is the distance from the inside solid surface of the pipe wall, it follows that $\frac{\partial r}{\partial \xi} = -1$ and

$$\tau = -\mu \frac{\partial v}{\partial r} \quad (2.12)$$

Equating Eqs. (2.11) and (2.12) and dividing both sides by μ leads to

$$\frac{\partial v}{\partial r} = -\frac{\rho g r S_f}{2\mu}$$

Integrating both sides with respect to r leads to

$$v = -\frac{\rho g r^2 S_f}{4\mu} + C$$

where C is an integration constant.

Noting that the fluid velocity at the wall of the pipe is zero, it follows that $v(r = \frac{D}{2}) = 0$, $C = \frac{\rho g D^2 S_f}{16\mu}$ and [2, p. 193]

$$v = \frac{\rho g S_f}{4\mu} \left(\frac{D^2}{4} - r^2 \right) \quad (2.13)$$

Challenge 2.6 Determine an expression for the flow rate and the mean velocity in the pipe.

The flow rate in the pipe, Q [$L^3 T^{-1}$], is found from [2, p. 194]

$$\begin{aligned} Q &= \int_0^{\frac{D}{2}} 2\pi r v dr \\ &= \left[\frac{\pi \rho g S_f}{2\mu} \left(\frac{D^2 r^2}{8} - \frac{r^4}{4} \right) \right]_0^{\frac{D}{2}} \\ &= \frac{\pi \rho g D^4 S_f}{128\mu} \end{aligned} \quad (2.14)$$

which is commonly referred to as Poiseuille's equation.

Given that the cross-sectional area, $A = \frac{\pi D^2}{4}$, it follows that the mean velocity

$$\hat{v} \equiv \frac{Q}{A} = \frac{\rho g D^2 S_f}{32\mu}. \quad (2.15)$$

2.4 Steady Turbulent Flow

Laminar flow conditions tends only to apply to slow moving fluids. As fluid velocities increases, water particle trajectories become more chaotic, leading to a breakdown in the smooth nature of velocity distributions described by Eqs. (2.7) and (2.13) and illustrated in Fig. 2.1a. This alternative model of flow is commonly referred to as turbulent flow conditions.

In this context, it is common to assume that fluid velocity is uniform across a cross-section of pipe. Frictional forces are then incorporated by invoking an infinitesimal skin of fluid along solid surface boundaries where the fluid remains static.

2.4.1 Turbulent Flow Through a Non-prismatic and Non-cylindrical Pipe

An incompressible fluid, of mass density, ρ [ML^{-3}], flows through a non-prismatic and non-cylindrical pipe, which is orientated at an angle, θ [–], to the horizontal. Consider a control-volume (CV) formed by isolating an interval of pipe of length, δs [L] (see Fig. 2.4). The fluid pressure acting on the inlet of the CV is p [$\text{ML}^{-1}\text{T}^{-2}$] whereas the pressure acting on the outlet is $p + \delta p$ [$\text{ML}^{-1}\text{T}^{-2}$]. The presence of an outer, infinitesimal, skin of static fluid gives rise to a wall shear stress, τ_0 , [$\text{ML}^{-1}\text{T}^{-2}$] acting in the opposite direction of the fluid flow.

Challenge 2.7 Apply the momentum equation to the CV, shown in Fig. 2.4, to derive a relationship between the wall shear stress, τ_0 , and friction slope, S_f .

The volumetric flow rate of fluid through the CV is Q . The momentum equation (recall Eq. (1.38)) therefore gives that

$$F = \rho Q \delta v \quad (2.16)$$

where F [MLT^{-1}] is the net-force acting on the CV, in the flow direction, found from

$$F = \sum_{i=1}^4 F_i \quad (2.17)$$

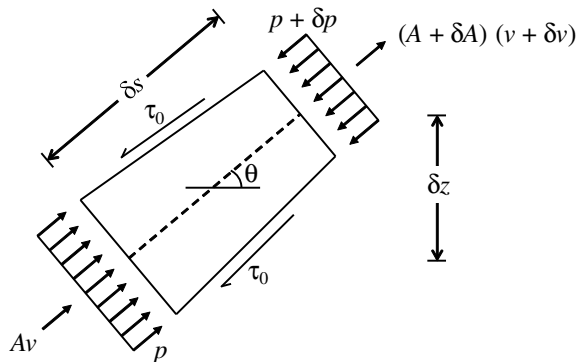
F_1 is the force due to the fluid pressure, p , on the inlet of the CV, found from

$$F_1 = Ap$$

F_2 is the force due to the fluid pressure on the outlet of the CV, found from

$$F_2 = -(A + \delta A)(p + \delta p)$$

Fig. 2.4 A control-volume located within a non-prismatic and non-cylindrical pipe



F_3 is the force due to the self-weight of the fluid within the CV, found from

$$F_3 = -\hat{A}\delta s \rho g \sin \theta = -\hat{A}\rho g \delta z$$

(recall again that $\sin \theta = \frac{\delta z}{\delta s}$) and F_4 is the force due to the wall shear stress, τ_0 , found from

$$F_4 = -\hat{P}\delta s \tau_0$$

where $\hat{A}$ is the mean cross-sectional area of the CV and $\hat{P}$ [L] is the mean wetted perimeter across the fluid column within the CV.

The wetted perimeter, P [L], of a fluid filled cylindrical pipe of diameter, D [L], would be the circumference, πD . The wetted perimeter for a fluid filled square section pipe of side, L [L], would be $4L$.

Equating Eqs. (2.17) and (2.16) leads to

$$Ap - (A + \delta A)(p + \delta p) - \hat{A}\rho g \delta z - \hat{P}\delta s \tau_0 = \rho Q \delta v$$

which can be simplified and rearranged to get

$$\tau_0 = -\frac{\rho g \hat{A}}{\hat{P}} \left(\frac{p}{\rho g \hat{A}} \frac{\delta A}{\delta s} + \frac{(A + \delta A)}{\hat{A} \rho g} \frac{\delta p}{\delta s} + \frac{Q}{\hat{A} g} \frac{\delta v}{\delta s} + \frac{\delta z}{\delta s} \right)$$

If the CV is infinitesimally small (i.e., $\delta s \rightarrow 0$, $\delta A \rightarrow 0$, $\hat{A} \rightarrow A$, $\hat{P} \rightarrow P$, $\frac{Q}{\hat{A}} \rightarrow v$) it can be further stated that

$$\tau_0 = -\frac{\rho g A}{P} \left(\frac{p}{\rho g A} \frac{\partial A}{\partial s} + \frac{1}{\rho g} \frac{\partial p}{\partial s} + \frac{v}{g} \frac{\partial v}{\partial s} + \frac{\partial z}{\partial s} \right)$$

Furthermore, for a pipe of smoothly varying cross-sectional area, $\frac{\partial A}{\partial s} \ll A$ and

$$\tau_0 = \rho g m S_f \quad (2.18)$$

where S_f is the friction slope (defined by Eq. (2.2)) and m [L] is the so-called hydraulic radius, found from

$$m = \frac{A}{P} \quad (2.19)$$

2.4.2 Linking Wall Shear Stress to Fluid Velocity

The frictional shear stress, τ_0 , can be determined from

$$\tau_0 = f p_n$$

where f [—] is known as the friction factor and p_n [$\text{ML}^{-1}\text{T}^{-2}$] is the normal stress acting on the static fluid skin by the interior column of moving fluid.

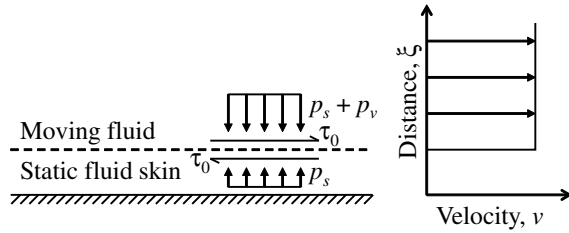
Note that the total head (Eq. (2.1)) can be usefully split up into two pressures:

$$E = \frac{p_s + p_v}{\rho g}$$

where p_s is referred to as the static pressure, found from

$$p_s = p + \rho g z$$

Fig. 2.5 Schematic diagram showing the pressures and shear stresses applied on a static fluid skin



and p_v is referred to as the velocity pressure, found from

$$p_v = \frac{\rho v^2}{2}$$

Both the static fluid skin and the interior column of moving fluid experience p_s (see Fig. 2.5). However, whereas the moving fluid also experiences p_v , the static fluid skin does not because it has no kinetic energy. Consequently, it is p_v that represents the friction inducing normal stress acting on the static fluid skin by the interior column of moving fluid. In this way it can be understood that $p_n = p_v$ and

$$\tau_0 = \frac{f \rho v^2}{2} \quad (2.20)$$

Equation (2.20) is referred to as the skin friction model, which tells us that skin friction shear stress is proportional to the square of the velocity of the moving body. In contrast, for a related model, the dry friction model (associated with solid objects sliding on a solid surface), friction shear stress is independent of the moving body velocity and purely a function of its weight instead.

Equating Eqs. (2.18) and (2.20) leads to the so-called Darcy–Weisbach equation [2, p. 248]:

$$S_f = \frac{f v^2}{2gm} \quad (2.21)$$

Furthermore, given that the fluid velocity is assumed constant across a cross-section, the cross-sectional mean velocity, $\hat{v} = v$, and

$$S_f = \frac{f \hat{v}^2}{2gm} \quad (2.22)$$

2.4.3 Friction Factor for Turbulent Flow Systems

Flow within a pipe will be either laminar or turbulent, depending on the Reynolds number, Re [–], defined by [3]

$$Re = \frac{4\rho m \hat{v}}{\mu} \quad (2.23)$$

where $\hat{v}$ [LT^{-1}] is the cross-sectional mean velocity and μ [$ML^{-1}T^{-1}$] is the dynamic viscosity of the fluid. Laminar flow is found to occur when $Re < 2000$. Turbulent

Table 2.2 Roughness values for a range of different materials (after [1, p. 371])

Material	Condition	κ (mm)	Uncertainty (%)
Steel	Sheet metal, new	0.05	± 60
	Stainless, new	0.002	± 50
	Commercial, new	0.046	± 30
	Riveted	3.0	± 70
	Rusted	2.0	± 50
Iron	Cast, new	0.26	± 50
	Wrought, new	0.046	± 20
	Galvanized, new	0.15	± 40
	Asphalted cast	0.12	± 50
Brass	Drawn, new	0.002	± 50
Plastic	Drawn tubing	0.0015	± 60
Concrete	Smoothed	0.04	± 60
	Rough	2.0	± 50
Rubber	Smoothed	0.01	± 60
Wood	Stave	0.5	± 40

flow is found to occur when $Re > 4000$. The region $Re \in [2000, 4000]$ is commonly referred to as the critical zone [2, p. 253].

Under turbulent flow conditions, the friction factor, f , can be determined from empirical equations. Below is an empirical equation due to [4] (see [2, p. 254]):

$$f = \left[3.6 \log_{10} \left(\frac{6.9}{Re} + \left(\frac{\kappa}{14.84m} \right)^{1.11} \right) \right]^{-2}, \quad Re > 4000 \quad (2.24)$$

where κ [L] is a measure of surface roughness (see Table 2.2 for a list of values).

Although Eq. (2.24) was derived from experiments using cylindrical pipes it is thought to apply to non-cylindrical pipes as well.

2.4.4 Friction Factor for Laminar Flow Systems

2.4.4.1 Laminar Flow Between Two Parallel Plates

Challenge 2.8 Given Eqs. (2.8), (2.22) and (2.23), derive an expression for the friction factor, f , describing steady laminar flow between two parallel plates in terms of Reynolds number, Re .

A friction factor for laminar flow between two parallel plates can be obtained by considering Eq. (2.8). Solving Eq. (2.8) for S_f leads to

$$S_f = \frac{12\mu\hat{v}}{\rho gb^2} \quad (2.25)$$

Equating Eqs. (2.22) and (2.25) and solving for f then give us

$$f = \frac{24m\mu}{\rho b^2 \hat{v}} \quad (2.26)$$

If we consider a flow channel of breadth, B [L], where $B \gg b$, the cross-sectional area, $A = Bb$, and the wetted perimeter, $P = 2B$. Therefore the hydraulic radius, $m = \frac{b}{2}$, which on substitution into Eq. (2.26) leads to

$$f = \frac{6\mu}{\rho m \hat{v}} \quad (2.27)$$

Substituting Eq. (2.23) into Eq. (2.27) gives us

$$f = \frac{24}{\text{Re}}, \quad \text{Re} < 2000 \quad (2.28)$$

2.4.4.2 Laminar Flow Through a Cylindrical Pipe

Challenge 2.9 Given Eqs. (2.15), (2.22) and (2.23), derive an expression for the friction factor, f , describing steady laminar flow through a cylindrical pipe in terms of Reynolds number.

A friction factor for laminar flow through a cylindrical pipe can be obtained by considering Eq. (2.15). Solving Eq. (2.15) for S_f leads to

$$S_f = \frac{32\mu \hat{v}}{\rho g D^2} \quad (2.29)$$

Equating Eqs. (2.22) and (2.29) and solving for friction factor then give us

$$f = \frac{64\mu m}{\rho D^2 \hat{v}} \quad (2.30)$$

In this case, the cross-sectional area, $A = \frac{\pi D^2}{4}$, and the wetted perimeter, $P = \pi D$. Therefore the hydraulic radius, $m = \frac{D}{4}$, which on substitution into Eq. (2.30) leads to

$$f = \frac{4\mu}{\rho m \hat{v}} \quad (2.31)$$

Substituting Eq. (2.23) into Eq. (2.31) gives us

$$f = \frac{16}{\text{Re}}, \quad \text{Re} < 2000 \quad (2.32)$$

2.4.4.3 Laminar Flow Through a Non-cylindrical Pipe

Given Eqs. (2.28) and (2.32) it can be understood that the friction factor for laminar flow through a non-cylindrical pipe takes the form

$$f = \frac{8c_0}{\text{Re}}, \quad \text{Re} < 2000 \quad (2.33)$$

where c_0 [–] is a geometrical factor equal to 3 for a parallel plate system and 2 for a cylindrical pipe. For intermediate geometries it is likely that $c_0 \in (2, 3)$.

2.5 Empirical Laws for Open Channel Flow

Open channel flow works in a very different way to pipe flow due to the presence of a free water surface. Importantly, this implies that the hydraulic radius is a function of fluid velocity and that pressure is not uniform within a given cross-section. Nevertheless, empirical laws used to describe open channel flow bare a startling resemblance to the Darcy–Weisbach equation for pipe flow.

2.5.1 Chezy Equation

Antoine de Chezy performed a series of flow monitoring experiments on canals and river channels associated with the River Seine in 1769 and derived the following empirical equation, referred to hereafter as the Chezy equation [2, p. 421]

$$S_f = \frac{v^2}{C^2 m} \quad (2.34)$$

where C [$L^{1/2}T^{-1}$] is an empirical constant known as the Chezy coefficient and m [L] is the hydraulic radius of the water filled channel.

2.5.2 Manning Equation

The Irish engineer, Robert Manning [5], performed a similar set of experiments and arrived at the following alternative equation [2, p. 422]

$$S_f = \frac{n^2 v^2}{m^{4/3}} \quad (2.35)$$

where n [$L^{-1/3}T$] is known as Manning’s roughness coefficient. Some typical values for the Manning coefficient are presented in Table 2.3.

Table 2.3 Some approximate values of the Manning coefficient, n , in $m^{-1/3}s$ [2, p. 422]

Smooth cement, planed timber	0.010
Rough timber, canvas	0.012
Cast iron, good ashlar masonry, brickwork	0.013
Vitrified clay, asphalt, good concrete	0.015
Rubble masonry	0.018
Firm gravel	0.020
Canals and rivers in good condition	0.025
Canals and rivers in bad condition	0.035

2.5.3 Expressions for Friction Factor

Challenge 2.10 Given Eqs. (2.21), (2.34) and (2.35), derive expressions relating the Darcy–Weisbach friction factor to the Chezy coefficient and the Manning coefficient.

Equating Eq. (2.34) with Eq. (2.21) reveals that the Chezy coefficient and the Darcy–Weisbach friction factor are related by

$$f = \frac{2g}{C^2} \quad (2.36)$$

and equating Eq. (2.35) with Eq. (2.21) reveals that the Manning coefficient and the Darcy–Weisbach friction factor are related by

$$f = \frac{2gn^2}{m^{1/3}} \quad (2.37)$$

2.5.4 An Expression for Total Head

When applying Darcy–Weisbach-type equations (e.g. Eqs. (2.21), (2.34) and (2.35)) to open channel flow problems, it is common to make the following assumptions:

1. Fluid velocity is uniform within a given cross-section.
2. Fluid pressure is hydrostatic.
3. The E term associated with S_f represents the total head at the base of the channel.

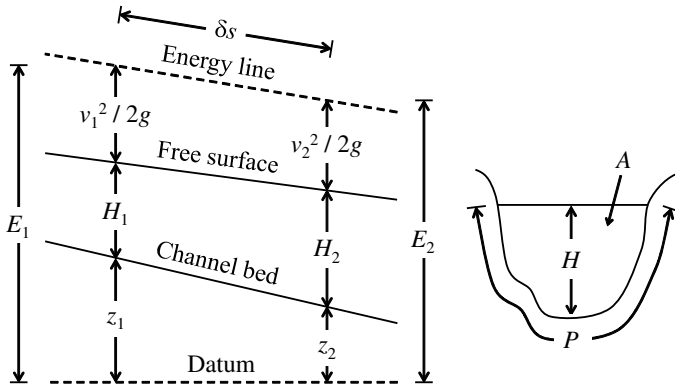
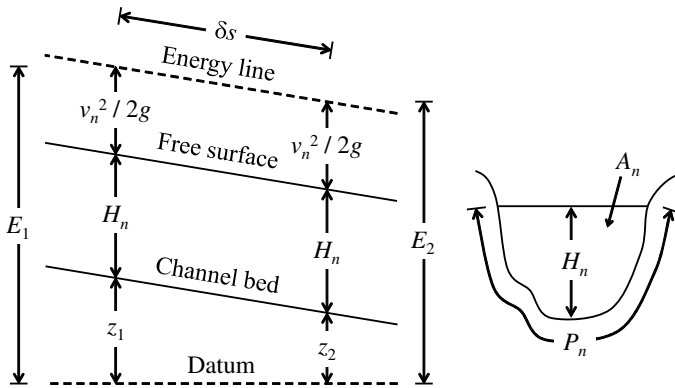
Given the hydrostatic pressure assumption, the pressure head at the base of the channel, ψ , is equal to the fluid depth above, H (see Fig. 2.6). It follows from Eq. (2.1) that

$$E = H + \frac{v^2}{2g} + z \quad (2.38)$$

2.5.5 Normal Flow Conditions

Under steady-state conditions within a sufficiently long prismatic open channel, the fluid velocity, v , is expected to be uniform in the flow direction. Such conditions are commonly referred to as normal flow conditions.

Noting that $Q = Av$ where Q is constant, it follows that the flowing cross-sectional area, A , will also be constant. For a prismatic channel, it can therefore be further asserted that the fluid depth, H , will be constant as well (see Fig. 2.7). As such

**Fig. 2.6** Gradually varied flow in an open channel**Fig. 2.7** Normal flow in an open channel

$$\frac{\partial E}{\partial s} = \frac{\partial z}{\partial s} \quad (2.39)$$

where z refers to the elevation of the channel bed in this context.

Equation (2.39) is often referred to as the normal flow assumption. Under normal flow conditions, the Darcy–Weisbach equation (Eq. (2.21)) gives that

$$S_0 = \frac{f v^2}{2gm} \quad (2.40)$$

where S_0 [–] is the bed slope found from

$$S_0 = -\frac{\partial z}{\partial s} \quad (2.41)$$

It is often convenient to compare real conditions to normal flow conditions. In this context, it is common to refer to the associated velocity, fluid depth, wetted perimeter, flowing cross-sectional area, friction factor and hydraulic radius as v_n , H_n , P_n , A_n , f_n and m_n , respectively (see Fig. 2.7). The n subscript denotes that these properties are those that would be expected under normal flow conditions (i.e., when $S_f = S_0$).

2.6 Problem Sheet

Problem 2.1 (see Worked Solution 2.1)

Water flows between two tanks via a 3 mm diameter cylindrical capillary tube of 4 m length. The elevation of the water surface in the downstream tank is 20 cm below the water surface in the upstream tank.

- (a) Determine the flow rate (in $\text{m}^3 \text{h}^{-1}$) through the pipe assuming laminar flow conditions and verify that the flow is indeed laminar.
- (b) Determine the capillary tube diameter required to yield a Reynolds number of 1900 and also quantify the corresponding flow rate (in $\text{m}^3 \text{h}^{-1}$).

Problem 2.2 (see Worked Solution 2.2)

A stainless steel cylindrical pipe of 3 cm diameter and 5 m length is used to transport water from one tank to another. Determine the total head loss across the pipe when the flow rate is $0.0012 \text{ m}^3 \text{s}^{-1}$.

Problem 2.3 (see Worked Solution 2.3)

Water flows along a symmetrical trapezoidal channel with a longitudinal slope of 1 in 2100 and a Chezy coefficient of $45 \text{ m}^{\frac{1}{2}} \text{s}^{-1}$. The breadth of the channel is 700 mm at the base and 1400 mm at an elevation of 800 mm above the base. The depth of water in the channel is 500 mm. Determine the flow rate in the channel assuming normal flow conditions.

Problem 2.4 (see Worked Solution 2.4)

An open channel of trapezoidal section, 2.2 m wide at the base with sides inclining at 60° to the horizontal, has a bed slope of 1 in 600. When the water depth is 300 mm, the flow rate in the channel is $0.95 \text{ m}^3 \text{s}^{-1}$. Assume normal flow conditions and use the Manning equation to determine the flow rate when the water depth is 450 mm.

Problem 2.5 (see Worked Solution 2.5)

Two reservoirs are connected by a cylindrical pipe of 0.9 m diameter and 3.2 km length. The pipe is laid at a uniform slope of 1 in 1400. When the reservoir levels

are low, the conduit runs partially full. When the depth is 320 mm, the steady-state rate of flow is $0.0720 \text{ m}^3 \text{ s}^{-1}$.

- (a) Determine a Manning coefficient for the pipe.
- (b) Determine the flow rate in the pipe when the water depth is 850 mm.
- (c) Determine the flow rate when the pipe is full and the difference between the reservoir levels is 4.2 m.

Problem 2.6 (see Worked Solution 2.6)

A conduit, of circular cross-section, is to deliver up to $0.11 \text{ m}^3 \text{ s}^{-1}$ of water under normal flow conditions. Another constraint is that the mean water velocity needs to be greater than 0.4 m s^{-1} when the water depth is one quarter of the conduit diameter. The conduit material has a Chezy coefficient of $45 \text{ m}^{1/2} \text{ s}^{-1}$. Determine the minimum required diameter and bed slope.

2.7 Worked Solutions

Worked Solution 2.1 (see Problem 2.1)

(a) Under laminar flow conditions, the flow rate in a cylindrical pipe is found from Eq. (2.14). Letting $D = 0.003 \text{ m}$, $S_f = \frac{0.2}{4}$, $\rho = 1000 \text{ kg m}^{-3}$, $\mu = 10^{-3} \text{ Pa s}$ and $g = 9.81 \text{ m s}^{-2}$ it follows that the flow rate, $Q = 0.00351 \text{ m}^3 \text{ h}^{-1}$.

For laminar flow conditions to apply, the Reynolds number, $\text{Re} < 2000$. Substituting Eq. (2.15) into Eq. (2.23) and remembering that $m = \frac{D}{4}$ leads to

$$\text{Re} = \frac{\rho^2 g D^3 S_f}{32 \mu^2} \quad (2.42)$$

Given the above values, it follows that $\text{Re} = 414$ which confirms that laminar flow conditions do indeed apply.

(b) Solving Eq. (2.42) for D leads to

$$D = \left(\frac{32 \mu^2 \text{Re}}{\rho^2 g S_f} \right)^{\frac{1}{3}}$$

Given $S_f = \frac{0.2}{4}$, $\rho = 1000 \text{ kg m}^{-3}$, $\mu = 10^{-3} \text{ Pa s}$, $g = 9.81 \text{ m s}^{-2}$ and $\text{Re} = 1900$, it follows that $D = 0.004986 \text{ m}$. So a 5 mm diameter capillary tube is required to yield a Reynolds number of 1900.

Substituting $Q = \frac{\pi D^2 \hat{v}}{4}$ and $m = \frac{D}{4}$ into Eq. (2.23) and solving for Q yields

$$Q = \frac{\pi \mu D \text{Re}}{4\rho}$$

which, given the values above, leads to a corresponding flow rate, $Q = 0.02679 \text{ m}^3 \text{ h}^{-1}$.

Worked Solution 2.2 (see Problem 2.2)

First we need to determine whether the flow is laminar or turbulent using the expression for Reynolds number (Eq. (2.23)). For water, $\rho = 1000 \text{ kg m}^{-3}$ and $\mu = 10^{-3} \text{ Pa s}$. For a cylindrical pipe, $\hat{v} = \frac{4Q}{\pi D^2}$ and $m = \frac{D}{4}$. Given the diameter, $D = 0.03 \text{ m}$ and the flow rate, $Q = 0.0012 \text{ m}^3 \text{ s}^{-1}$, it follows that the Reynolds number, $\text{Re} = 50,930$, which is > 4000 so the flow is turbulent.

The friction slope, S_f , can therefore be found using the Darcy–Weisbach equation (Eq. (2.22)) with Haaland’s friction factor equation (Eq. (2.24)). For a stainless steel pipe, the roughness, $\kappa = 0.002 \times 10^{-3} \text{ m}$ (see Table 2.2). It follows that the friction factor, $f = 0.005203$, and the friction slope, $S_f = 0.1019$. Given that the pipe length, $L = 5 \text{ m}$, the total head loss across the pipe is

$$S_f L = 0.510 \text{ m}$$

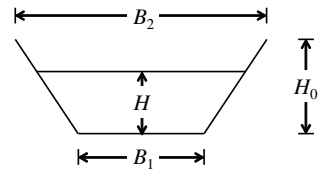
Worked Solution 2.3 (see Problem 2.3)

Let $H_0 = 0.8 \text{ m}$, $B_1 = 0.7 \text{ m}$, $B_2 = 1.4 \text{ m}$, $H = 0.5 \text{ m}$, $C = 45 \text{ m}^{1/2} \text{ s}^{-1}$ and $S_0 = \frac{1}{2100}$. The flowing area, A , and the wetted perimeter, P , are found from (see Fig. 2.8):

$$A = B_1 H + (B_2 - B_1) \frac{H^2}{2H_0} = 0.4594 \text{ m}^2$$

$$P = B_1 + 2 \left[\left[(B_2 - B_1) \frac{H}{2H_0} \right]^2 + H^2 \right]^{\frac{1}{2}} = 1.792 \text{ m}$$

Fig. 2.8 Open channel with a trapezoidal cross-section



The hydraulic radius, $m = A/P = 0.2564$ m

Invoking the Chezy equation (Eq. (2.34)), setting $Q = Av$ and assuming normal flow conditions (i.e. setting $S_f = S_0$) leads to

$$Q = AC\sqrt{mS_0} = 0.2284 = 0.228 \text{ m}^3\text{s}^{-1}$$

Worked Solution 2.4 (see Problem 2.4)

Let $B = 2.2$ m, $\theta = 60^\circ$, $S_0 = \frac{1}{600}$, $Q_1 = 0.95 \text{ m}^3\text{s}^{-1}$, $H_1 = 0.3$ m and $H_2 = 0.45$ m. The first step is to determine a Manning coefficient, n , for the H_1 scenario. Then we will be able to determine the flow rate using the Manning equation for the H_2 scenario.

The flowing area, A_1 , wetted perimeter, P_1 , and hydraulic radius, m_1 , for the H_1 scenario are (see Fig. 2.9):

$$A_1 = BH_1 + H_1^2 \cot \theta = 0.7120 \text{ m}^2$$

$$P_1 = B + 2H_1 \csc \theta = 2.893 \text{ m}$$

$$m_1 = \frac{A_1}{P_1} = 0.2461 \text{ m}$$

Rearranging the Manning equation (Eq. (2.35)) and assuming normal flow conditions (i.e., setting $S_f = S_0$) leads to

$$n = \frac{A_1 m_1^{2/3}}{Q_1} \sqrt{S_0} = 0.01202 \text{ m}^{-1/3} \text{ s}$$

The flowing area, A_2 , wetted perimeter, P_2 , and hydraulic radius, m_2 , for the H_2 scenario are:

$$A_2 = BH_2 + H_2^2 \cot \theta = 1.107 \text{ m}^2$$

$$P_2 = B + 2H_2 \csc \theta = 3.239 \text{ m}$$

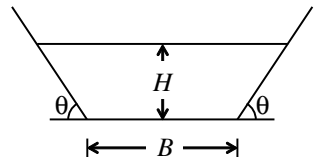
$$m_2 = \frac{A_2}{P_2} = 0.3417 \text{ m}$$

and from the Manning equation

$$Q_2 = \frac{A_2 m_2^{2/3}}{n} \sqrt{S_0} = 1.838 \text{ m}^3\text{s}^{-1}$$

So the flow rate when the depth is 450 mm will be $1.84 \text{ m}^3\text{s}^{-1}$.

Fig. 2.9 Another open channel with a trapezoidal cross-section



Worked Solution 2.5 (see Problem 2.5)

(a) Let $D = 0.9$ m, $S_0 = \frac{1}{1400}$, $H_1 = 0.32$ m and $Q_1 = 0.0720$ m³s⁻¹. To determine the Manning coefficient, n , we need to determine the flowing area, A_1 , wetted perimeter, P_1 , and hydraulic radius, m_1 , for the H_1 scenario.

Let $\theta_1 = \arccos\left(1 - \frac{2H_1}{D}\right) = 1.278$ radians. It follows that (see Fig. 2.10):

$$A_1 = \frac{D^2}{4} \left(\theta_1 - \frac{\sin 2\theta_1}{2} \right) = 0.2027 \text{ m}^2$$

$$P_1 = \theta_1 D = 1.150 \text{ m}$$

$$m_1 = \frac{A_1}{P_1} = 0.1763 \text{ m}$$

Rearranging the Manning equation (Eq. (2.35)) and assuming normal flow conditions (i.e., $S_f = S_0$) then leads to

$$n = \frac{A_1 m_1^{\frac{2}{3}}}{Q_1} \sqrt{S_0} = 0.02366 \text{ m}^{-\frac{1}{3}} \text{ s}$$

So the Manning coefficient of the pipe is $0.0237 \text{ m}^{-\frac{1}{3}} \text{ s}$.

(b) Let $H_2 = 0.85$ m. It follows that:

$$\theta_2 = \arccos\left(1 - \frac{2H_2}{D}\right) = 2.666 \text{ radians}$$

$$A_2 = \frac{D^2}{4} \left(\theta_2 - \frac{\sin 2\theta_2}{2} \right) = 0.6223 \text{ m}^2$$

$$P_2 = \theta_2 D = 2.399 \text{ m}$$

$$m_2 = \frac{A_2}{P_2} = 0.2594 \text{ m}$$

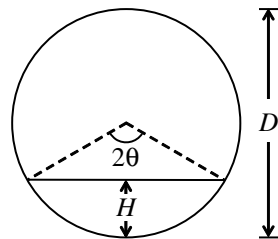
and from the Manning equation

$$Q_2 = \frac{A_2 m_2^{\frac{2}{3}}}{n} \sqrt{S_0} = 0.2859 \text{ m}^3 \text{ s}^{-1}$$

So the flow rate when the depth is 850 mm will be $0.286 \text{ m}^3 \text{ s}^{-1}$.

(c) Let $L = 3200$ m and $\Delta E = 4.2$ m. For the case when the pipe is full we can say that $H_3 = D$. It follows that $A_3 = \pi D^2/4$, $P_3 = \pi D$ and $m_3 = D/4$. Furthermore,

Fig. 2.10 Free surface flow in a cylindrical pipe



the pipe is now pressured up, so rather than taking $S_f = S_0$, we should say instead that $S_f = \Delta E/L$. The Manning equation then leads to

$$Q_3 = \frac{A_3 m_3^{2/3}}{n} \sqrt{\frac{\Delta E}{L}} = 0.3603 \text{ m}^3 \text{ s}^{-1}$$

So the flow rate when the pipe is completely full and there is a 4.2 m water level difference between the two reservoirs will be $0.360 \text{ m}^3 \text{ s}^{-1}$.

Worked Solution 2.6 (see Problem 2.6)

Let $Q_1 = 0.11 \text{ m}^3 \text{ s}^{-1}$, $v_2 = 0.4 \text{ m s}^{-1}$, $C = 45 \text{ m}^{1/2} \text{ s}^{-1}$, D be the pipe diameter and S_0 be the slope. Under normal flow conditions, $S_f = S_0$.

The Q_1 scenario represents an upper bound so we should assume that the conduit is operating at full capacity in this case. It follows that the area and wetted perimeter for the Q_1 scenario are found from $A_1 = \pi D^2/4$ and $m_1 = D/4$, respectively. The Chezy equation (Eq. (2.34)) gives that

$$S_0 = \frac{v^2}{C^2 m}$$

from which it follows that

$$\frac{Q_1^2}{C^2 S_0} = m_1 A_1^2 = \frac{\pi^2 D^5}{4^3} \quad (2.43)$$

For the v_2 scenario, the water depth, denoted H_2 , is a quarter of the pipe diameter and therefore:

$$\theta_2 = \arccos\left(1 - \frac{2H_2}{D}\right) = \arccos\left(\frac{1}{2}\right) = \frac{\pi}{3}$$

$$A_2 = \frac{D^2}{4} \left(\theta_2 - \frac{\sin 2\theta_2}{2}\right)$$

$$P_2 = \theta_2 D$$

$$m_2 = \frac{A_2}{P_2} = \frac{D}{4} \left(1 - \frac{\sin 2\theta_2}{2\theta_2}\right)$$

From the Chezy equation it can then be stated that

$$\frac{v_2^2}{C^2 S_0} = m_2 = \frac{D}{4} \left(1 - \frac{\sin 2\theta_2}{2\theta_2}\right) \quad (2.44)$$

To obtain D , we need to first eliminate S_0 by dividing Eq. (2.44) by Eq. (2.43) to get

$$\frac{v_2^2}{Q_1^2} = \frac{4^2}{\pi^2 D^4} \left(1 - \frac{\sin 2\theta_2}{2\theta_2}\right)$$

It follows that

$$D = 2 \left(\frac{Q_1}{\pi v_2}\right)^{1/2} \left(1 - \frac{\sin 2\theta_2}{2\theta_2}\right)^{1/4} = 0.5178 \text{ m}$$

Equation (2.43) then gives that

$$S_0 = \frac{4^3 Q_1^2}{\pi^2 C^2 D^5} = \frac{1}{961.0}$$

So the slope should be 1 in 961 and the conduit diameter should be 518 mm.

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Gradually Varied Flow in Open Channels

3

Abstract

This chapter explains how to solve steady-state gradually varied open channel flow problems. The gradually varied flow (GVF) equation is obtained by differentiating an expression for total head with respect to distance. The concept of sub-critical and supercritical flow are discussed in the context of the Froude number. The special case of a rectangular cross-section channel is studied using the Darcy-Weisbach equation, the Chezy equation and the Manning equation. A classification scheme for channel bed slope (mild, critical and steep) is developed in terms of normal and critical water depths. This in turn leads to the classical GVF profile classification scheme (A2, A3, M1, M2, etc.). A numerical solution for the GVF equation is developed using MATLAB's ODE (ordinary differential equation) solver, ode45. Practical applications are presented through worked examples and a problem sheet with worked solutions.

Notation

A	Area [L^2].
A_n	Normal area [L^2].
A_c	Critical area [L^2].
B	Breadth [L].
C	Chezy coefficient [$L^{1/2} T^{-1}$].
E	Total head [L].
f	Friction factor [–].
f_n	Normal friction factor [–].
f_c	Critical friction factor [–].
Fr	Froude number [–].
g	Gravitational acceleration [LT^{-2}].
H	Depth [L].
H_n	Normal depth [L].

H_c	Critical depth [L].
L	Length [L].
m	Hydraulic radius [L].
m_n	Normal hydraulic radius [L].
m_c	Critical hydraulic radius [L].
n	Manning coefficient [$L^{-\frac{1}{3}}T$].
P	Wetted perimeter [L].
P_n	Normal wetted perimeter [L].
P_c	Critical wetted perimeter [L].
Q	Flow rate [L^3T^{-1}].
s	Distance along a channel [L].
S_0	Bed slope [–].
S_f	Friction slope [–].
v	Fluid velocity [LT^{-1}].
v_c	Critical velocity [LT^{-1}].
v_n	Normal velocity [LT^{-1}].
z	Elevation [L].

3.1 Introduction

In Chap. 2 we looked at steady normal flow in open channels. Normal flow conditions implies that the friction slope is equal to the channel bed slope. A result of this assumption is that, for prismatic channels, both the velocity and fluid depth remain constant with distance along the channel. For non-normal flow conditions, velocity and fluid depth will vary along an open channel. Generally we distinguish between gradually varied flow and rapidly varied flow. Gradually varied flow includes flow scenarios where fluid velocity and fluid depth vary slowly and continuously with distance (i.e., $\frac{dh}{ds} \ll 1$). Rapidly varied flow includes flow scenarios where fluid velocity and fluid depth vary rapidly and potentially discontinuously. This chapter focuses on gradually varied flow (see Chap. 4 for detail about rapidly varied flow).

First we derive the gradually varied flow (GVF) equation for fluid depth gradient in terms of bed slope, friction slope and Froude number. Special cases are developed for rectangular cross-section channels with the Chezy equation and the Manning equation. A discussion is presented concerning the classification of different types of GVF profiles. A numerical solution for the GVF equation is presented using MATLAB's ODE (ordinary differential equation) solver, `ode45`. Some examples are demonstrated based on various scenarios around a channel bed slope change.

3.2 Gradually Varied Flow (GVF) Equation

3.2.1 Fluid Depth Gradient

Recall the definition of total head, E [L], for open channel systems given by Eq. (2.38)

$$E = H + \frac{v^2}{2g} + z \quad (3.1)$$

where H [L] is fluid depth, v [LT^{-1}] is fluid velocity, g [LT^{-2}] is gravitational acceleration and z [L] is the elevation of the channel bed.

Challenge 3.1 Differentiate the expression in Eq. (3.1) with respect to distance, s [L], and use the continuity equation to derive an expression for fluid depth gradient, $\frac{\partial H}{\partial s}$, in terms of channel bed slope, S_0 [–], friction slope, S_f [–], fluid velocity, v [LT^{-1}], gravitational acceleration, g [LT^{-2}], flowing cross-sectional area, A [L^2], and $\frac{\partial A}{\partial H}$ [L].

Differentiating Eq. (3.1) with respect to s leads to

$$S_f = S_0 - \frac{\partial H}{\partial s} - \frac{v}{g} \frac{\partial v}{\partial s} \quad (3.2)$$

where

$$S_f = -\frac{\partial E}{\partial s} \quad \text{and} \quad S_0 = -\frac{\partial z}{\partial s}$$

which represent the friction slope and channel bed slope, respectively.

The continuity equation (Eq. (1.32)) gives that the volumetric flow rate, Q [L^3T^{-1}], is found from

$$Q = Av \quad (3.3)$$

Given that Q is constant

$$v \frac{\partial A}{\partial s} + A \frac{\partial v}{\partial s} = 0$$

and therefore

$$\frac{\partial v}{\partial s} = -\frac{v}{A} \frac{\partial A}{\partial s}$$

Given that $A = f(H)$ it follows that

$$\frac{\partial v}{\partial s} = -\frac{v}{A} \frac{\partial A}{\partial H} \frac{\partial H}{\partial s} \quad (3.4)$$

Substituting Eq. (3.4) into Eq. (3.2) therefore leads to

$$\frac{\partial H}{\partial s} = \frac{S_0 - S_f}{1 - \frac{v^2}{gA} \frac{\partial A}{\partial H}} \quad (3.5)$$

which is widely referred to as the gradually varied flow (GVF) equation. Note that S_f can be obtained from the Darcy-Weisbach equation (recall Eq. (2.21)).

3.2.2 The Froude Number

The parameter group in the denominator of Eq. (3.5) is commonly lumped together as a dimensionless group known as the Froude number, Fr [–]. In this way, Eq. (3.5) reduces to

$$\frac{\partial H}{\partial s} = \frac{S_0 - S_f}{1 - Fr^2} \quad (3.6)$$

where

$$Fr = \sqrt{\frac{v^2}{gA} \frac{\partial A}{\partial H}} \quad (3.7)$$

It is useful to distinguish between sub-critical, critical and supercritical flow conditions. Sub-critical flow conditions occur when $Fr < 1$. Supercritical flow conditions occur when $Fr > 1$. Critical flow conditions occur when $Fr = 1$; note that Eq. (3.6) has a singularity at $Fr = 1$. The physical meaning of these different conditions is explored further in Chap. 4.

It is often convenient to compare actual conditions to critical flow conditions. In this context, it is common to refer to the associated velocity, fluid depth, wetted perimeter, flowing cross-sectional area, friction factor and hydraulic radius as v_c , H_c , P_c , A_c , f_c and m_c , respectively. The c subscript denotes that these properties are those that would be expected under critical flow conditions (i.e., when $Fr = 1$).

3.3 Rectangular Cross-Sections

Consider a rectangular cross-section channel of breadth, B [L], whereby:

$$A = BH, \quad \frac{\partial A}{\partial H} = B, \quad m = \frac{BH}{B + 2H} \quad (3.8)$$

Substituting Eqs. (3.3) and (3.8) into the Darcy-Weisbach equation (Eq. (2.21)) leads to

$$S_f = \frac{f(B + 2H)Q^2}{2gB^3H^3} \quad (3.9)$$

Substituting Eqs. (3.3) and (3.8) into the Froude number equation (Eq. (3.7)) leads to

$$Fr = \sqrt{\frac{Q^2}{gB^2H^3}} \quad (3.10)$$

Substituting Eqs. (3.9) and (3.10) into Eq. (3.6) leads to

$$\frac{\partial H}{\partial s} = \frac{S_0 - \frac{f(B+2H)Q^2}{2gB^3H^3}}{1 - \frac{Q^2}{gB^2H^3}} \quad (3.11)$$

3.3.1 Incorporating Critical Depth

Challenge 3.2 Determine an expression for critical fluid depth, H_c , in terms of flow rate, Q , and use this to eliminate Q from Eq. (3.11).

Solving Eq. (3.10) for H^3 leads to

$$H^3 = \frac{Q^2}{gB^2\text{Fr}^2} \quad (3.12)$$

Under critical flow conditions, $\text{Fr} = 1$, $H = H_c$ and therefore

$$H_c^3 = \frac{Q^2}{gB^2} \quad (3.13)$$

Substituting Eq. (3.13) into Eq. (3.11) leads to

$$\frac{\partial H}{\partial s} = \frac{S_0 - \frac{f(B+2H)}{2B} \left(\frac{H_c}{H}\right)^3}{1 - \left(\frac{H_c}{H}\right)^3} \quad (3.14)$$

3.3.2 Incorporating Normal Depth

Challenge 3.3 Determine an expression for critical fluid depth, H_c , in terms of normal fluid depth, H_n , and substitute this into the numerator of Eq. (3.14).

Under normal flow conditions $S_f = S_0$ and $H = H_n$. Equation (3.9) therefore leads to

$$S_0 = \frac{f_n(B + 2H_n)Q^2}{2gB^3H_n^3} \quad (3.15)$$

Substituting Eq. (3.13) into Eq. (3.15) and solving for H_c yields

$$H_c^3 = \frac{2S_0BH_n^3}{f_n(B + 2H_n)} \quad (3.16)$$

Substituting Eq. (3.16) into the numerator of Eq. (3.14) then leads to

$$\frac{\partial H}{\partial s} = S_0 \left(\frac{1 - \frac{f}{f_n} \left(\frac{B+2H}{B+2H_n} \right) \left(\frac{H_n}{H} \right)^3}{1 - \left(\frac{H_c}{H} \right)^3} \right), \quad S_0 > 0 \quad (3.17)$$

Note that the concept of a normal depth only makes sense when $S_0 > 0$. When $S_0 \leq 0$ we should use Eq. (3.14) instead.

3.3.3 Application of the Chezy Equation

According to the Chezy equation, the friction factor, f , is found from Eq. (2.36). Substituting Eq. (2.36) into Eqs. (3.14), (3.16) and (3.17) leads to:

$$\frac{\partial H}{\partial s} = \frac{S_0 - \frac{g(B+2H)}{C^2 B} \left(\frac{H_c}{H}\right)^3}{1 - \left(\frac{H_c}{H}\right)^3} \quad (3.18)$$

$$H_c^3 = \frac{S_0 C^2 B H_n^3}{g(B + 2H_n)} \quad (3.19)$$

$$\frac{\partial H}{\partial s} = S_0 \left(\frac{1 - \left(\frac{B+2H}{B+2H_n}\right) \left(\frac{H_n}{H}\right)^3}{1 - \left(\frac{H_c}{H}\right)^3} \right), \quad S_0 > 0 \quad (3.20)$$

3.3.4 Application of the Manning Equation

According to the Manning equation, the friction factor, f , is found from Eq. (2.37). Substituting Eq. (2.37) into Eqs. (3.14), (3.16) and (3.17) leads to:

$$\frac{\partial H}{\partial s} = \frac{S_0 - \left(\frac{B+2H}{B}\right)^{\frac{4}{3}} \frac{gn^2 H_c^3}{H^{\frac{10}{3}}}}{1 - \left(\frac{H_c}{H}\right)^3} \quad (3.21)$$

$$H_c^3 = \left(\frac{B}{B + 2H_n}\right)^{\frac{4}{3}} \frac{S_0 H_n^{\frac{10}{3}}}{gn^2} \quad (3.22)$$

$$\frac{\partial H}{\partial s} = S_0 \left(\frac{1 - \left(\frac{B+2H}{B+2H_n}\right)^{\frac{4}{3}} \left(\frac{H_n}{H}\right)^{\frac{10}{3}}}{1 - \left(\frac{H_c}{H}\right)^3} \right), \quad S_0 > 0 \quad (3.23)$$

3.4 Classification of Flow Profiles

From Eq. (3.6) it can be understood that the sign of $\frac{\partial H}{\partial s}$ depends strongly on the slope of the channel bed, S_0 , and whether or not the flow is sub-critical ($Fr < 1$) or supercritical ($Fr > 1$). There are four important categories of channel bed slope, as identified in Table 3.1.

Given that $S_f \geq 0$, it is clear (considering Eq. (3.6)) that when $S_0 \leq 0$, supercritical flow leads to $\frac{\partial H}{\partial s} < 0$ whereas sub-critical flow leads to $\frac{\partial H}{\partial s} > 0$. These conditions are referred to as A2 and A3, respectively (see Table 3.2). However, when

Table 3.1 Classification of channel slopes

Classification	Channel slope
Adverse or horizontal (A)	$S_0 \leq 0$
Mild (M)	$S_0 \in (0, S_f)$
Critical (C)	$S_0 = S_f$
Steep (S)	$S_0 > S_f$

Table 3.2 Classification of gradually varied flow profiles

Classification	Channel slope	Fluid depth	Surface slope
A2	$S_0 \leq 0$	$H > H_c$	$\frac{\partial H}{\partial s} < 0$
A3	$S_0 \leq 0$	$H < H_c$	$\frac{\partial H}{\partial s} > 0$
M1	$H_n > H_c$	$H > H_n$	$\frac{\partial H}{\partial s} > 0$
M2	$H_n > H_c$	$H \in (H_c, H_n)$	$\frac{\partial H}{\partial s} < 0$
M3	$H_n > H_c$	$H < H_c$	$\frac{\partial H}{\partial s} > 0$
C1	$H_n = H_c$	$H > H_c$	$\frac{\partial H}{\partial s} > 0$
C3	$H_n = H_c$	$H < H_c$	$\frac{\partial H}{\partial s} > 0$
S1	$H_n \in (0, H_c)$	$H > H_c$	$\frac{\partial H}{\partial s} > 0$
S2	$H_n \in (0, H_c)$	$H \in (H_n, H_c)$	$\frac{\partial H}{\partial s} < 0$
S3	$H_n \in (0, H_c)$	$H < H_n$	$\frac{\partial H}{\partial s} > 0$

$S_0 > 0$, the sign of $\frac{\partial H}{\partial s}$ depends on S_f . Further insight can be obtained by comparing the fluid depth, H , to that expected under normal flow conditions, H_n .

Challenge 3.4 Determine the relationship between H_n and H_c for the limit when $S_f \rightarrow S_0$.

From Eq. (3.6) it can be understood that

$$\lim_{S_f \rightarrow S_0} \text{Fr}^2 = 1$$

and therefore

$$\lim_{S_f \rightarrow S_0} H = H_c$$

Given Eq. (3.9), it can be further stated that

$$\lim_{S_f \rightarrow S_0} S_f = \frac{f_c(B + 2H_c)Q^2}{2gB^2H_c^3} \quad (3.24)$$

Comparing Eq. (3.24) with Eq. (3.15) then reveals that

$$\lim_{S_f \rightarrow S_0} H_n = H_c \quad (3.25)$$

Consequently it can be understood that:

$$\begin{aligned} H_n &> H_c, & S_0 < S_f & \text{(Mild slopes)} \\ H_n &= H_c, & S_0 &= S_f & \text{(Critical slopes)} \\ H_n &\in (0, H_c), & S_0 &> S_f & \text{(Steep slopes)} \end{aligned}$$

Equation (3.17) then reveals eight important conditions governing the sign of $\frac{\partial H}{\partial s}$ when $S_0 > 0$, denoted M1, M2, M3, C1, C3, S1, S2 and S3. All the possible conditions are listed Table 3.2.

3.5 Solving the GVF Equation

Here we will focus on providing fast and accurate numerical solutions for the gradually varied flow (GVF) equation with rectangular prismatic cross-section channels and Manning equation (i.e., Eq. (3.21)).

Often we want to determine the distance at which a certain fluid depth applies. It is therefore useful to choose s as the dependent variable and H as the independent variable. Consequently, we will specifically seek to solve

$$\frac{\partial s}{\partial H} = \frac{1 - \left(\frac{H_c}{H}\right)^3}{S_0 - \left(\frac{B+2H}{B}\right)^{\frac{4}{3}} \frac{gn^2 H_c^3}{H^{\frac{10}{3}}}} \quad (3.26)$$

Accurate solutions to first-order ordinary differential equations (ODE), such as Eq. (3.26), can be obtained using MATLAB's ODE solver, `ode45`, which is based on an explicit Runge–Kutta (4, 5) formula, the Dormand-Prince pair [1,2].

`ode45` users can specify the initial value of the dependent variable, s_1 , and the initial and final values of the independent variable, H_1 and H_2 , respectively. `ode45` will then solve for s at a set of discrete points for $H \in [H_1, H_2]$. The location of the solution points are optimally selected to minimise computation time whilst maintaining error, between 4th and 5th order Runge–Kutta approximations, below a pre-defined tolerance.

The MATLAB function, `GVFaFun`, given in Listing 3.1, can be used to obtain solutions for Eq. (3.26) using `ode45`. `GVFaFun` provides $s(H \in [H_1, H_2])$ subject to the initial value constraint, $s(H = H_1) = s_1$. The first line defines the ODE function, `ODEFUN`, which directly represents Eq. (3.26). The second line calls `ode45`, providing `ODEFUN` as the function containing the ODE to be solved, the values of H_1 and H_2 to solve between and the value of s_1 , which represents the initial value of s . The output from `ode45` includes an array of solution point locations, representing H , and a corresponding array of solution values, representing s .

Listing 3.1 Solution for the GVF equation, with distance as dependant variable, assuming a rectangular prismatic cross-section channel (Eq. (3.26)).

```
function [H,s]=GVFaFun(H1,H2,s1,B,g,Hc,n,S0)
%Solves gradually varied flow equation using ode45
%providing the location of points associated with
%an array of fluid depths ranging from H1 and H2.
%H1 - Fluid depth at s = s1 (m)
%H2 - Fluid depth at s = s2 (m)
%s1 - Location of H1 (m)
%B - Breadth of rectangular channel (m)
%g - Gravitational acceleration (m/s^2)
%Hc - Critical fluid depth (m)
%n - Manning coefficient (m^(-1/3) s)
%S0 - Channel bed slope (-)
%H - Vector of fluid depths between H1 and H2
%s - Location of s values between s1 and s2
ODEFUN=@(H,s) (1-(Hc/H)^3)/(S0-...
((B+2*H)/B)^(4/3)*g*n^2*Hc^3/H^(10/3));
[H,s]=ode45(ODEFUN,[H1 H2],s1);
```

Note that Eq. (3.21) is singular at $H = H_c$. Furthermore, considering Eq. (3.23), it can be understood that for $S_0 > 0$, Eq. (3.26) is singular at $H = H_n$. Consequently GVFaFun can only be used within the specific regions defined in Table 3.2.

3.5.1 Solutions for Adverse Slopes

The MATLAB code below provides the example set of A2 and A3 profiles shown in Fig. 3.1a using the GVFaFun code given in Listing 3.1:

```
B=2; %Breadth of channel (m)
g=9.81; %Gravitational acceleration (m/s^2)
Hc=1; %Critical fluid depth (m)
n=0.015; %Manning coefficient (m^(-1/3) s)
%Adverse slope examples (A2 and A3):
S0A=-1e-3; %Define channel bed slope
%Determine A3 profile 0<H<Hc with H(s=0)=Hc
[HA3,sA3]=GVFaFun(Hc,0.01,0,B,g,Hc,n,S0A);
%Determine A2 profile H>Hc with H(s=0)=Hc
[HA2,sA2]=GVFaFun(Hc,5,0,B,g,Hc,n,S0A);
```

The first step involves specifying the various model parameters to describe a rectangular concrete channel with a breadth of 2 m and a flow rate that corresponds to a critical fluid depth of 1 m. Because the slope is adverse, S_0 is set to a negative number. We have arbitrarily chosen $S_0 = -10^{-3}$.

The set of H and s values defining the A3-type profile are obtained by calling GVFaFun with $H_1 = H_c$ and $H_2 = 0.01$ m (it is better not to go all the way down

to zero because this leads to unnecessary numerical problems). The s_1 value is set to zero such that $H = H_c$ at $s = 0$. The results are shown as a red line in Fig. 3.1a.

The set of H and s values defining the A2-type profile are obtained by calling GVFafun with $H_1 = H_c$ and $H_2 = 5$ m (this is some arbitrary number greater than H_c). Again, the s_1 value is set to zero such that $H = H_c$ at $s = 0$. The results are shown as a green line in Fig. 3.1a.

3.5.2 Solutions for Mild Slopes

When tackling situations where $S_0 > 0$ it is important to first calculate the normal flow depth, H_n , by iteratively solving Eq. (3.22). The MATLAB code given in Listing 3.2 provides a function, HnFun, for achieving this purpose.

Listing 3.2 Function to obtain normal flow depth by iterative solution of Eq. (3.22).

```
function Hn=HnFun(B,g,Hc,n,S0)
%Determine the depth under normal flow conditions
%B - Breadth of rectangular channel (m)
%g - Gravitational acceleration (m/s^2)
%Hc - Critical fluid depth (m)
%n - Manning coefficient (m^(-1/3) s)
%S0 - Channel bed slope (-)
%Hn - Normal flow depth (m)
FUN=@(Hn) Hc^3-(B/(B+2*Hn))^(4/3)*S0*Hn^(10/3)/g/n^2;
Hn=fzero(FUN,Hc);
```

The MATLAB code listed below utilizes Listings 3.1 and 3.2 to provide the example set of M1, M2 and M3 profiles shown in Fig. 3.1b:

```
%Mild slope examples (M1, M2 and M3):
S0M=2e-3; %Define channel bed slope
HnM=HnFun(B,g,Hc,n,S0M); %Normal flow depth
%Determine M3 profile 0<H<Hc with H(s=0)=Hc
[HM3,sM3]=GVFaFun(Hc,0.01,0,B,g,Hc,n,S0M);
%Determine M2 profile Hc<H<Hn with H(s=0)=Hc
[HM2,sM2]=GVFaFun(Hc,0.99*HnM,0,B,g,Hc,n,S0M);
%Determine M1 profile H>Hn with H(s=sM2(end))=Hn
[HM1,sM1]=GVFaFun(1.01*HnM,2,sM2(end),B,g,Hc,n,S0M);
```

The channel bed slope, S_0 , is set to a relatively small positive value of 2×10^{-3} . Following on from this, the HnFun function is called to determine the associated normal flow depth, H_n , shown as a black dash-dot line in Fig. 3.1b. The set of H and s values defining the M3-type profile are then obtained by calling GVFafun with $H_1 = H_c$, $H_2 = 0.01$ m and $s_1 = 0$ (such that $H = H_c$ at $s = 0$). The results are shown as a red line in Fig. 3.1b.

The set of H and s values defining the M2-type profile are obtained by calling GVFafun with $H_1 = H_c$, $H_2 = 0.99H_n$ and $s_1 = 0$. It is important not to go right

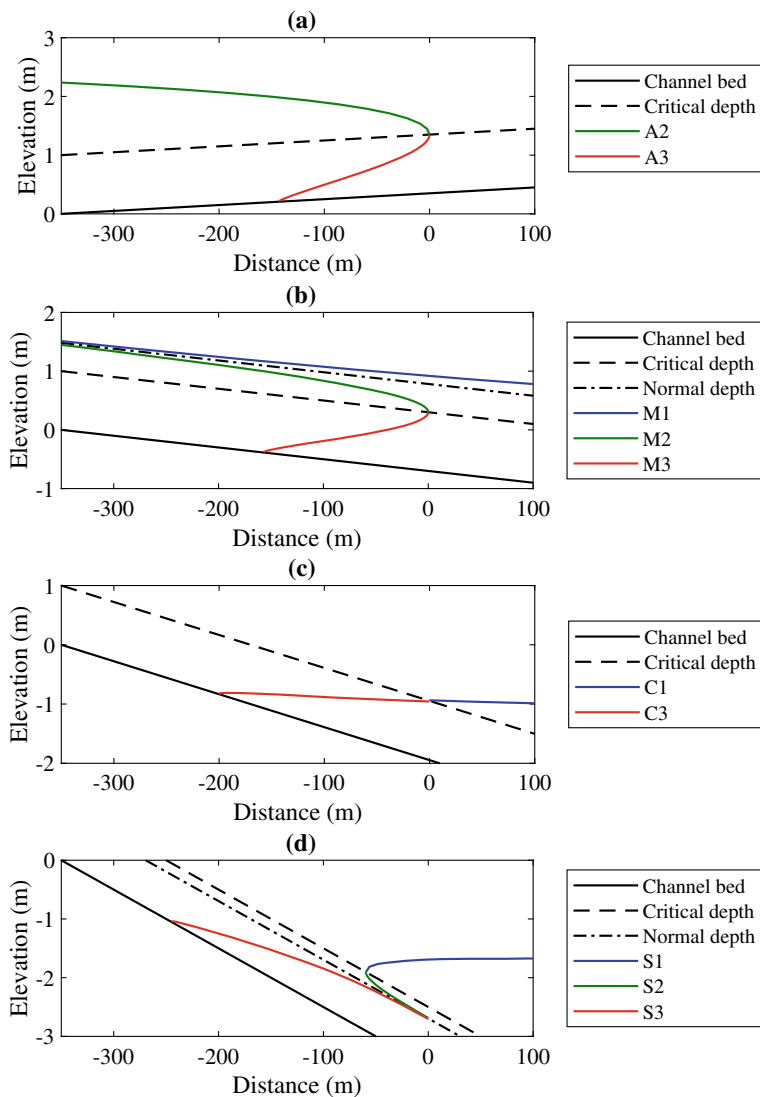


Fig. 3.1 Example water surface profiles for the ten gradually varied flow classifications listed in Table 3.2, assuming a 2 m wide rectangular concrete channel. **a** Adverse slope examples. **b** Mild slope examples. **c** Critical slope examples. **d** Steep slope examples

up to H_n because of the singularity present at $H = H_n$. The results are shown as a green line in Fig. 3.1b.

The set of H and s values defining the M1-type profile are obtained by calling `GVFaFun` with $H_1 = 1.01H_n$ and $H_2 = 2$ m (this is some arbitrary number greater than H_c). Here, the s_1 value is set to the s value where the M2-type profile reaches $H = 0.99H_n$. The results are shown as a blue line in Fig. 3.1b.

3.5.3 Solutions for Critical Slopes

The critical channel bed slope, $S_0 = S_{0c}$, that leads to $H_n = H_c$ is found by setting $H_n = H_c$ and solving Eq. (3.22) for S_0 to get

$$S_{0c} = \left(\frac{B + 2H_c}{B} \right)^{\frac{4}{3}} \frac{gn^2}{H_c^{\frac{1}{3}}} \quad (3.27)$$

The MATLAB code listed below utilizes Listing 3.1 to provide the example set of C1 and C3 profiles shown in Fig. 3.1c where S_{0c} is found from Eq. (3.27):

```
%Critical slope examples (C1 and C3):
%Determine critical channel bed slope
S0C=( (B+2*Hc)/B)^(4/3)*g*n^2/Hc^(1/3);
%Determine C3 profile 0<H<Hc with H(s=0)=Hc
[HC3,sC3]=GVFaFun(0.99*Hc,0.01,0,B,g,Hc,n,S0C);
%Determine C1 profile H>Hc with H(s=sC3(end))=Hn
[HC1,sC1]=GVFaFun(1.01*Hc,5,0,B,g,Hc,n,S0C);
```

The set of H and s values defining the C3-type profile are obtained by calling `GVFaFun` with $H_1 = 0.99H_c$, $H_2 = 0.01$ m and $s_1 = 0$. It is necessary to only go up to $0.99H_c$ for this example because $H_c = H_n$ where there is a singularity. The results are shown as a red line in Fig. 3.1c.

The set of H and s values defining the C1-type profile are obtained by calling `GVFaFun` with $H_1 = 1.01H_c$, $H_2 = 5$ m and $s_1 = 0$. The results are shown as a blue line in Fig. 3.1c.

3.5.4 Solutions for Steep Slopes

The MATLAB code below utilizes Listings 3.1 and 3.2 to provide the example set of S1, S2 and S3 profiles shown in Fig. 3.1d.

```
%Steep slope examples (S1, S2 and S3):
S0S=1e-2; %Define channel bed slope
HnS=HnFun(B,g,Hc,n,S0S); %Normal flow depth
%Determine S3 profile 0<H<Hn with H(s=0)=Hc
[HS3,sS3]=GVFaFun(0.99*HnS,0.01,0,B,g,Hc,n,S0S);
%Determine S2 profile Hn<H<Hc with H(s=0)=Hc
```

```
[HS2, sS2] = GVFaFun(1.01*HnS, Hc, 0, B, g, Hc, n, S0S);
%Determine S1 profile H>Hc with H(s=sS2(end))=Hc
[HS1, sS1] = GVFaFun(Hc, 6, sS2(end), B, g, Hc, n, S0S);
```

The channel bed slope, S_0 , is set to a relatively large positive value of 10^{-2} . Following on from this, the $HnFun$ function is called to determine the associated normal flow depth, H_n , shown as a black dash-dot line in Fig. 3.1d.

A set of H and s values defining the S3-type profile are obtained by calling $GVFaFun$ with $H_1 = 0.99H_n$, $H_2 = 0.01$ m and $s_1 = 0$. The results are shown as a red line in Fig. 3.1d.

A set of H and s values defining the S2-type profile are obtained by calling $GVFaFun$ with $H_1 = 1.01H_n$, $H_2 = H_c$ and $s_1 = 0$. The results are shown as a green line in Fig. 3.1d.

A set of H and s values defining the S1-type profile are obtained by calling $GVFaFun$ with $H_1 = H_c$ and $H_2 = 6$ m (an arbitrary number greater than H_c). Here, the s_1 value is set to the s value where the S2-type profile reaches $H = H_c$. The results are shown as a blue line in Fig. 3.1d.

3.6 Development of Composite Profiles

In practice, gradually varied flow water levels often take the form of a composite set of different gradually varied flow profiles (S1, S2, M1, M2 etc.) combined with normal flow water levels. A set of useful rules to help determine how these fit together are presented in Table 3.3. Some examples of how gradually varied flow progresses over different channel bed slope changes are shown in Fig. 3.2.

Figure 3.2a shows an example where a mild channel bed slope transitions into a milder channel bed slope. According to Rule 3 in Table 3.3, flow is normal far away from the slope transition. The nature of mild slopes is that the normal flow depth is greater than the critical flow depth (recall Table 3.1). It follows that flow over both slopes is sub-critical. According to Rule 1, flow over the upstream slope is controlled

Table 3.3 Useful rules to combine gradually varied flow and normal flow profiles (modified from [3, p. 104])

1. Sub-critical flow is controlled by downstream boundary conditions.
2. Supercritical flow is controlled by upstream boundary conditions.
3. Far away from flow controls, flow tends to become normal in prismatic channels.
4. Flow is sub-critical upstream of a sluice gate and supercritical downstream.
5. When sub-critical flow is present in a channel terminating at a free fall, the depth at the free fall will be approximately equal to the critical depth.
6. The change from supercritical to sub-critical flow in a prismatic channel is only possible through a hydraulic jump (which is explained in more detail in Chap. 4).

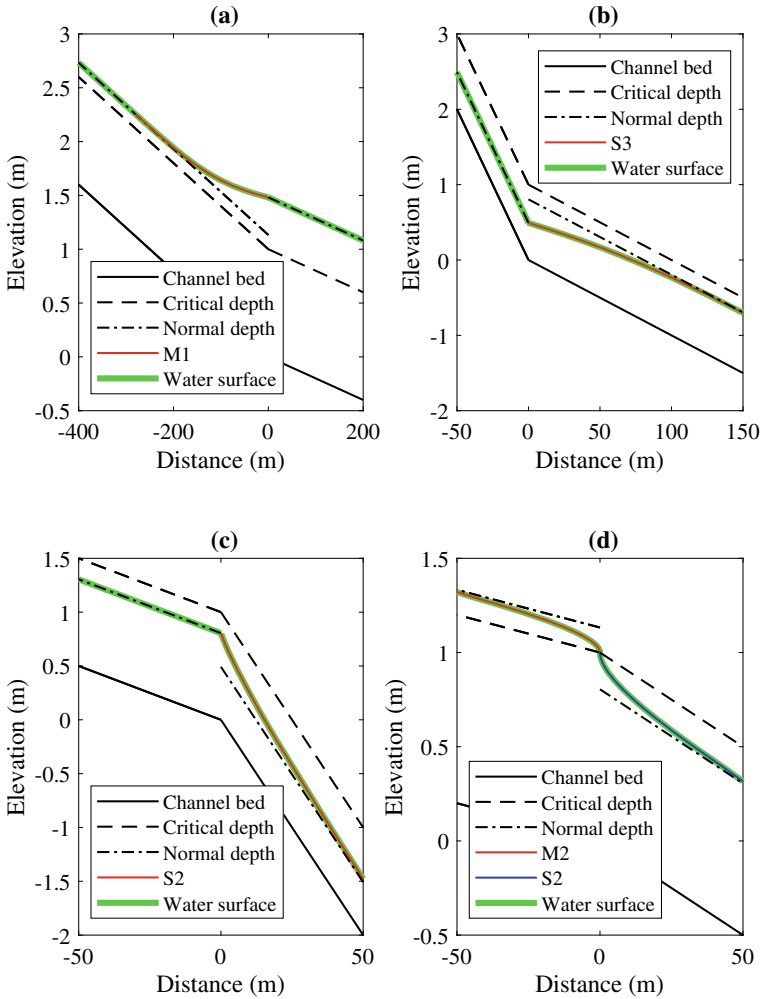


Fig. 3.2 Gradually varied flow over a change in channel bed slope assuming a 2 m wide rectangular concrete channel. **a** A mild slope followed by a milder slope. **b** A steep slope preceded by a steeper slope. **c** A steep slope followed by a steeper slope. **d** A mild slope followed by a steep slope

by the slope transition whereas flow over the downstream slope is unaffected. It follows that flow over the upstream slope must transition from the upstream slope normal flow depth to the downstream slope normal flow depth (which occurs at the slope transition). The associated gradually varied flow profile is of M1-type (see Table 3.2).

Figure 3.2b shows an example where a steep channel bed slope is preceded by a steeper channel bed slope. Again, flow is normal far away from the slope transition. The nature of steep slopes is that the normal flow depth is less than the critical

flow depth (recall Table 3.2). It follows that flow over both slopes is supercritical. According to Rule 2, flow over the downstream slope is controlled by the slope transition whereas flow over the upstream slope is unaffected. Again, it follows that flow over the downstream slope must transition from the upstream slope normal flow depth (which occurs at the slope transition) to the downstream slope normal flow depth. However, this time, the associated gradually varied flow profile is of S3-type (see Table 3.2).

Figure 3.2c shows an example where a steep channel bed slope transitions into a steeper channel bed slope. Flow is normal far away from the slope transition. Flow is supercritical with the normal flow depth being less than the critical depth for both slopes, due their steep nature. Again, according to Rule 2, flow over the downstream slope is controlled by the slope transition whereas flow over the upstream slope is unaffected. It follows that flow over the downstream slope must transition from the upstream slope normal flow depth (which occurs at the slope transition) to the downstream slope normal flow depth. The associated gradually varied flow profile is of S2-type (see Table 3.2).

Figure 3.2d shows an example where a mild channel bed slope transitions into a steep channel bed slope. Flow is normal far away from the slope transition. Flow is sub-critical with the normal flow depth being less than the critical depth upstream of the transition. Flow is supercritical with the normal flow depth being greater than the critical depth downstream of the transition. According to Rules 1 and 2, flow over both the upstream and downstream slope is controlled by the slope transition. The steepening of the slope is analogous to a free fall. Therefore by Rule 5, the fluid depth at the transition should be the critical depth. Flow over the upstream slope transitions from the upstream normal flow depth to the critical depth at the bed slope transition. The associated gradually varied flow profile is of M2-type (see Table 3.2). Flow over the downstream slope transitions from the critical depth at the bed slope transition to the downstream normal flow depth. The associated gradually varied flow profile is of S2-type (see Table 3.2).

3.7 Problem Sheet

Problem 3.1 (see Worked Solution 3.1)

A reservoir is fed with water, at a rate of $2.1 \text{ m}^3 \text{ s}^{-1}$, via a rectangular cross-section open channel with a breadth of 2.6 m, a downwards slope of 1 in 600 and a Manning coefficient of $0.017 \text{ m}^{-\frac{1}{3}} \text{ s}$. The depth of water in the channel at the reservoir inlet is 1.2 m. Upstream of the reservoir inlet, flow is normal and sub-critical. Determine the distance upstream of the reservoir inlet where the water depth is within 1% of that expected for normal flow.

Problem 3.2 (see Worked Solution 3.2)

Water flows, under sub-critical flow conditions, along a rectangular cross-section open channel with a breadth of 0.4 m, an upwards slope of 1 in 50 and a Manning coefficient of $0.012 \text{ m}^{-\frac{1}{3}} \text{ s}$. The channel terminates with a free fall outlet. The water depth immediately upstream of outlet is 0.1 m. Determine the water depth 10 m upstream of the outlet.

Problem 3.3 (see Worked Solution 3.3)

Two water reservoirs are connected by a rectangular cross-section open channel with a breadth of 0.5 m, a length of 300 m, a downwards slope of 1 in 500 and a Manning coefficient of $0.015 \text{ m}^{-\frac{1}{3}} \text{ s}$. The water depth in the channel adjacent to the upstream reservoir is 1.8 m. The channel slope is mild and the flow is sub-critical.

(a) Determine the flow rate in the channel when the water surface at the downstream end of the channel is 0.3 m below that of the upstream end. Verify your answer by plotting water elevation against distance and checking that a change in water surface elevation of 0.3 m is achieved at 300 m distance from the upstream reservoir.

(b) Repeat part (a) assuming the water surface at the downstream end of the channel is 1.3 m below that of the upstream end.

3.8 Worked Solutions**Worked Solution 3.1** (see Problem 3.1)

Let $Q = 2.1 \text{ m}^3 \text{ s}^{-1}$, $B = 2.6 \text{ m}$, $S_0 = \frac{1}{600}$, $n = 0.017 \text{ m}^{-\frac{1}{3}} \text{ s}$ and $H_2 = 1.2 \text{ m}$. A value for the critical depth, H_c , can be obtained from Eq. (3.13). A corresponding value for the normal flow water depth, H_n , can be obtained using the function, HnFun, given in Listing 3.2. The water depth will be within 1% of that expected under normal flow conditions where $H_1 = 1.01 H_n$.

If we set $H = H_1$ at $s = s_1$ and $H = H_2$ at $s = s_2$, then the distance upstream of the reservoir inlet where the water depth is within 1% of that expected for normal flow is found from $L = s_2 - s_1$. The MATLAB code below utilises HnFun in Listing 3.2 and GVFaFun in Listing 3.1 to determine the value of L :

```
Q=2.1; %Flow rate (m3/s)
B=2.6; %Breadth of channel (m)
S0=1/600; %Channel slope (-)
```

```

n=0.017; %Manning coefficient (m-1/3 s)
g=9.81; %Gravitational acceleration (m/s2)
H2=1.2; %Downstream boundary fluid depth (m)
%Determine critical fluid depth
Hc=(Q2/g/B2)(1/3);
%Determine normal depth
Hn=HnFun(B,g,Hc,n,S0);
H1=1.01*Hn; %Set H1 to be within 1% of Hn
s1=0; %Location on s where H=H1
%Evaluate water surface profile
[H,s]=GVFaFun(H1,H2,s1,B,g,Hc,n,S0);
s2=s(end); %Location on s where H=H2
L=s2-s1 %Distance to upstream point (m)

```

Execution of the above MATLAB code reveals that $L = 700$ m.

Worked Solution 3.2 (see Problem 3.2)

From Table 3.3 we know that the water depth above a free fall outlet is the critical depth, H_c . It follows that $H_c = 0.1$ m. We also have that $B = 0.4$ m, $S_0 = -\frac{1}{50}$ and $n = 0.012 \text{ m}^{-\frac{1}{3}} \text{ s}$.

We need to determine the water depth, H_1 , at a distance, $L = 10$ m, upstream of the outlet. The function, GVFaFun (Listing 3.1), is inappropriate for this task because it provides a distance, s , for a given water depth, H . Instead, we need to determine a water depth, H , for a given location, s , by solving Eq. (3.21). A MATLAB code, which solves Eq. (3.21) using ode45 is provided in Listing 3.3.

Listing 3.3 Solution for the GVF equation, with fluid depth as dependant variable, assuming a rectangular prismatic cross-section channel (Eq. (3.21)).

```

function [H,s]=GVFbFun(s1,s2,H1,B,g,Hc,n,S0)
%Solves gradually varied flow equation using ode45
%providing the location of points associated with
%an array of fluid depths ranging from H1 and H2.
%s1 - Location of H1 (m)
%s2 - Location of H2 (m)
%H1 - Fluid depth at s = s1 (m)
%B - Breadth of rectangular channel (m)
%g - Gravitational acceleration (m/s2)
%Hc - Critical fluid depth (m)
%n - Manning coefficient (m-1/3 s)
%S0 - Channel bed slope (-)
%H - Vector of fluid depths between H1 and H2
%s - Location of s values between s1 and s2
ODEFUN=@(s,H) (S0-((B+2*H)/B)^(4/3)*g*n^2*...
Hc^3/H^(10/3))/(1-(Hc/H)^3);

```

```
[s, H] = ode45(ODEFUN, [s1 s2], H1);
```

Let s_1 and s_2 be the locations of the outlet and the upstream point, respectively. It follows that $H = H_1$ at $s = s_1$ and $H = H_2$ at $s = s_2$. Furthermore, $s_1 = L$, $s_2 = 0$ and $H_1 = 1.001H_c$ (it is not possible to set $H_1 = H_c$ because the GVF equation is singular at this location). The MATLAB code below utilises GVFbFun in Listing 3.3 to determine the value of H_2 :

```
B=0.4; %Breadth of channel (m)
S0=-1/50; %Channel slope (-)
n=0.012; %Manning coefficient (m-1/3 s)
Hc=0.1; %Critical fluid depth (m)
L=10; %Distance (m)
g=9.81; %Gravitational acceleration (m/s2)
H1=1.001*Hc; %Downstream fluid depth (m)
s1=L; %Location where H=H1
s2=0; %Location where H=H2
%Evaluate water surface profile
[H, s]=GVFbFun(s1, s2, H1, B, g, Hc, n, S0);
H2=H(end) %Value of H at s=s2
```

The resulting answer for H_2 is 0.353 m.

Worked Solution 3.3 (see Problem 3.3)

Let $B = 0.5$ m, $L = 300$ m, $S_0 = \frac{1}{500}$, $n = 0.015$ m^{-1/3} s and $H_1 = 1.8$ m. Solving Eq. (3.13) for the flow rate, Q , leads to

$$Q = B\sqrt{gH_c^3}$$

Let s_1 and s_2 be the distance at which $H = H_1$ and $H = H_2$, respectively. The critical depth, H_c , can be found by iteratively changing the H_c value in GVFaFun (Listing 3.1) until $s_2 - s_1 = L$. Here we will use MATLAB's optimisation scheme, `fminsearch`, to iteratively choose a value of H_c such that the objective function, $F = |s_2 - s_1 - L|$ is minimised.

Given that the slope is mild and the flow is sub-critical we know that the water surface profile in the channel will be either M1 or M2 (see Table 3.2). Whether it will be an M1 or and M2 is important for our decision concerning an initial guess for H_c . We want to avoid a corresponding normal depth, H_n , such that $H_n \in (H_1, H_2)$ because it is not possible for the water elevation to pass through H_n (see Fig. 3.1b). It follows that we should first provide a reasonable initial guess for H_n and then calculate a corresponding initial guess for H_c using Eq. (3.22).

Listing 3.4 Function to obtain flow rate and critical depth for sub-critical flow in mild sloping rectangular open channels.

```
function [Q,Hc]=GVFQfun(Hn,H1,H2,B,g,n,S0,L)
%Determines flow rate and critical depth for
%sub-critical flow in mild sloping channels
%Hn - Initial guess for normal depth (m)
%H1 - Fluid depth at s = s1 (m)
%H2 - Fluid depth at s = s2 (m)
%B - Breadth of rectangular channel (m)
%g - Gravitational acceleration (m/s^2)
%n - Manning coefficient (m^(-1/3) s)
%S0 - Channel bed slope (-)
%L - Distance between s1 and s2 (m)
%Q - Flow rate (m^3/s)
%Hc - Critical fluid depth (m)
%Determine initial guess for Hc using Hn
Hc=( (B/(B+2*Hn))^(4/3)*S0*Hn^(10/3)/g/n^2)^(1/3);
%Determine actual value of Hc by iterative solution
Hc=fminsearch(@GVFQobjFun,Hc,[],H1,H2,B,g,n,S0,L);
%Determine flow rate from Hc
Q=B*sqrt(g*Hc^3);
%*****
function F=GVFQobjFun(Hc,H1,H2,B,g,n,S0,L)
%Contains the objective function to be minimised
%by fminsearch in GVFQfun
s1=0; %Let H=H1 at s=s1 and s1=0
%Solve GVF equation
[H,s]=GVFaFun(H1,H2,s1,B,g,Hc,n,S0);
s2=s(end); %Let s=s2 where H=H2
F=abs(s2-s1-L); %Define objective function
```

(a) Let Δh [L], Δz [L] and ΔH [L] be the losses in water surface elevation, channel bed elevation and fluid depth that occur over a distance, L [L], in the flow direction along the channel. Note that channel slope, $S_0 = \frac{\Delta z}{L}$. It follows that

$$\Delta H = \Delta h - S_0 L \quad (3.28)$$

In this case, $\Delta h = 0.3$ m such that $\Delta H = -0.3$ m. Consequently $\frac{\partial H}{\partial s} > 0$ and an M1 profile will apply (see Table 3.2). Furthermore, $H_2 = H_1 - \Delta H = 2.1$ m.

For an M1 profile, $H > H_n$ and $H_2 > H_1$. Therefore an initial guess for H_n should be less than H_1 . Here we will choose it to be 90% of H_1 . The MATLAB script listed below, utilises GVFafun in Listing 3.1 and GVFQfun in Listing 3.4 to determine Q and plot the resulting water surface elevation profile:

```

B=0.5; %Breadth of channel (m)
L=300; %Channel length (m)
S0=1/500; %Channel slope (-)
H1=1.8; %Upstream boundary fluid depth (m)
n=0.015; %Manning coefficient (m-1/3 s)
g=9.81; %Gravitational acceleration (m/s2)
dh=0.3; %Loss in water surface elevation (m)
dH=dh-S0*L %Loss in fluid depth (m)
H2=H1-dH %Downstream fluid depth (m)
Hn0=0.9*H1; %Initial guess for normal depth
%Evaluate flow rate and critical depth
[Q,Hc]=GVFQfun(Hn0,H1,H2,B,g,n,S0,L)
%Evaluate water surface profile
[H,s]=GVFaFun(H1,H2,0,B,g,Hc,n,S0);
figure(1);clf;hold on;box on %Plot results
plot([0 L],-S0*[0 L],'k') %Channel bed
plot(s,H-S0*s,'b') %Water surface
%Boundary conditions
plot([0 L],[H1 H2]-S0*[0 L],'bo')
xlabel('Distance (m)')
ylabel('Elevation (m)')
xlim([0 L])

```

The resulting flow rate is $0.759 \text{ m}^3 \text{ s}^{-1}$. The resulting water surface profile is shown as a blue line in Fig. 3.3.

(b) In this case, $\Delta h = 1.3 \text{ m}$ such that $\Delta H = 0.7 \text{ m}$. Consequently $\frac{\partial H}{\partial s} < 0$ and an M2 profile will apply (see Table 3.2). Furthermore, $H_2 = H_1 - \Delta H = 1.1 \text{ m}$.

For an M2 profile, $H < H_n$ and $H_2 < H_1$. Therefore an initial guess for H_n should be greater than H_1 . Here we will chose it to be 110% of H_1 . The additional

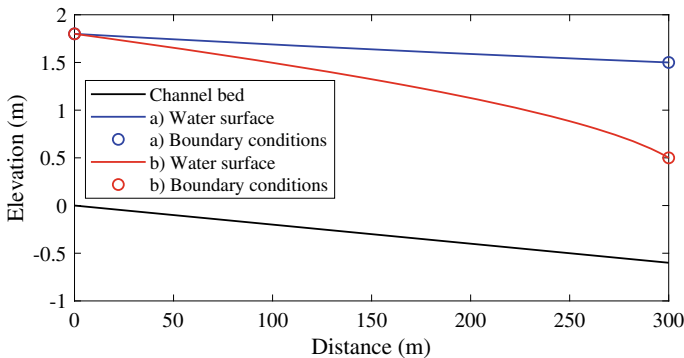


Fig. 3.3 Plots of water surface elevation resulting from a total water surface elevation decline of **a** 0.3 m (blue line) and **b** 1.3 m (red line)

MATLAB script listed below utilizes GVF_aFun in Listing 3.1 and GVF_Qfun in Listing 3.4 to determine Q and plot the resulting water surface elevation profile:

```
dh=1.3; %Loss in water surface elevation (m)
dH=dh-S0*L %Loss in fluid depth (m)
H2=H1-dH %Downstream fluid depth (m)
Hn0=1.1*H1; %Initial guess for normal depth
%Evaluate flow rate and critical depth
[Q,Hc]=GVFQfun(Hn0,H1,H2,B,g,n,S0,L)
%Evaluate water surface profile
[H,s]=GVFaFun(H1,H2,0,B,g,Hc,n,S0);
plot(s,H-S0*s,'r') %Plot water surface
%Plot boundary conditions
plot([0 L],[H1 H2]-S0*[0 L],'ro')
%Add a legend
legend('Channel bed','a) Water surface',...
'a) Boundary conditions',...
'b) Water surface',...
'b) Boundary conditions')
```

The resulting flow rate is $1.15 \text{ m}^3 \text{ s}^{-1}$. The resulting water surface profile is shown as a red line in Fig. 3.3.

References

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Rapidly Varied Flow in Open Channels

4

Abstract

This chapter explains how to solve steady-state rapidly varied open channel flow problems. The continuity and momentum equations are used to derive expressions for conjugate depths on either side of a hydraulic jump. An expression is derived to predict the total head lost within a hydraulic jump. A moving control-volume, following a countercurrent wave-front, is used to derive an expression for the speed of a shallow-water wave. It is shown how to determine the location of a hydraulic jump using the gradually varied flow equation. Practical applications are presented through worked examples and a problem sheet with worked solutions.

Notation

B	Breadth [L].
c	Wave speed [LT^{-1}].
E	Total head [L].
F	Force [MLT^{-2}].
Fr	Froude number [-].
g	Gravitational acceleration [LT^{-2}].
H	Depth [L].
H_n	Normal depth [L].
H_c	Critical depth [L].
L	Length [L].
n	Manning coefficient [$\text{L}^{-\frac{1}{3}}\text{T}$].
Q	Flow rate [L^3T^{-1}].
s	Distance along a channel [L].
s_{12}	Location of a hydraulic jump [L].
S_0	Bed slope [-].
v	Fluid velocity [LT^{-1}].
v_c	Critical velocity [LT^{-1}].

v_n	Normal velocity [LT^{-1}].
z	Elevation [L].
ρ	Mass density of a fluid [ML^{-3}].

4.1 Introduction

In Chap. 3 we studied gradually varied flow (GVF). The Froude number was used to distinguish between three different types of open channel flow: (1) sub-critical, (2) critical and (3) supercritical.

Providing the flow regime stays as being sub-critical or supercritical, the (theoretical) fluid surface is expected to be smooth and gradually varied. However, there are many situations that lead to flow transitioning from sub-critical to supercritical or vice versa. Sub-critical flow can smoothly transition into supercritical flow (e.g. Fig. 3.2d). However, the change from supercritical flow to sub-critical flow is only possible through a discontinuity, referred to as a hydraulic jump (recall Rule 6 in Table 3.3).

Systems involving hydraulic jumps are commonly referred to as rapidly varied flow systems (in contrast to gradually varied flow systems). Energy is lost within a hydraulic jump due to turbulence. Therefore, engineers often induce hydraulic jumps to take energy out of flowing fluids in a controlled manner so as to avoid scouring and erosion further downstream. The objective of this chapter is to derive theoretical equations to determine the location and energy consumption of hydraulic jumps.

First we explore how critical flow conditions represents a minimum total head state. Equations are derived to relate the fluid depths before and after a hydraulic jump. An equation is then derived to determine the total head loss within a hydraulic jump. An expression is derived for the speed of a moving surface wave in a shallow-water environment. Finally, it is shown how we can use the GVF equation to locate the occurrence of a hydraulic jump.

4.2 Critical Flow Conditions

Recall the expression for total head, E [L], for an open channel flow system (Eq. (2.38))

$$E = H + \frac{v^2}{2g} + z \quad (4.1)$$

where H [L] is fluid depth, v [LT^{-1}] is velocity, g [LT^{-2}] is gravitational acceleration and z [L] is the elevation of the channel bed.

Consider a rectangular cross-section channel of breadth, B [L]. The flow rate, Q [L^3T^{-1}], is found from

$$Q = vBH \quad (4.2)$$

which on substitution into Eq. (4.1) leads to

$$E = H + \frac{Q^2}{2gB^2H^2} + z \quad (4.3)$$

Challenge 4.1 Use Eq. (4.3) to determine H_c whereby setting $H = H_c$ yields the minimum value for E .

Differentiating Eq. (4.3) with respect to H twice leads to

$$\frac{\partial E}{\partial H} = 1 - \frac{Q^2}{gB^2H^3}$$

and

$$\frac{\partial^2 E}{\partial H^2} = \frac{3Q^2}{gB^2H^4}$$

Noting that the second derivative is always positive, it follows that any stationary point found from the first derivative will be a minimum. Let H_c [L] be the fluid depth when the total head, E , is minimized. Setting $H = H_c$ and $\frac{\partial E}{\partial H} = 0$ leads to [1, p. 433]

$$H_c^3 = \frac{Q^2}{gB^2} \quad (4.4)$$

Note that Eq. (4.4) is identical to Eq. (3.13), suggesting that H_c is the critical fluid depth that leads to critical flow conditions. It follows that $H = H_c$ represents a special state where the total head, E , is minimised for a given flow rate, Q .

Challenge 4.2 Determine an expression for v_c in terms of H_c and g , whereby $v = v_c$ when $H = H_c$.

Let $v = v_c$ when $H = H_c$. From Eq. (4.2) we have

$$Q = v_c B H_c \quad (4.5)$$

Substituting Eq. (4.5) into Eq. (4.4) and solving for v_c leads to [1, p. 433]

$$v_c = \sqrt{gH_c} \quad (4.6)$$

It turns out that $\sqrt{gH}$ is a universal wave speed expected for small surface waves travelling under shallow-water conditions. The interesting thing about Eq. (4.6) is that it tells us that the total head is minimised when water particles are moving at the same velocity as any waves or ripples occurring at the surface.

This idea is encapsulated in the Froude number, Fr [-], which for rectangular cross-section channels takes the form (obtained by substituting Eq. (4.2) into Eq. (3.10))

$$Fr = \frac{v}{\sqrt{gH}} \quad (4.7)$$

Recall that:

- Sub-critical flow is when $Fr < 1$.
- Critical flow is when $Fr = 1$.
- Supercritical flow is when $Fr > 1$.

During sub-critical flow, the velocity of water particles is less than the shallow-water wave speed. During supercritical flow, the velocity of water particles is greater than the shallow-water wave speed.

We expect sub-critical flow to be controlled by downstream boundaries because surface waves reflected upstream from a downstream boundary move faster than downstream moving water particles (hence Rule 1 in Table 3.3). In contrast, we expect supercritical flow to be controlled by upstream boundaries because surface waves reflected upstream from a downstream boundary move slower than downstream moving water particles (hence Rule 2 in Table 3.3).

4.3 Hydraulic Jumps

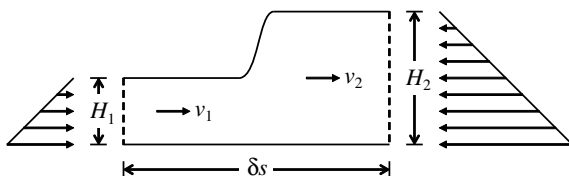
When flow is supercritical, a change can occur whereby the water level suddenly increases such that downstream of this discontinuity, flow is sub-critical. Such a discontinuity is referred to as a hydraulic jump.

Consider a hydraulic jump present within a flowing horizontal open channel of rectangular cross-section with a breadth, B [L] (Fig. 4.1). Let the fluid depth and velocity upstream of the hydraulic jump be H_1 [L] and v_1 [LT^{-1}], respectively. Let the fluid depth and velocity downstream of the hydraulic jump be H_2 [L] and v_2 [LT^{-1}], respectively. Let Q [L^3T^{-1}] be the total volumetric flow rate within the channel. Fluid pressure within the channel is assumed to be hydrostatic.

4.3.1 Conjugate Depths

Challenge 4.3 Use both the continuity equation and the momentum equation to determine an expression for H_1 as a function of H_2 and the critical depth, H_c . Then determine an equivalent expression for H_2 as a function of H_1 and the critical depth, H_c .

Fig. 4.1 Schematic diagram of a hydraulic jump



From the continuity equation (Eq. (1.32)) we have

$$Q = BH_1v_1 = BH_2v_2 \quad (4.8)$$

and from the momentum equation we have

$$F = \rho Q(v_2 - v_1)$$

where F is the net-force in the s -direction acting on the CV.

Eliminating the velocity terms in the momentum equation using the continuity equation leads to

$$F = \frac{\rho Q^2}{BH_1H_2}(H_1 - H_2) \quad (4.9)$$

Because the fluid is assumed to be hydrostatic, the vertical pressure distribution within the fluid will be triangular (consider Eq. (1.6)). The force acting on the upstream face of the CV due to fluid pressure will be $\frac{\rho g B H_1^2}{2}$. Similarly, the force acting on the downstream face of the CV due to fluid pressure will be $\frac{\rho g B H_2^2}{2}$. The net-force in the s -direction acting on the CV is therefore

$$F = \frac{\rho g B H_1^2}{2} - \frac{\rho g B H_2^2}{2}$$

which can be rearranged to obtain

$$F = \frac{\rho g B}{2}(H_1 + H_2)(H_1 - H_2) \quad (4.10)$$

Equating Eqs. (4.9) with (4.10) and substituting Eq. (4.4) then gives us

$$H_1^2 H_2 + H_1 H_2^2 - 2H_c^3 = 0 \quad (4.11)$$

which is a quadratic equation in terms of either H_1 or H_2 .

It follows that

$$H_1 = \frac{H_2}{2} \left[-1 \pm \sqrt{1 + 8 \left(\frac{H_c}{H_2} \right)^3} \right]$$

and

$$H_2 = \frac{H_1}{2} \left[-1 \pm \sqrt{1 + 8 \left(\frac{H_c}{H_1} \right)^3} \right]$$

Noting that both H_1 and H_2 must be positive, it can be further stated that

$$H_1 = \frac{H_2}{2} \left[-1 + \sqrt{1 + 8 \left(\frac{H_c}{H_2} \right)^3} \right] \quad (4.12)$$

and

$$H_2 = \frac{H_1}{2} \left[-1 + \sqrt{1 + 8 \left(\frac{H_c}{H_1} \right)^3} \right] \quad (4.13)$$

Challenge 4.4 Write both Eqs. (4.12) and (4.13) in terms of Froude numbers.

Let Fr_1 and Fr_2 be the Froude numbers upstream and downstream of the hydraulic jump, respectively. Given Eq. (4.7), we have

$$Fr_1 = \frac{v_1}{\sqrt{gH_1}} \quad \text{and} \quad Fr_2 = \frac{v_2}{\sqrt{gH_2}}$$

Application of the continuity equation enables the Froude numbers to be written in terms of Q as opposed to v :

$$Fr_1 = \frac{Q}{BH_1\sqrt{gH_1}} \quad \text{and} \quad Fr_2 = \frac{Q}{BH_2\sqrt{gH_2}}$$

Substituting Eq. (4.4) then leads to

$$Fr_1^2 = \left(\frac{H_c}{H_1}\right)^3 \quad \text{and} \quad Fr_2^2 = \left(\frac{H_c}{H_2}\right)^3$$

which on substitution into Eqs. (4.12) and (4.13) gives us [1, p. 441]

$$H_1 = \frac{H_2}{2} \left(-1 + \sqrt{1 + 8Fr_2^2} \right) \quad (4.14)$$

and

$$H_2 = \frac{H_1}{2} \left(-1 + \sqrt{1 + 8Fr_1^2} \right) \quad (4.15)$$

Note that when $Fr_2 = 1$, flow upstream of the “hydraulic jump” (which does not really exist in this case) is critical and $H_1 = H_2$. When $Fr_2 < 1$, flow downstream of the hydraulic jump is sub-critical and $H_1 < H_2$. When $Fr_2 > 1$, flow downstream of the hydraulic jump (which also does not really exist in this case) is supercritical and $H_2 < H_1$.

The value of H_1 given by Eqs. (4.12) or (4.14) for a given value of H_2 is referred to as the conjugate depth of H_2 . Similarly, the value of H_2 given by Eqs. (4.13) or (4.15) for a given value of H_1 is referred to as the conjugate depth of H_1 .

4.3.2 Total Head Loss Due to a Hydraulic Jump

Challenge 4.5 Use Eq. (4.11) to determine an expression for the total head loss due to the hydraulic jump (which also does not really exist in this case) as a function of H_1 and H_2 .

Let E_1 and E_2 be the total head upstream and downstream of the hydraulic jump, respectively, found from (recall Eq. (4.3)):

$$E_1 = H_1 + \frac{Q^2}{2gB^2H_1^2} + z_1$$

$$E_2 = H_2 + \frac{Q^2}{2gB^2H_2^2} + z_2$$

where z_1 [L] and z_2 [L] are the elevations of the channel bed upstream and downstream of the hydraulic jump, respectively.

The total head loss, $\Delta E = E_1 - E_2$, is found from

$$\Delta E = H_1 - H_2 + \frac{Q^2}{2gB^2} \left(\frac{1}{H_1^2} - \frac{1}{H_2^2} \right) + \Delta z \quad (4.16)$$

where $\Delta z = z_1 - z_2$.

From Eq. (4.11) we have

$$\frac{Q^2}{2gB^2} = \frac{H_1^2 H_2 + H_1 H_2^2}{4}$$

which on substitution into Eq. (4.16) leads to [1, p. 440]

$$\begin{aligned} \Delta E &= H_1 - H_2 + \frac{H_1^2 H_2 + H_1 H_2^2}{4} \left(\frac{1}{H_1^2} - \frac{1}{H_2^2} \right) + \Delta z \\ &= \frac{4H_1^2 H_2^2 (H_1 - H_2) + (H_2^2 - H_1^2)(H_1^2 H_2 + H_1 H_2^2)}{4H_1^2 H_2^2} + \Delta z \\ &= \frac{H_2^3 + 3H_1^2 H_2 - 3H_1 H_2^2 - H_1^3}{4H_1 H_2} + \Delta z \\ &= \frac{(H_2 - H_1)^3}{4H_1 H_2} + \Delta z \end{aligned} \quad (4.17)$$

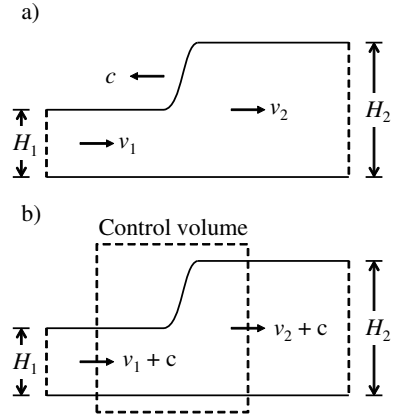
Note that for a horizontal channel, $\Delta z = 0$.

4.4 Shallow-Water Waves

Consider fluid movement along a horizontal open channel of uniform rectangular section of breadth, B [L]. A wave-front is propagating upstream at a velocity of c [LT^{-1}] (Fig. 4.2a). The fluid depths in the channel upstream and downstream of the wave-front are constant and denoted H_1 and H_2 , respectively. The fluid velocities in the channel upstream and downstream of the wave-front are also constant and denoted v_1 and v_2 , respectively. It is of interest to determine a relationship between c , v_1 and H_1 .

Challenge 4.6 Determine an expression for the velocity of the wave-front relative to the velocity of flowing water particles upstream of the wave-front (i.e., $v_1 + c$) in terms of H_1 and gravitational acceleration, g .

Fig. 4.2 **a** Schematic diagram of a wave-front propagating upstream in a horizontal open channel. **b** A moving control-volume that moves with the wave-front



This problem becomes more straightforward if we choose a control-volume (CV) that moves upstream with the wave-front (Fig. 4.2b).

Invoking the continuity equation, rate of water movement in and out of the CV, Q [L^3T^{-1}], is found from

$$Q = BH_1(v_1 + c) = BH_2(v_2 + c) \quad (4.18)$$

The momentum equation provides that

$$F = \rho Q(v_2 - v_1)$$

The Q and v_2 terms in the momentum equation can be eliminated using Eq. (4.18). But to eliminate v_2 , Eq. (4.18) needs to be first slightly rearranged to get

$$v_2 = \frac{H_1}{H_2}(v_1 + c) - c \quad (4.19)$$

Substituting Eqs. (4.18) and (4.19) into the momentum equation then leads to

$$F = \rho B \frac{H_1}{H_2}(v_1 + c)^2(H_1 - H_2) \quad (4.20)$$

But recall from Eq. (4.10) that the net-force in the s -direction acting on the CV can also be found from

$$F = \frac{\rho g B}{2}(H_1 + H_2)(H_1 - H_2) \quad (4.21)$$

Equating Eqs. (4.20) and (4.21) then leads to

$$(v_1 + c)^2 = g \left(\frac{H_1 + H_2}{2} \right) \frac{H_2}{H_1} \quad (4.22)$$

For small perturbations (i.e., $H_2 - H_1 \ll 1$)

$$v_1 + c = \sqrt{gH_1} \quad (4.23)$$

which is the shallow-water wave speed we saw earlier in the definition of the Froude number given in Eq. (4.7).

4.5 Locating Hydraulic Jumps

The gradually varied flow (GVF) equation (Eq.(3.5)) can be used to determine the location at which a hydraulic jump is likely to occur [2,3].

4.5.1 Supercritical to Normal Sub-critical Flow

The easiest case to consider is where supercritical flow transitions into a normal sub-critical flow (e.g. [2, p. 199]). Note that normal sub-critical flow is a characteristic of a mild slope (see Table 3.2). Consider the following scenario.

Water flows, under a sluice gate at a rate of $5.5 \text{ m}^3 \text{ s}^{-1}$, into a rectangular cross-section open channel with a breadth of 3 m, a downward slope of 1 in 1000 and a Manning coefficient of $0.014 \text{ m}^{-\frac{1}{3}} \text{ s}$. The depth of water immediately downstream of the sluice gate is 0.3 m. Normal flow conditions are achieved downstream of a hydraulic jump.

Let $Q = 5.5 \text{ m}^3 \text{ s}^{-1}$, $B = 3 \text{ m}$, $S_0 = 10^{-3}$, $n = 0.014 \text{ m}^{-\frac{1}{3}} \text{ s}$ and $H_0 = 0.3 \text{ m}$. Furthermore, let $s_0 = 0$ be the location of the sluice gate, s_{12} be the location of the hydraulic jump, H_1 be the fluid depth immediately upstream of the hydraulic jump and H_2 be the fluid depth immediately downstream of the hydraulic jump.

Given that normal flow conditions are achieved immediately downstream of the hydraulic jump, $H_2 = H_n$ where H_n is the normal depth (which can be obtained using the `HnFun` function given in Listing 3.2). A value for H_1 can be found from Eq.(4.12). The location of the hydraulic jump, s_{12} , can then be found using the `GVFaFun` function given in Listing 3.1. The above calculations are achieved using the MATLAB code below:

```
Q=5.5; %Flow rate (m3/s)
B=3; %Breadth of channel (m)
S0=1/1000; %Channel slope (-)
n=0.014; %Manning coefficient (m^(-1/3) s)
g=9.81; %Gravitational acceleration (m/s2)
H0=0.3; %Upstream boundary fluid depth (m)
s0=0; %Location on s where H=H0 (m)
Hc=(Q^2/g/B^2)^(1/3); %Determine critical depth
H2=HnFun(B,g,Hc,n,S0); %Determine normal depth
%Determine depth upstream of hydraulic jump
H1=H2/2.*(-1+sqrt(1+8*(Hc./H2).^3));
%Evaluate GVF water surface profile
[H,s]=GVFaFun(H0,H1,s0,B,g,Hc,n,S0);
s12=s(end) %Location of hydraulic jump (m)
```

It turns out that the location of the hydraulic jump is 28.0 m downstream of the sluice gate. A plot of the corresponding water surface is shown in Fig. 4.3a.

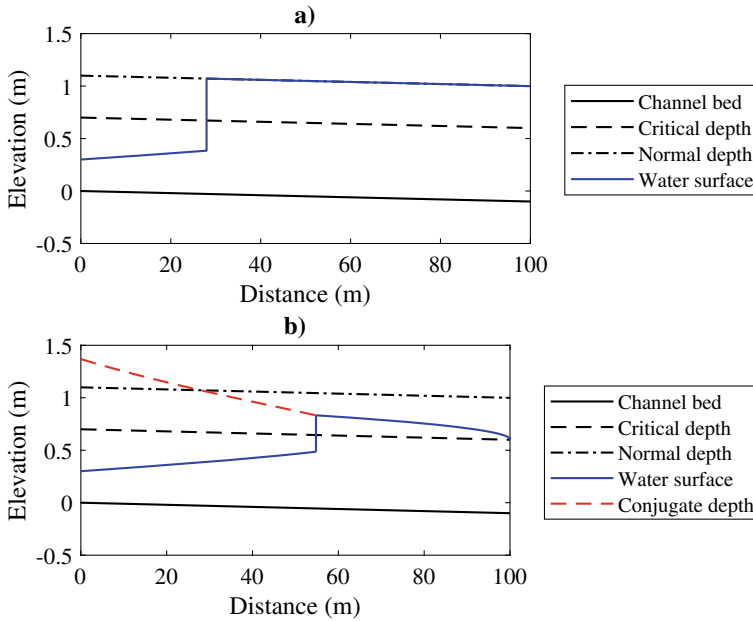


Fig. 4.3 Examples of GVF water surfaces interacting with a hydraulic jump. **a** Supercritical flow into normal sub-critical flow. **b** Supercritical flow into non-normal sub-critical flow

4.5.2 Supercritical to Non-normal Sub-critical Flow

The situation where supercritical flow transitions into a non-normal subcritical flow is much more complicated because there is a GVF profile either side of the hydraulic jump. In this case, the location of the hydraulic jump must be found by iterative solution [3].

Consider again the scenario described in Sect. 4.5.1 but this time with the rectangular cross-section open channel terminating with a free-fall outlet at a distance of 100 m from the sluice gate. Table 3.3 tells us to expect the fluid depth at the outlet to be equal to the critical depth.

Let $Q = 5.5 \text{ m}^3 \text{ s}^{-1}$, $B = 3 \text{ m}$, $S_0 = 10^{-3}$, $n = 0.014 \text{ m}^{-\frac{1}{3}} \text{ s}$, $H_0 = 0.3 \text{ m}$ and $H_3 = 1.001H_c$ (recall that the GVF equation is singular at $H = H_c$ so it is better to solve from just above H_c in this case). Furthermore, let $s_0 = 0$ be the location of the sluice gate, s_{12} be the location of the hydraulic jump, $s_3 = 100 \text{ m}$ be the location of the free-fall outlet, H_1 be the fluid depth immediately upstream of the hydraulic jump and H_2 be the fluid depth immediately downstream of the hydraulic jump.

To solve the GVF problem we need to split the domain into two regions. Let $H = H_a$ for $s \in [s_0, s_{12})$ and $H = H_b$ for $s \in (s_{12}, s_3]$. Furthermore, let $H_{1a} = H_a(s = s_{12})$ and $H_{2b} = H_b(s = s_{12})$. The value of H_{2b} can be compared to the conjugate value of H_{1a} (obtained from Eq. (4.13)), referred to as H_{2a} . Providing the hydraulic jump is correctly located, $H_{2a} = H_{2b}$.

The correct location of the hydraulic jump can be found by iteratively changing s_{12} until the difference between H_{2a} and H_{2b} has been minimised [3]. The MATLAB function, `s12ObjFun`, given in Listing 4.1, utilizes the `GVFbFun` function, given in Listing 3.3, to determine the fluid depth either side of a proposed hydraulic jump and calculates the absolute difference between H_{2a} and H_{2b} .

Listing 4.1 Function to determine the error between the fluid depths at a proposed hydraulic jump derived from GVF profiles either side of the hydraulic jump.

```
function [F,H1a,H2b,sa,sb,Ha,Hb,HaCONJ]...
=s12ObjFun(s12,s0,s3,H0,H3,B,g,Hc,n,S0)
%Obtains objective function to be minimized when
%locating a hydraulic jump
%s12 - Proposed location of hydraulic jump (m)
%s0 - Location of H0 (m)
%s3 - Location of H3 (m)
%H0 - Fluid depth at sa = s0 (m)
%H3 - Fluid depth at sb = s3 (m)
%B - Breadth of rectangular channel (m)
%g - Gravitational acceleration (m/s2)
%Hc - Critical fluid depth (m)
%n - Manning coefficient (m^(-1/3) s)
%S0 - Channel bed slope (-)
%F - Absolute error to be minimized
%H1a - Fluid depth at sa = s12 (m)
%H2b - Fluid depth at sb = s12 (m)
%sa - Location of s values between s0 and s12
%sb - Location of s values between s12 and s3
%Ha - Fluid depth for s<s12 (m)
%Hb - Fluid depth for s>s12 (m)
%HaCONJ - Conjugate values of Ha
%Evaluate GVF profile upstream of hydraulic jump
[Ha,sa]=GVFbFun(s0,s12,H0,B,g,Hc,n,S0);
H1a=Ha(end); %Extract H1a=Ha(sa=s12)
%Evaluate GVF profile downstream of hydraulic jump
[Hb,sb]=GVFbFun(s3,s12,H3,B,g,Hc,n,S0);
H2b=Hb(end); %Extract H2b=Hb(sb=s12)
%Determine conjugate of Ha
HaCONJ=Ha/2.*(-1+sqrt(1+8*(Hc./Ha).^3));
H2a=HaCONJ(end); %Extract H2a=Hb(sb=s12)
F=abs(H2a-H2b); %Absolute error to be minimized
```

For a first iteration we can assume that the hydraulic jump occurs at the midpoint between the sluice gate and the hydraulic jump, i.e. $s_{12} \approx \frac{s_3-s_0}{2}$. The MATLAB code below minimizes the `s12ObjFun` function (in Listing 4.1) using MATLAB's optimization function, `fminsearch`, to determine the actual location of the hydraulic jump for the scenario described above:

```

Q=5.5; %Flow rate (m3/s)
B=3; %Breadth of channel (m)
S0=1/1000; %Channel slope (-)
n=0.014; %Manning coefficient (m-1/3 s)
g=9.81; %Gravitational acceleration (m/s2)
H0=0.3; %Upstream boundary fluid depth (m)
s0=0; %Location on s where H=H0 (m)
s3=100; %Location of free-fall outlet
Hc=(Q2/g/B2)(1/3); %Determine critical depth
H3=1.001*Hc; %Downstream boundary fluid depth (m)
%Initial guess for hydraulic jump location (m)
s12guess=(s3-s0)/2;
%Determine location of hydraulic jump (m)
s12=fminsearch(@s12ObjFun,s12guess,[],s0,s3,...
H0,H3,B,g,Hc,n,S0)

```

The location of the hydraulic jump turns out to be 54.8 m downstream from the sluice gate in this case.

The water surface profile for the free-fall outlet scenario (as described in the current section) is shown in Fig. 4.3b. The effect of the free-fall outlet, as compared to the normal flow scenario (as described in Sect. 4.5.1 and shown in Fig. 4.3a), is to reduce the fluid depth on the downstream side of the hydraulic jump, which in turn leads to the hydraulic jump moving further away from the sluice gate.

The conjugate fluid depth, corresponding to the supercritical portion of the water surface profile, and the normal fluid depth are plotted in Fig. 4.3b as a red dashed line and a black dash-dot line, respectively. Not surprisingly, it can be seen that the hydraulic jump in Fig. 4.3a occurs exactly where the conjugate fluid depth coincides with the normal fluid depth in Fig. 4.3b.

4.6 Problem Sheet

Problem 4.1 (see Worked Solution 4.1)

In a long rectangular channel 3 m wide the total head relative to the base of the channel (i.e., $E - z$) is 1.8 m and the rate of flow is $12 \text{ m}^3 \text{ s}^{-1}$. Calculate two possible depths of flow and the corresponding Froude numbers.

Problem 4.2 (see Worked Solution 4.2)

Water flows at a depth of 1.2 m in a rectangular prismatic channel 2.7 m wide. However, it is observed that there is a 200 mm high smooth hump on the channel

bed where a drop of 150 mm in the water surface can be seen to occur. Neglecting frictional effects, use the Bernoulli equation and the continuity equation to calculate the rate of flow.

Problem 4.3 (see Worked Solution 4.3)

A sluice across a rectangular prismatic channel, 6 m wide, discharges a stream of water, 1.2 m deep.

- (a) Determine the flow rate when the upstream depth is 6 m.
- (b) The conditions downstream cause a hydraulic jump to occur at a place where concrete blocks have been placed on the bed. Determine the force exerted on the water by the blocks if the depth after the jump is 3.1 m.

Problem 4.4 (see Worked Solution 4.4)

Water flows at $5.4 \text{ m}^3 \text{ s}^{-1}$ under a wide sluice gate into a rectangular prismatic channel 3.5 m wide. A hydraulic jump is formed just downstream of a section where the depth is 380 mm. Calculate the depth downstream of the jump and the power dissipated in it.

Problem 4.5 (see Worked Solution 4.5)

A long horizontal rectangular prismatic channel has a base width of 1.5 m. When the flow in the channel is $0.85 \text{ m}^3 \text{ s}^{-1}$ the depth is 500 mm. The discharge is suddenly reduced so that a surge wave of amplitude 150 mm is propagated upstream. Determine the velocity of the wave and new rate of flow.

Problem 4.6 (see Worked Solution 4.6)

Water flows along a rectangular channel with a base width of 3 m. The Manning coefficient is $0.02 \text{ m}^{-\frac{1}{3}} \text{ s}$. The channel features two distinct bed slopes. The upstream portion of the channel is steep with a slope of 0.02. The downstream portion of the channel is mild with a slope of 0.005. The channel system is sufficiently long such that flow is normal both upstream and downstream of the bed slope change. Determine the location of a hydraulic jump that occurs, relative to the location of the bed slope change, when the flow rate is (a) $15 \text{ m}^3 \text{ s}^{-1}$ and (b) $40 \text{ m}^3 \text{ s}^{-1}$.

4.7 Worked Solutions

Worked Solution 4.1 (see Problem 4.1)

The total head, E , is found from Eq. (4.3). The total head relative to the base of the channel, $e = E - z$ where z is the elevation of the channel bed. It follows that

$$e = H + \frac{Q^2}{2B^2H^2g}$$

where $B = 3$ m, $e = 1.8$ m and $Q = 12$ m³s⁻¹.

The above equation can be rearranged to obtain a cubic polynomial:

$$H^3 - eH^2 + \frac{Q^2}{2B^2g} = 0$$

The relevant fluid depths will be the two positive roots which can be found using the following MATLAB code:

```
%Define input variables
B=3; %Channel breadth (m)
e=1.8; %Total head relative to base of channel (m)
Q=12; %Flow rate (m3/s)
g=9.81; %Gravitational acceleration (m/s2)
%Find roots of polynomial
H=roots([1 -e 0 Q^2/2/B^2/g]);
%Exclude negative roots
H(H<0)=[];
%Display result
num2str(H)
```

The two positive values of H , when $e = 1.8$ m, are 1.357 m and 1.027 m, respectively.

Substituting Eq. (4.2) into Eq. (4.7) leads to

$$\text{Fr} = \frac{Q}{BH\sqrt{Hg}}$$

which yields corresponding Froude numbers of 0.808 and 1.23, respectively.

Worked Solution 4.2 (see Problem 4.2)

Let $H_1 = 1.2$ m, $B = 2.7$ m, $\Delta z = 0.2$ m and $\Delta h = 0.15$ m. The Bernoulli equation implies that the total head, E , is constant (see Sect. 1.3.4). In this context, Eq. (4.1) gives that

$$H_1 + \frac{v_1^2}{2g} = H_2 + \frac{v_2^2}{2g} + \Delta z$$

where v_1 and v_2 are the fluid velocities upstream of the hump and above the hump, respectively, and H_2 is the fluid depth above the hump.

From the continuity equation we have that (recall Eq. (4.8))

$$v_1 = \frac{Q}{BH_1} \quad \text{and} \quad v_2 = \frac{Q}{BH_2}$$

where Q is the flow rate, to be determined.

It follows that

$$H_1 + \frac{Q^2}{2B^2H_1^2g} = H_2 + \frac{Q^2}{2B^2H_2^2g} + \Delta z$$

which can be rearranged to get

$$Q = \sqrt{\frac{2B^2g(H_1 - H_2 - \Delta z)}{H_2^{-2} - H_1^{-2}}} \quad (4.24)$$

Furthermore, $H_2 = H_1 - \Delta z - \Delta h$, such that

$$Q = \sqrt{\frac{2B^2g\Delta h}{(H_1 - \Delta z - \Delta h)^{-2} - H_1^{-2}}} = 5.578 \text{ m}^3\text{s}^{-1}$$

So the flow rate is $5.58 \text{ m}^3\text{s}^{-1}$.

Worked Solution 4.3 (see Problem 4.3)

(a) Let $B = 6$, $H_1 = 6 \text{ m}$, $H_2 = 1.2 \text{ m}$. Similar to as in Eq. (4.24), a combination of the Bernoulli equation and the continuity equation (i.e., Eqs. (4.1) and (4.8)) reveals that

$$Q = \sqrt{\frac{2B^2g(H_1 - H_2)}{H_2^{-2} - H_1^{-2}}}$$

which in this case (because $\Delta z = 0$) reduces further to

$$Q = BH_1H_2\sqrt{\frac{2g}{H_1 + H_2}} = 71.31 \text{ m}^3\text{s}^{-1}$$

So the flow rate is $71.3 \text{ m}^3\text{s}^{-1}$.

(b) Let $H_3 = 3.1 \text{ m}$. Also recall that the density of water, $\rho = 1000 \text{ kg m}^{-3}$. The force, F , exerted on the water by the blocks is found using the momentum equation combined with an assumption of hydrostatic pressure:

$$\frac{\rho g BH_2^2}{2} - \frac{\rho g BH_3^2}{2} - F = \rho Q(v_3 - v_2)$$

From the continuity equation we have that

$$v_2 = \frac{Q}{BH_2} \quad \text{and} \quad v_3 = \frac{Q}{BH_3}$$

so

$$\frac{\rho g B H_2^2}{2} - \frac{\rho g B H_3^2}{2} - F = \rho Q^2 \left(\frac{1}{B H_3} - \frac{1}{B H_2} \right)$$

which can be rearranged to get

$$F = \rho B (H_2 - H_3) \left[\frac{g(H_2 + H_3)}{2} - \frac{Q^2}{B^2 H_2 H_3} \right] = 192,400 \text{ N}$$

So the force exerted on the blocks is 192 kN.

Worked Solution 4.4 (see Problem 4.4)

Let $Q = 5.4 \text{ m}^3 \text{ s}^{-1}$, $B = 3.5 \text{ m}$, $H_1 = 0.38 \text{ m}$ and assume that the density of water, $\rho = 1000 \text{ kg m}^{-3}$.

Recall that total head is an energy per unit weight of fluid. Let ΔE be the total head lost in the hydraulic jump. The volume rate of flow is defined by Q . The mass rate of flow is defined by ρQ . It follows that the power dissipated by the hydraulic jump is found from $\rho g Q \Delta E$.

From Eq. (4.13), the downstream depth, $H_2 = 0.9560 \text{ m}$. The total head lost in the hydraulic jump is found from Eq. (4.17) with $\Delta z = 0$ because the channel is horizontal. It follows that

$$\rho g Q \Delta E = \frac{\rho g Q (H_2 - H_1)^3}{4 H_1 H_2} = 6965 \text{ W}$$

So the power dissipated by the jump is 6.97 kW.

Worked Solution 4.5 (see Problem 4.5)

Let $B = 1.5 \text{ m}$, $Q_1 = 0.85 \text{ m}^3 \text{ s}^{-1}$, $H_1 = 0.5 \text{ m}$ and $\Delta h = 0.15 \text{ m}$. Equation (4.22) gives us

$$(v_1 + c)^2 = g \left(\frac{H_1 + H_2}{2} \right) \frac{H_2}{H_1}$$

where v_1 is the upstream fluid velocity, c is the wave speed and H_2 is the downstream fluid depth.

Noting that

$$v_1 = \frac{Q_1}{B H_1} \quad \text{and} \quad H_2 = H_1 + \Delta h$$

it can be shown that

$$c = -\frac{Q_1}{B H_1} + \sqrt{g(H_1 + \Delta h) \left(1 + \frac{\Delta h}{2 H_1} \right)} = 1.575 \text{ m s}^{-1}$$

So the velocity of the wave is 1.56 m s^{-1} .

Recall from Eq.(4.18) that

$$BH_1(v_1 + c) = BH_2(v_2 + c)$$

where v_2 is the downstream velocity, which in turn is found from

$$v_2 = \frac{Q_2}{BH_2}$$

where Q_2 is the new flow rate we are seeking to determine.

It follows that

$$Q_2 = Q_1 - Bc\Delta h = 0.4957 \text{ m}^3\text{s}^{-1} = 0.496 \text{ m}^3\text{s}^{-1}$$

Worked Solution 4.6 (see Problem 4.6)

Let $B = 3 \text{ m}$, $n = 0.02 \text{ m}^{-\frac{1}{3}} \text{ s}$, $g = 9.81 \text{ m s}^{-2}$, $S_{0U} = 0.02$, $S_{0D} = 0.005$, $Q_a = 15 \text{ m}^3\text{s}^{-3}$ and $Q_b = 40 \text{ m}^3\text{s}^{-3}$. In this case, S_{0U} and S_{0D} represent the slope of the channel bed in the upstream and downstream portion of the channel system, respectively, whilst Q_a and Q_b represent the flow rates for scenario (a) and (b), respectively.

Recall that hydraulic jumps represent a transition from supercritical flow to sub-critical flow. Given that a hydraulic jump is present, the normal flow in the upstream channel portion must be supercritical (suggesting that the upstream bed slope should be classified as a steep slope, recall Table 3.2) whereas the the normal flow in the downstream channel portion must be sub-critical (suggesting that the downstream bed slope should be classified as a mild slope, recall Table 3.2).

In both cases (a) and (b), the hydraulic jump transforms a supercritical flow to a normal sub-critical flow. The hydraulic jumps locations can therefore be determined using the method described in Sect. 4.5.1. However, it is first necessary to determine whether the hydraulic jump occurs upstream or downstream of the bed slope change.

The critical fluid depth, H_c , can be obtained using Eq.(4.4). The normal fluid depths for the upstream and downstream slopes, H_{nU} and H_{nD} , respectively, can be determined using the `HnFun` function detailed in Listing 3.2. The associated conjugate fluid depths, $H_{nU\text{conj}}$ and $H_{nD\text{conj}}$, can be determined using Eq.(4.12).

The values of H_{nU} , H_{nD} , $H_{nU\text{conj}}$ and $H_{nD\text{conj}}$ can be used to determine whether the hydraulic jump occurs in the upstream or the downstream portion of the channel system.

If the hydraulic jump occurs in the mild downstream slope, a GVF profile will occur with $H \in [H_{nU}, H_{nD\text{conj}}]$. Furthermore, the GVF profile will be of M3 type (see Fig. 3.1), with fluid depth monotonically increasing with distance. Therefore a necessary condition for the hydraulic jump to occur in the downstream portion of the channel system is that $H_{nU} < H_{nD\text{conj}}$.

If the hydraulic jump occurs in the steep upstream slope, a GVF profile will occur with $H \in [H_{nU\text{conj}}, H_{nD}]$. Furthermore, the GVF profile will be of S1 type (see Fig. 3.1), with fluid depth monotonically increasing with distance. Therefore a

necessary condition for the hydraulic jump to occur in the upstream portion of the channel system is that $H_{nUconj} < H_{nD}$.

Similar to in Sect. 4.5.1, the exact location of the hydraulic jump can be determined using the GVFaFun function given in Listing 3.1.

If the hydraulic jump is in the downstream portion, we can set $S_0 = S_{0D}$, $s_1 = 0$ m (the location of the bed slope change), $H_1 = H_{nU}$ (because the fluid depth will be normal at the bed slope change) and $H_2 = H_{nDconj}$. The location, $s = s_{12}$, at which $H = H_{nDconj}$ represents the distance from the bed slope change to the hydraulic jump.

If the hydraulic jump is in the upstream portion, we can set $S_0 = S_{0U}$, $s_1 = 0$ m (the location of the bed slope change), $H_1 = H_{nD}$ (because the fluid depth will be normal at the bed slope change) and $H_2 = H_{nUconj}$. The location, $s = s_{12}$ [L], at which $H = H_{nUconj}$ represents the distance from the bed slope change to the hydraulic jump. Note that s_{12} will be negative in this case because the hydraulic jump is upstream of the bed slope change.

The above problem can be solved using the MATLAB code listed below:

```
B=3; %Breadth of channel (m)
n=0.02; %Manning coefficient (m-1/3 s)
g=9.81; %Gravitational acceleration (m/s2)
S0U=0.02; %Upstream bed slope (-)
S0D=0.005; %Downstream bed slope (-)
Qa=15; %Flow rate for part a) (m3/s)
Qb=40; %Flow rate for part b) (m3/s)
%Locate hydraulic jump for part a)
s12a=s12Fun(Qa,B,n,g,S0U,S0D)
%Locate hydraulic jump for part b)
s12b=s12Fun(Qb,B,n,g,S0U,S0D)
```

where the s12Fun function reads as follows:

```
function s12=s12Fun(Q,B,n,g,S0U,S0D)
%Determine the critical depth
Hc=(Q2/g/B2)(1/3);
%Determine the normal depths
HnU=HnFun(B,g,Hc,n,S0U); %Upstream slope
HnD=HnFun(B,g,Hc,n,S0D); %Downstream slope
%Determine corresponding conjugate depths
HnUCONJ=HnU/2*(-1+sqrt(1+8*(Hc/HnU)3));
HnDCONJ=HnD/2*(-1+sqrt(1+8*(Hc/HnD)3));
if HnU<HnDCONJ %Evaluate GVF on downstream slope
[H,s]=GVFaFun(HnU,HnDCONJ,0,B,g,Hc,n,S0D);
elseif HnUCONJ<HnD %Evaluate GVF on upstream slope
[H,s]=GVFaFun(HnD,HnUCONJ,0,B,g,Hc,n,S0U);
end
s12=s(end); %Location of hydraulic jump (m)
```

Table 4.1 Results for Problem 4.6

	(a)	(b)
$Q \text{ (m}^3 \text{ s}^{-1}\text{)}$	15	40
$H_{nU} \text{ (m)}$	0.9957	2.07
$H_{nUconj} \text{ (m)}$	1.819	3.276
$H_c \text{ (m)}$	1.366	2.627
$H_{nDconj} \text{ (m)}$	1.11	1.832
$H_{nD} \text{ (m)}$	1.658	3.625
$s_{12} \text{ (m)}$	11.15	−13.53

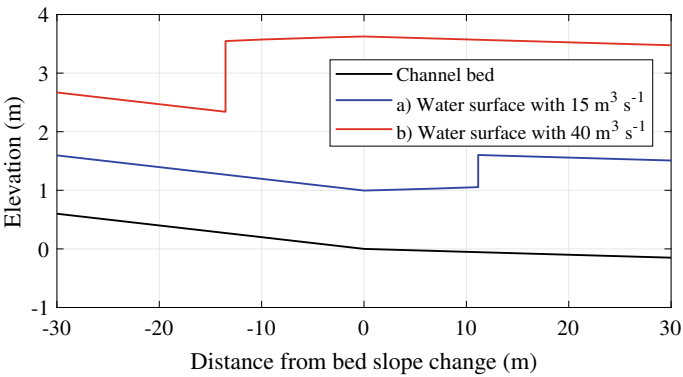


Fig. 4.4 Hydraulic jumps occurring due to a channel bed slope change with different flow rates

Key numerical results are shown in Table 4.1. Plots of water surface elevation against distance are shown in Fig. 4.4. When the flow rate is $15 \text{ m}^3 \text{ s}^{-1}$, $H_{nU} < H_{nDconj}$ and therefore the hydraulic jump occurs at a distance of 11.2 m downstream from the bed slope change. When the flow rate is $40 \text{ m}^3 \text{ s}^{-1}$, $H_{nUconj} < H_{nD}$ and therefore the hydraulic jump occurs at a distance of 13.5 m upstream from the bed slope change.

References

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Airy Waves and Basic Coastal Defence Design

5

Abstract

This chapter focuses on the derivation of Airy wave equations and how they can be used for coastal defence design. The steady-state Bernoulli equation is extended to account for transient flow conditions. A Laplace equation is derived by combining the concepts of mass conservation and velocity potential. Two dimensional Airy wave equations are derived using a separation of variables technique. Assumptions of constant wave-period and constant wave-power are used to derive shoaling equations for wavelength and wave-height. Empirical equations are provided to estimate deep-water wavelength and deep-water wave-height from wind-speed and wind-fetch data. A simple design method for sloped coastal defence systems is presented, based on wave-breaking and wave run-up criteria. Practical applications are presented through a problem sheet with worked solutions.

Notation

a	Acceleration [LT^{-2}].
A	Area [L^2].
$\hat{A}$	Mean cross-sectional area [L^2].
$c = \frac{L}{T}$	Wave celerity (i.e., wave speed) [LT^{-1}].
E_T	A transient form of total head [L].
F	Force [MLT^{-2}].
F_W	Wind-fetch [L].
g	Gravitational acceleration [LT^{-2}].
H	Wave-height [L].
H_0	Deep-water wave-height [L].
H_s	Significant wave-height [L].
$k = \frac{2\pi}{L}$	Wave number [L^{-1}].
L	Wavelength [L].
L_0	Deep-water wavelength [L].

p	Fluid pressure [$\text{ML}^{-1}\text{T}^{-2}$].
Q	Flow rate [L^3T^{-1}].
R	Wave-power [MLT^{-3}].
R_c	Mean freeboard [L].
R_{u2}	Run-up distance [L].
s	Distance along a streamtube [L].
t	Time [T].
T	Wave-period [T].
T_s	Significant wave-period [T].
u	Fluid velocity in the x -direction [LT^{-1}].
U_{10}	Wind-speed measured at 10 m above still-water level [LT^{-1}].
v	Fluid velocity in the y -direction or s -direction [LT^{-1}].
w	Fluid velocity in the z -direction [LT^{-1}].
x	Horizontal distance in the x -direction [L].
y	Horizontal distance in the y -direction [L].
z	Elevation [L].
β	Angle of a sloped sea-wall to the horizontal [-].
γ_f	Dimensionless roughness reduction factor [-].
ζ	Vertical displacement [L].
η	Water depth [L].
η_0	Still-water depth [L].
ξ	Horizontal displacement [L].
ξ_p	Iribarren number [-].
ρ	Mass density of a fluid [ML^{-3}].
φ	Velocity potential [L^2T^{-1}].

5.1 Introduction

Coastal defence is required to protect property from coastal flooding and to reduce coastal erosion of important coastline features. Coastal defence systems are generally designed to deal with a specified storm event in terms of wind speed and wind-fetch (the uninterrupted distance of open water over which the wind blows). Empirical equations are generally used to determine a deep-water wavelength and wave-height that will result from a given wind speed and wind-fetch.

As waves approach the shoreline, wavelengths decrease and the wave-heights increase. This process is known as shoaling. Shoaling equations are used to determine the wave-height that will be expected at the shoreline for a given deep-water wavelength and wave-height. Empirical equations are then used to estimate how far up a slope a wave will run once it reaches the shoreline. Estimates of wave run-up can be used to design key features of a coastal defence system.

This chapter concerns itself with the derivation of shoaling equations for basic coastal defence design using Airy wave theory. Section 5.2 details the derivation of the Airy wave equations. Section 5.3 derives shoaling equations to predict near-shore

wavelengths and wave-heights. Section 5.4 introduces important empirical equations commonly used to estimate wave run-up and wave breaking criteria for sloped coastal defence design.

5.2 Airy Wave Theory

Airy wave theory refers to linearised mathematical equations used to describe the spatial and temporal distribution of fluid velocity underneath sinusoidal waves imposed at a liquid surface. In this section, the concept of Bernoulli equation is extended to account for transient effects associated with transient waves, giving rise to a new term referred to as velocity potential. A Laplace equation, in terms of velocity potential, is then derived using the principle of mass conservation. An analytical solution for velocity potential is formed based on a linearised set of boundary conditions. This is finally used to derive a relationship between wave speed and fluid depth, often referred to as the Airy wave dispersion relation.

5.2.1 The Transient Bernoulli Equation

The Bernoulli equation gives that, for steady-state, incompressible and inviscid flow, the sum of the hydraulic head and velocity head is constant along a streamtube (see Sect. 1.3.4). However, the process of ocean waves moving to the shoreline is not a steady-state process. An analysis of ocean waves requires an alternative transient momentum equation and corresponding transient Bernoulli equation.

Consider again the control-volume (CV) in a streamtube described in Sect. 1.3.1. Under transient conditions, the expression for fluid acceleration, a [LT^{-2}], given by Eq. (1.36), becomes

$$a = \frac{\partial \hat{v}}{\partial t} + \frac{Q}{\hat{A}} \frac{\delta v}{\delta s} \quad (5.1)$$

where $\hat{v}$ [LT^{-1}] is the mean fluid velocity in the CV, t [T] is time, Q [L^3T^{-1}] is the volumetric flow rate of fluid through the streamtube, $\hat{A}$ [L^2] is the mean cross-sectional area of the CV, δv [LT^{-1}] is the change in fluid velocity that occurs along the CV and δs [L] is the length of the CV (see Fig. 1.11).

Substituting Eqs. (5.1) and (1.37) into Eq. (1.33) leads to

$$F = \rho \hat{A} \delta s \frac{\partial \hat{v}}{\partial t} + \rho Q \delta v \quad (5.2)$$

where F [MLT^{-2}] is the net-force acting on the CV in the s -direction and ρ [ML^{-3}] is the fluid density. Equation (5.2) represents a transient form of the momentum equation, given by Eq. (1.38).

Equating Eqs. (1.39) and (5.2) leads to

$$\rho \hat{A} \delta s \frac{\partial \hat{v}}{\partial t} + \rho Q \delta v = -\delta A p - (A + \delta A) \delta p - \hat{A} \rho g \delta z \quad (5.3)$$

where p [$\text{ML}^{-1}\text{T}^{-2}$] is fluid pressure, g [LT^{-2}] is gravitational acceleration and δz [L] is the change in elevation that occurs within the CV (see Fig. 1.11).

Equation (5.3) can be rearranged to get

$$\frac{p}{\hat{A}\rho g} \frac{\delta A}{\delta s} + \frac{(A + \delta A)}{\hat{A}\rho g} \frac{\delta p}{\delta s} + \frac{1}{g} \frac{\partial \hat{v}}{\partial t} + \frac{Q}{\hat{A}g} \frac{\delta v}{\delta s} + \frac{\delta z}{\delta s} = 0$$

If the CV is infinitesimally small (i.e., $\delta s \rightarrow 0$, $\delta A \rightarrow 0$, $\hat{A} \rightarrow A$, $\hat{v} \rightarrow v$) it can be further stated that

$$\frac{p}{A\rho g} \frac{\partial A}{\partial s} + \frac{1}{\rho g} \frac{\partial p}{\partial s} + \frac{1}{g} \frac{\partial v}{\partial t} + \frac{v}{g} \frac{\partial v}{\partial s} + \frac{\partial z}{\partial s} = 0$$

Furthermore, because a streamtube should be smoothly varying in cross-sectional area, $\frac{\partial A}{\partial s} \ll A$ and

$$\frac{1}{\rho g} \frac{\partial p}{\partial s} + \frac{1}{g} \frac{\partial v}{\partial t} + \frac{v}{g} \frac{\partial v}{\partial s} + \frac{\partial z}{\partial s} = 0 \quad (5.4)$$

where z [L] is elevation and s [L] is distance along the streamtube.

Integrating both sides of Eq. (5.4) with respect to s leads to the so-called transient Bernoulli equation [1, p. 578]

$$\frac{p}{\rho g} + \frac{1}{g} \frac{\partial \varphi}{\partial t} + \frac{v^2}{2g} + z = E_T \quad (5.5)$$

where E_T [L] is a term that is constant along the streamtube (analogous to total head) and φ [L^2T^{-1}] is known as the velocity potential and is defined by

$$\varphi = \int v ds. \quad (5.6)$$

5.2.2 Derivation of a Mass Conservation Equation

Now consider a new three-dimensional control-volume (CV) of fluid of dimensions, δx [L], δy [L] and δz [L], during a time-period, δt [T] (Fig. 5.1).

The mass of fluid entering the CV from outside is

$$\delta y \delta z \rho u \delta t + \delta x \delta z \rho v \delta t + \delta x \delta y \rho w \delta t$$

where u [LT^{-1}], v [LT^{-1}] and w [LT^{-1}] are the velocities in the x , y and z directions, respectively.

The mass of fluid exiting the CV is

$$\delta y \delta z [\rho u + \delta(\rho u)] \delta t + \delta x \delta z [\rho v + \delta(\rho v)] \delta t + \delta x \delta y [\rho w + \delta(\rho w)] \delta t$$

The consequential change in mass within the CV is

$$\delta x \delta y \delta z \delta \rho$$

The principle of mass conservation dictates that this change in mass is equal to the mass into the CV minus the mass out of the CV.

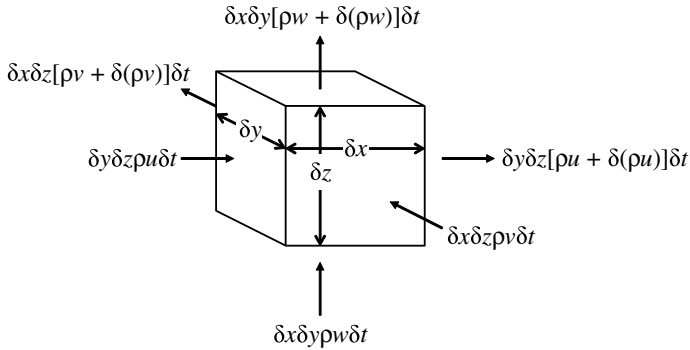


Fig. 5.1 Mass conservation for a three-dimensional control-volume

Challenge 5.1 Apply the principle of mass conservation to the CV shown in Fig. 5.1 to derive a partial differential equation (PDE) relating u , v and w for an incompressible fluid.

Applying the principle of mass conservation to the CV shown in Fig. 5.1 therefore leads to

$$\begin{aligned} \delta x \delta y \delta z \delta \rho &= \delta y \delta z \rho u \delta t + \delta x \delta z \rho v \delta t + \delta x \delta y \rho w \delta t \\ &\quad - \delta y \delta z [\rho u + \delta(\rho u)] \delta t - \delta x \delta z [\rho v + \delta(\rho v)] \delta t \\ &\quad - \delta x \delta y [\rho w + \delta(\rho w)] \delta t \end{aligned}$$

which can be rearranged and simplified to get

$$\frac{\delta \rho}{\delta t} = -\frac{\delta(\rho u)}{\delta x} - \frac{\delta(\rho v)}{\delta y} - \frac{\delta(\rho w)}{\delta z}$$

If both the time-period and the CV are taken to be infinitesimally small (i.e., $\delta t \rightarrow 0$, $\delta x \rightarrow 0$, $\delta y \rightarrow 0$, $\delta z \rightarrow 0$) then

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho u)}{\partial x} - \frac{\partial(\rho v)}{\partial y} - \frac{\partial(\rho w)}{\partial z}$$

and for an incompressible fluid

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \quad (5.7)$$

5.2.3 Transformation to a Laplace Equation

Recall the velocity potential term in the transient Bernoulli equation, Eq. (5.5). For a three-dimensional system, the velocity potential, φ [$L^2 T^{-1}$], is related to all three velocities as follows:

$$\frac{\partial \varphi}{\partial x} = u, \quad \frac{\partial \varphi}{\partial y} = v, \quad \frac{\partial \varphi}{\partial z} = w \quad (5.8)$$

Substituting Eq. (5.8) into Eq. (5.7) yields the Laplace equation

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} = 0 \quad (5.9)$$

The advantage of Eq. (5.9) as compared to Eq. (5.7) is that it has only one dependent variable and is therefore more straightforward to solve.

5.2.4 Conceptual Model for Airy Waves

Imagine a semi-infinite continuum of incompressible fluid with a free upper surface and bounded at $z = 0$ by a horizontal and impermeable base. The depth of the water, η [L], is described by

$$\eta = \eta_0 + \frac{H}{2} \sin \left[2\pi \left(\frac{x}{L} - \frac{t}{T} \right) \right] \quad (5.10)$$

where η_0 [L] is the still-water depth and H [L], L [L] and T [T] are the wave-height, wavelength and period of waves on the fluid surface (Fig. 5.2). Here we will use the Laplace equation, Eq. (5.9), to derive an analytical solution that describes the spatial and temporal distribution of velocity potential in such a system.

The first step is to recognise that there will be no velocity potential variation in the y -direction such that Eq. (5.9) reduces to

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial z^2} = 0 \quad (5.11)$$

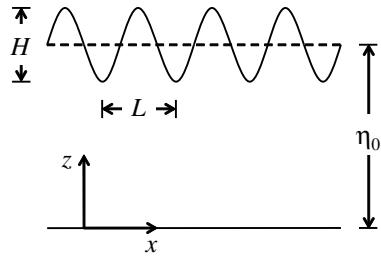
The next step is to recognise the boundary conditions:

$$\begin{aligned} w &= 0, \quad z = 0 \\ w &= \frac{d\eta}{dt}, \quad z = \eta \end{aligned}$$

The transient Bernoulli equation must also be satisfied (recall Eq. (5.5))

$$\frac{p}{\rho g} + \frac{1}{g} \frac{\partial \varphi}{\partial t} + \frac{u^2}{2g} + \frac{v^2}{2g} + \frac{w^2}{2g} + z = E_T$$

Fig. 5.2 Conceptual model for Airy waves



Making the assumptions that $H \ll L$ and $H \ll \eta_0$ leads to a linearisation of the boundary conditions (in which the smaller, higher order and product terms are neglected), which are then applied at the still-water level such that [2, p. 25]

$$\begin{aligned} w &= 0, \quad z = 0 \\ w &= \frac{\partial \eta}{\partial t}, \quad z = \eta_0 \end{aligned}$$

and the transient Bernoulli equation reduces to

$$\frac{p}{\rho g} + \frac{1}{g} \frac{\partial \phi}{\partial t} + z = \eta_0. \quad (5.12)$$

5.2.5 Analytical Solution

5.2.5.1 Separation of Variables

Challenge 5.2 Most methods of solving PDEs involve transforming a given PDE to a set of ordinary differential equations (ODE) and then using an ODE solution procedure. Assume that $\phi(x, z) = F(x)G(z)$. Then substitute $\phi(x, z) = F(x)G(z)$ into Eq. (5.11) and derive the two associated ODEs for F and G .

Let $\phi(x, z) = F(x)G(z)$ such that it can be said that

$$\frac{\partial^2 \phi}{\partial x^2} = G \frac{\partial^2 F}{\partial x^2} \quad \text{and} \quad \frac{\partial^2 \phi}{\partial z^2} = F \frac{\partial^2 G}{\partial z^2}$$

which, on substitution into Eq. (5.11) lead to

$$G \frac{\partial^2 F}{\partial x^2} + F \frac{\partial^2 G}{\partial z^2} = 0$$

Separating the z -factors and x -factors then gives us

$$\frac{1}{G} \frac{\partial^2 G}{\partial z^2} = -\frac{1}{F} \frac{\partial^2 F}{\partial x^2}$$

Since the left-hand-side of the above equation contains only z -factors and the right-hand-side of the above equation contains only x -factors both sides of the equation must in fact be constant in both x and z . Therefore let us say that

$$\frac{1}{G} \frac{\partial^2 G}{\partial z^2} = -\frac{1}{F} \frac{\partial^2 F}{\partial x^2} = k^2$$

where k is an, as yet, undetermined constant. With some further rearranging, the following set of ODEs (ordinary differential equations) is arrived:

$$\frac{\partial^2 F}{\partial x^2} = -k^2 F \quad (5.13)$$

$$\frac{\partial^2 G}{\partial z^2} = k^2 G. \quad (5.14)$$

5.2.5.2 General Solution

The general solution of an ODE of the form

$$a \frac{d^2 y}{dx^2} + b \frac{dy}{dx} + cy = 0 \quad (5.15)$$

is [3, p. 1093]

$$y(x) = A_1 \exp \left[\left(\frac{-b + \sqrt{b^2 - 4ac}}{2a} \right) x \right] + A_2 \exp \left[\left(\frac{-b - \sqrt{b^2 - 4ac}}{2a} \right) x \right] \quad (5.16)$$

where A_1 and A_2 are unknown constants defined by any associated boundary conditions.

Also note that:

$$\cos x = \frac{e^{ix} + e^{-ix}}{2} \quad \text{and} \quad \sin x = \frac{e^{ix} - e^{-ix}}{i2} \quad (5.17)$$

$$\cosh x = \frac{e^x + e^{-x}}{2} \quad \text{and} \quad \sinh x = \frac{e^x - e^{-x}}{2}. \quad (5.18)$$

Challenge 5.3 Determine general solutions for the ODEs given by Eqs. (5.13) and (5.14) and consequently a general solution for the PDE given by Eq. (5.11). Your final answers should be written in terms of trigonometric and hyperbolic functions.

By comparing Eqs. (5.13) and (5.15), it can be seen that $a = 1$, $b = 0$ and $c = k^2$. Equation (5.16) therefore gives that

$$F(x) = A_1 \exp(ikx) + A_2 \exp(-ikx)$$

Considering Eq. (5.17), it can be further stated that

$$F(x) = a_1 \cos(kx) + a_2 \sin(kx)$$

where $A_1 = \frac{a_1 - ia_2}{2}$ and $A_2 = \frac{a_1 + ia_2}{2}$.

By comparing Eqs. (5.14) and (5.15), it can be seen that $a = 1$, $b = 0$ and $c = -k^2$. Equation (5.16) therefore gives that

$$G(z) = B_1 \exp(kz) + B_2 \exp(-kz)$$

Considering Eq. (5.18), it can be further stated that

$$G(z) = b_1 \cosh(kz) + b_2 \sinh(kz)$$

where $B_1 = \frac{b_1 + b_2}{2}$ and $B_2 = \frac{b_1 - b_2}{2}$.

Given that $\varphi(x, z) = F(x)G(z)$, the general solution for Eq. (5.11) is therefore

$$\varphi = [a_1 \cos(kx) + a_2 \sin(kx)] [b_1 \cosh(kz) + b_2 \sinh(kz)] \quad (5.19)$$

where a_1 , a_2 , b_1 , b_2 and k are unknown constants yet to be determined.

5.2.5.3 Application of Boundary Conditions

Challenge 5.4 Eliminate one of the unknown constants in Eq. (5.19) by imposing the impermeable boundary condition at $z = 0$.

Given that the base of the domain is impermeable it can be said that

$$w = 0 \quad \text{at} \quad z = 0$$

and, recalling that $w = \partial\varphi/\partial z$,

$$\frac{\partial\varphi}{\partial z} = 0 \quad \text{at} \quad z = 0 \quad (5.20)$$

Partially differentiating Eq. (5.19) with respect to z leads to

$$\frac{\partial\varphi}{\partial z} = k [a_1 \cos(kx) + a_2 \sin(kx)] [b_1 \sinh(kz) + b_2 \cosh(kz)]$$

such that imposing Eq. (5.20) reveals that $b_2 = 0$ and

$$\varphi = b_1 \cosh(kz) [a_1 \cos(kx) + a_2 \sin(kx)]. \quad (5.21)$$

Challenge 5.5 Eliminate the remaining unknown constants in Eq. (5.21) by imposing that $w = \frac{\partial\eta}{\partial t}$ at $z = \eta_0$. You will benefit from applying the trigonometric identity $\cos(A + B) = \cos A \cos B - \sin A \sin B$.

We now wish to impose that $w = \frac{\partial\eta}{\partial t}$ at $z = \eta_0$. Partially differentiating Eq. (5.10) with respect to t yields

$$\frac{\partial\eta}{\partial t} = -\frac{\pi H}{T} \cos \left[2\pi \left(\frac{x}{L} - \frac{t}{T} \right) \right] \quad (5.22)$$

Partially differentiating Eq. (5.21) with respect to z yields

$$w = \frac{\partial\varphi}{\partial z} = kb_1 \sinh(kz) [a_1 \cos(kx) + a_2 \sin(kx)]$$

According to our boundary condition, $\frac{\partial\eta}{\partial t} = w$ at $z = \eta_0$, therefore

$$\frac{\partial\eta}{\partial t} = kb_1 \sinh(k\eta_0) [a_1 \cos(kx) + a_2 \sin(kx)] \quad (5.23)$$

Comparing Eqs. (5.22) and (5.23) it is clear that we should utilize the trigonometric identity

$$\cos(A + B) = \cos A \cos B - \sin A \sin B \quad (5.24)$$

because this enables us to say

$$\begin{aligned} \cos \left[2\pi \left(\frac{x}{L} - \frac{t}{T} \right) \right] &= \cos \left(\frac{2\pi x}{L} \right) \cos \left(-\frac{2\pi t}{T} \right) - \sin \left(\frac{2\pi x}{L} \right) \sin \left(-\frac{2\pi t}{T} \right) \\ &= \cos \left(\frac{2\pi x}{L} \right) \cos \left(\frac{2\pi t}{T} \right) + \sin \left(\frac{2\pi x}{L} \right) \sin \left(\frac{2\pi t}{T} \right) \end{aligned}$$

and therefore Eq. (5.22) can be written as

$$\frac{\partial \eta}{\partial t} = -\frac{\pi H}{T} \left[\cos\left(\frac{2\pi t}{T}\right) \cos\left(\frac{2\pi x}{L}\right) + \sin\left(\frac{2\pi t}{T}\right) \sin\left(\frac{2\pi x}{L}\right) \right] \quad (5.25)$$

Comparing Eqs. (5.23) and (5.25) it can then be seen that:

$$ka_1 b_1 \sinh(k\eta_0) = -\frac{\pi H}{T} \cos\left(\frac{2\pi t}{T}\right)$$

$$ka_2 b_1 \sinh(k\eta_0) = -\frac{\pi H}{T} \sin\left(\frac{2\pi t}{T}\right)$$

$$k = \frac{2\pi}{L}$$

and therefore:

$$a_1 b_1 = -\frac{cH \cos(-kct)}{2 \sinh(k\eta_0)}$$

$$a_1 b_2 = \frac{cH \sin(-kct)}{2 \sinh(k\eta_0)}$$

where $c = \frac{L}{T}$ [LT^{-1}], which is referred to as the wave celerity (or wave speed).

Substituting the above identities into Eq. (5.21) leads to

$$\varphi = -\frac{cH \cosh(kz)}{2 \sinh(k\eta_0)} [\cos(kx) \cos(-kct) - \sin(kx) \sin(-kct)]$$

Imposing the trigonometric identity in Eq. (5.24) again then leads to [1, p. 579]

$$\varphi(x, z, t) = -\frac{cH \cosh(kz) \cos[k(x - ct)]}{2 \sinh(k\eta_0)} \quad (5.26)$$

where

$$k = \frac{2\pi}{L} \quad (5.27)$$

and

$$c = \frac{L}{T}. \quad (5.28)$$

5.2.6 Displacement of Particles

Challenge 5.6 Determine expressions for the horizontal and vertical displacement, ξ [L] and ζ [L], respectively, of particles within the liquid.

Recall that

$$u = \frac{\partial x}{\partial t} = \frac{\partial \varphi}{\partial x}$$

and

$$w = \frac{\partial z}{\partial t} = \frac{\partial \varphi}{\partial z}$$

It follows that

$$\xi = \int u dt$$

and

$$\zeta = \int w dt$$

From Eq. (5.26) we have

$$u = \frac{ckH \cosh(kz) \sin[k(x - ct)]}{2 \sinh(k\eta_0)} \quad (5.29)$$

$$w = -\frac{ckH \sinh(kz) \cos[k(x - ct)]}{2 \sinh(k\eta_0)} \quad (5.30)$$

It follows that [1, p. 582]

$$\xi = \frac{H \cosh(kz) \cos[k(x - ct)]}{2 \sinh(k\eta_0)} \quad (5.31)$$

$$\zeta = \frac{H \sinh(kz) \sin[k(x - ct)]}{2 \sinh(k\eta_0)}. \quad (5.32)$$

5.2.7 The Airy Wave Dispersion Equation

Challenge 5.7 Substitute Eq. (5.26) into Eq. (5.12) for $z = \eta$ and derive a simplified equation relating c , k and η_0 .

At $z = \eta$, the pressure is atmospheric, which means the fluid pressure is zero, such that Eq. (5.12) reduces to

$$\frac{1}{g} \frac{\partial \varphi}{\partial t} \Big|_{z=\eta} + \eta = \eta_0 \quad (5.33)$$

Partially differentiating Eq. (5.26) with respect to time leads to

$$\frac{\partial \varphi}{\partial t} = -\frac{kc^2 H \cosh(kz) \sin[k(x - ct)]}{2 \sinh(k\eta_0)} \quad (5.34)$$

Because Eq. (5.26) is only valid for $z \in [0, \eta_0]$, it is necessary to assume that

$$\frac{\partial \varphi}{\partial t} \Big|_{z=\eta} = \frac{\partial \varphi}{\partial t} \Big|_{z=\eta_0} = -\frac{kc^2 H \sin[k(x - ct)]}{2 \tanh(k\eta_0)}$$

which on substitution into Eq. (5.33) along with Eq. (5.10) gives

$$-\frac{kc^2 H \sin[k(x - ct)]}{2g \tanh(k\eta_0)} + \eta_0 + \frac{H}{2} \sin[k(x - ct)] = \eta_0$$

from which it follows that [1, p. 579]

$$kc^2 = g \tanh(k\eta_0) \quad (5.35)$$

which is often referred to as the Airy wave dispersion equation.

5.2.8 Shallow-Water Approximation

Substituting the Maclaurin series, $\tanh x = x + O(x^3)$, into Eq. (5.35) leads to

$$c^2 = g\eta_0 + O(\eta_0^3) \quad (5.36)$$

which is analogous to our expression for shallow-water wave speed given by Eq. (4.23).

5.3 Wave Shoaling

As waves move from deep water conditions to a shoreline, they experience progressively shallower water depths. Wave shoaling is a term used to describe how water waves change with decreasing still-water depth, η_0 [L]. The wave-period, T [T], and wave-power, R [MLT^{-3}], are thought to remain constant whereas the wavelength, L [L], is expected to decrease whilst the wave-height, H [L], is expected to increase. Although Airy wave theory involves assuming a horizontal and impermeable base, it is often used to derive relevant shoaling equations to predict these processes [1,2].

Consider a set of waves moving towards a shoreline with η_0 becoming progressively smaller as the waves approach the shore. Let L_0 [L] and H_0 [L] be the wavelength and wave-height of the waves under deep-water conditions, respectively, i.e.,

$$\lim_{\eta_0 \rightarrow \infty} L = L_0 \quad \text{and} \quad \lim_{\eta_0 \rightarrow \infty} H = H_0$$

In what follows, we will use the Airy wave theory, derived in Sect. 5.2, in conjunction with the assumptions of constant T and constant R , to derive expressions for L and H in terms of L_0 , H_0 and η_0 .

5.3.1 Wave-Power

The wave power, R [MLT^{-3}], represents the mean rate (averaged over the wave-period) at which wave energy moves in the direction of wave propagation per unit-length of wave crest. It is given by

$$R = \frac{1}{T} \int_0^{\eta_0} \int_0^T p u d t d z. \quad (5.37)$$

Challenge 5.8 Use the transient Bernoulli equation, Eq. (5.12), to derive an expression for the pressure distribution within the liquid described by Eq. (5.26).

Substituting Eq. (5.34) into Eq. (5.12) leads to

$$\frac{p}{\rho g} - \frac{1}{g} \frac{k c^2 H \cosh(kz) \sin[k(x - ct)]}{2 \sinh(k\eta_0)} + z = \eta_0$$

which can be rearranged to get

$$p = \frac{\rho k c^2 H \cosh(kz) \sin[k(x - ct)]}{2 \sinh(k\eta_0)} + \rho g(\eta_0 - z)$$

Substituting Eq. (5.35) then leads to

$$p = \frac{\rho g H}{2} \frac{\cosh(kz)}{\cosh(k\eta_0)} \sin[k(x - ct)] + \rho g(\eta_0 - z). \quad (5.38)$$

Challenge 5.9 Evaluate an expression for R given Eqs. (5.29), (5.37) and (5.38).

To obtain an expression for R we need to integrate the product, pu , with respect to t . Multiplying the expression for p in Eq. (5.38) by the expression for u in Eq. (5.29) and integrating with respect to t from zero to T leads to

$$\begin{aligned} \int_0^T p u dt &= \int_0^T \left[\frac{\rho g H}{2} \frac{\cosh(kz)}{\cosh(k\eta_0)} \sin[k(x - ct)] + \rho g(\eta_0 - z) \right] \frac{ck H \cosh(kz) \sin[k(x - ct)]}{2 \sinh(k\eta_0)} dt \\ &= \frac{\rho g ck H}{2} \int_0^T \left[\frac{H \cosh^2(kz) \sin^2[k(x - ct)]}{2 \cosh(k\eta_0) \sinh(k\eta_0)} + \frac{(\eta_0 - z) \cosh(kz) \sin[k(x - ct)]}{\sinh(k\eta_0)} \right] dt \end{aligned}$$

Noting that

$$\int \sin^2[k(x - ct)] dt = \frac{t}{2} + \frac{\sin[2k(x - ct)]}{4kc}$$

we then get

$$\begin{aligned} \int_0^T p u dt &= \frac{\rho g ck H}{2} \left[\frac{H \cosh^2(kz) [2kct + \sin[2k(x - ct)]]}{8kc \cosh(k\eta_0) \sinh(k\eta_0)} + \frac{(\eta_0 - z) \cosh(kz) \cos[k(x - ct)]}{kc \sinh(k\eta_0)} \right]_0^T \\ &= \frac{\rho g ck H^2 \cosh^2(kz) T}{8 \cosh(k\eta_0) \sinh(k\eta_0)} \end{aligned} \quad (5.39)$$

Substituting Eq. (5.39) into Eq. (5.37) finally leads to

$$\begin{aligned} R &= \frac{\rho g ck H^2}{8 \cosh(k\eta_0) \sinh(k\eta_0)} \int_0^{\eta_0} \cosh^2(kz) dz \\ &= \frac{\rho g ck H^2}{8 \cosh(k\eta_0) \sinh(k\eta_0)} \left[\frac{z}{2} + \frac{\sinh(2kz)}{4k} \right]_0^{\eta_0} \\ &= \frac{\rho g ck H^2}{8 \cosh(k\eta_0) \sinh(k\eta_0)} \left[\frac{\eta_0}{2} + \frac{\sinh(2k\eta_0)}{4k} \right] \end{aligned}$$

Noting that $\sinh(2k\eta_0) = 2 \cosh(k\eta_0) \sinh(k\eta_0)$ it further follows that [1, p. 584]

$$R = \frac{\rho g c H^2}{16} [1 + 2k\eta_0 \operatorname{csch}(2k\eta_0)]. \quad (5.40)$$

5.3.2 Wavelength Equation

Challenge 5.10 Use the constant wave-period assumption in conjunction with the Airy wave dispersion equation, Eq. (5.35), to derive a relationship between wavelength, L , still-water depth, η_0 , and deep-water wavelength, L_0 .

Here we will derive a relationship between wavelength, L , still-water depth, η_0 and deep-water wavelength, L_0 . Our starting point is the Airy wave dispersion equation, Eq. (5.35). Substituting Eqs. (5.27) and (5.28) into Eq. (5.35) leads to

$$L = \frac{gT^2}{2\pi} \tanh\left(\frac{2\pi\eta_0}{L}\right) \quad (5.41)$$

Recall that

$$\lim_{\eta_0 \rightarrow \infty} L = L_0$$

where L_0 is the deep-water wavelength.

It turns out that

$$\lim_{x \rightarrow \infty} \tanh x = 1$$

from which it follows that

$$L_0 = \frac{gT^2}{2\pi} \quad (5.42)$$

Given that we can assume the wave-period is constant, substituting Eq. (5.42) into Eq. (5.41) leads to

$$L = L_0 \tanh\left(\frac{2\pi\eta_0}{L}\right) \quad (5.43)$$

Values of L for given values of η_0 and L_0 can be obtained by iterative solution of Eq. (5.43). Alternatively, L can be interpolated from the data given in Table 5.1.

Table 5.1 Corresponding values of L/L_0 and η_0/L_0 according to Eq. (5.43)

L/L_0	η_0/L_0
0.05	0.0003982
0.1	0.001597
0.2	0.006453
0.3	0.01478
0.4	0.02697
0.5	0.04371
0.6	0.06619
0.7	0.09662
0.8	0.1399
0.9	0.2109
0.95	0.2770

5.3.3 Wave-Height Equation

Challenge 5.11 Use the constant wave-period and constant wave-power assumptions in conjunction with the wave-power equation, Eq. (5.40), to derive a relationship between wave-height, H , wavelength, L , still-water depth, η_0 , deep-water wavelength, L_0 , and deep-water wave-height, H_0 .

Here we will derive a relationship between wave-height, H , wavelength, L , still-water depth, η_0 , deep-water wavelength, L_0 , and deep-water wave-height, H_0 . Our starting point is the wave-power equation, Eq. (5.40). Substituting Eqs. (5.27) and (5.28) into Eq. (5.40) leads to

$$R = \frac{\rho g L H^2}{16T} \left[1 + \frac{4\pi\eta_0}{L} \operatorname{csch} \left(\frac{4\pi\eta_0}{L} \right) \right] \quad (5.44)$$

Recall that

$$\lim_{\eta_0 \rightarrow \infty} L = L_0 \quad \text{and} \quad \lim_{\eta_0 \rightarrow \infty} H = H_0$$

It turns out that

$$\lim_{x \rightarrow \infty} x \operatorname{csch} x = 0$$

from which it follows that

$$R = \frac{\rho g L_0 H_0^2}{16T} \quad (5.45)$$

Given that we can assume both the wave-period and wave-power are constant, substituting Eq. (5.45) into Eq. (5.44) and solving for H leads to

$$H = H_0 \sqrt{\frac{L_0}{L} \left[1 + \frac{4\pi\eta_0}{L} \operatorname{csch} \left(\frac{4\pi\eta_0}{L} \right) \right]^{-1}} \quad (5.46)$$

where L should be determined by iterative solution of Eq. (5.43) or interpolated from the data provided in Table 5.1.

5.3.4 Shallow-Water Approximation

Under shallow-water conditions, η_0 is small. Noting the Maclaurin series

$$\tanh x = x + O(x^3)$$

Equation (5.43) can be expanded as follows

$$L = \frac{2\pi L_0 \eta_0}{L} + O \left(\frac{2\pi \eta_0}{L} \right)^3$$

and therefore

$$L = \sqrt{2\pi L_0 \eta_0} + O \left(\frac{2\pi \eta_0}{L} \right)$$

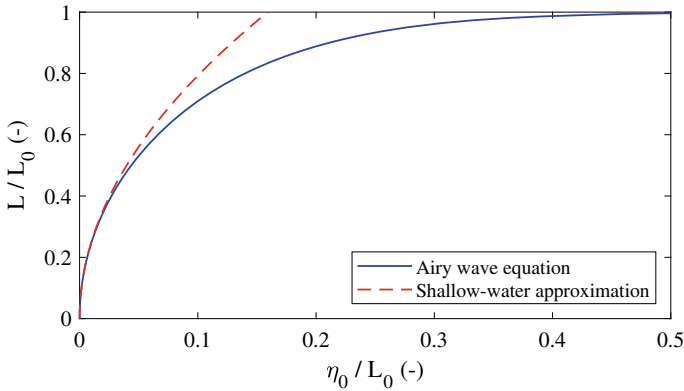


Fig. 5.3 Plot of normalised wavelength, L/L_0 , against normalized fluid depth, η_0/L_0 , using both the Airy wave equation, Eq. (5.43), and the shallow-water approximation, Eq. (5.47)

The shallow-water approximation of Eq. (5.43) is therefore

$$L \approx \sqrt{2\pi L_0 \eta_0} \quad (5.47)$$

which has the obvious advantage over Eq. (5.43), in that L can be determined explicitly from η_0 and L_0 .

A graphical comparison of Eqs. (5.43) and (5.47) is presented in Fig. 5.3, from which it can be seen that the shallow-water approximation becomes reasonable when $\frac{\eta_0}{L_0} < 0.03$.

5.4 Empirical Equations for Design

5.4.1 Significant Wave-Period and Wave-Height

Marine waves are largely treated as a stochastic process and characterised by statistical distributions. An important piece of work in this context is the Joint North Sea Wave Project (JONSWAP), which enables the estimation of significant wave-period, T_s [T], and significant wave-height, H_s [L], for a given wind-speed (measured at 10 m above still-water level), U_{10} [LT^{-1}] and wind-fetch, F_W [L].

The wind-fetch represents the uninterrupted distance of open water over which the wind blows. In this context, the significant wave-period and wave-height are generally defined as the mean wave-period and wave-height of the highest third of waves in a sample.

The relevant equations read as follows [1, pp. 598 and 600]:

$$T_s = \frac{0.777}{f_m} \quad (5.48)$$

and

$$H_s = \frac{0.552g\alpha^{1/2}}{\pi^2 f_m^2} \quad (5.49)$$

where

$$f_m = \frac{3.5g}{U_{10}} \left(\frac{U_{10}^2}{gF_W} \right)^{0.33} \quad (5.50)$$

and

$$\alpha = 0.076 \left(\frac{U_{10}^2}{gF_W} \right)^{0.22} \quad (5.51)$$

The significant wave-height, H_s , is thought to represent the deep-water wave-height, H_0 (i.e., $H_s = H_0$). The significant wave-period, T_s , is thought to be independent of fluid depth (i.e., $T_s = T$). Therefore the corresponding deep-water wavelength, $L_0 = gT_s^2/(2\pi)$ (recall Eq. (5.42)). Wave-height, H , and wavelength, L , for a given still-water depth, η_0 , can be found from Eqs. (5.46) and (5.43), respectively.

5.4.2 Critical Slope for Wave-Breaking

Wave-breaking is an important aspect of coastal protection. It enables the energy of the waves to be dissipated in turbulence within a controlled region, which can be protected by armour material, thus reducing the effects of coastal erosion elsewhere. Vertical sea-walls lead to wave reflection. Wave-breaking can be induced by reducing the slope of sea-walls.

Whether or not waves break is strongly controlled by the so-called Iribarren number, ξ_p [-], defined by [4, p. 492]

$$\xi_p = \frac{\tan \beta}{\sqrt{H/L_0}} \quad (5.52)$$

where β [-] is the angle of a sloped sea-wall to the horizontal and H is the wave-height at the foot of a sloped sea-wall and L_0 is the corresponding deep-water wavelength.

The critical slope for wave-breaking is generally found by ensuring that

$$\xi_p < 2. \quad (5.53)$$

5.4.3 Wave Run-Up

The height of a sea-wall is often constrained by the amount that incoming breaking waves run-up the sea-side slope. A commonly applied empirical equation in this context is that of [5] (see [4, p. 492]):

$$R_{u2} = \begin{cases} 1.6\gamma_f \xi_p, & \xi_p < 2.5 \\ \gamma_f(4.5 - 0.2\xi_p), & \xi_p > 2.5 \end{cases} \quad (5.54)$$

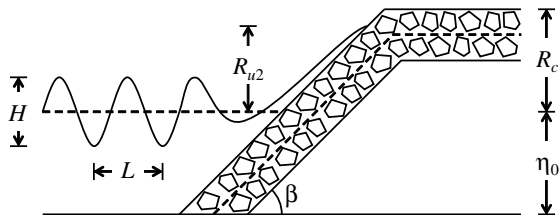


Fig. 5.4 Schematic diagram of a sloped coastal defence with a two layer armourstone revetment

Table 5.2 Values of roughness reduction factor, γ_f [4, p. 494]

Armour unit	γ_f (–)
Concrete, asphalt and grass	1.0
Pitched stone	0.80–0.95
One layer of armourstone	0.70
Two layers of armourstone	0.55

where R_{u2} [L] is the run-up distance and γ_f [–] is a dimensionless roughness reduction factor. The run-up distance, R_{u2} , is defined as the vertical height above sea-water level beyond which only 2% of incoming waves are expected to over-top (Fig. 5.4). The roughness factor, γ_f , describes the energy absorbing capacity of different materials and can be determined from Table 5.2.

5.5 Problem Sheet

Problem 5.1 (see Worked Solution 5.1)

A surface-water wave is characterised by a wavelength of 4 m, a wave-height of 0.6 m and a wave-period of 100 s. The still-water level is 1 m above the sea-bed.

- (a) Write a MATLAB code to show 20 equal-interval contours of velocity potential over one full wavelength from sea-bed to seawater surface when $t = 0$. Also plot the elevation of the seawater surface on top of the velocity potential contours for comparison.
- (b) Extend your MATLAB code to show the pathways of four particles located with mean elevations of 0.1, 0.3, 0.5 and 0.9 m above the sea-bed and a mean x -value of 1.0 m.

Problem 5.2 (see Worked Solution 5.2)

Write a MATLAB code to determine the wavelength that would be expected for a still-water depth of 4 m, given a deep-water wavelength of 34.5 m.

Problem 5.3 (see Worked Solution 5.3)

At a depth of 20 m, waves of height 1.31 m and period 7 s are observed to travel inshore. Determine the wavelength and wave-height that would be expected (a) in deep-water conditions, and (b) at the toe of a sloped sea-wall where the water depth is 4 m.

Problem 5.4 (see Worked Solution 5.4)

A storm in deep water generates waves which travel towards the shore impinging on a breakwater where the still-water depth is 8 m. The storm is fetch-limited and has a wind speed of 10 m s^{-1} and a wind-fetch of 100 km. The breakwater is protected by rock revetment with a slope of $1/3$. Determine the wavelength and wave-height to be expected at the breakwater location and assess whether the waves will break on the revetment.

Problem 5.5 (see Worked Solution 5.5)

Estimate the wave run-up on a concrete embankment, with a slope of $1/4$, resulting from waves of height 0.8 m with a period of (a) 10 s and (b) 3 s.

Problem 5.6 (see Worked Solution 5.6)

Design a sloped sea-wall to deal with wind speeds of up to 50 km h^{-1} assuming a wind-fetch of 100 km and a still-water depth of 3.5 m. Specifically, determine the maximum slope to ensure wave-breaking and the minimum crest-height to prevent 98% of waves from over-topping and choose an appropriate level of precision.

5.6 Worked Solutions

Worked Solution 5.1 (see Problem 5.1)

(a) The following MATLAB code generates a φ contour plot using Eq. (5.26):

```
%Specify input parameters:
L=4; %Wavelength (m)
T=100; %Wave-period (s)
H=0.6; %Wave-height (m)
eta0=1; %Still-water depth (m)
%Specify location of points
x=linspace(0,L,100);
z=linspace(0,eta0,50);
%Replicate points to enable array
multiplication
[z,x]=ndgrid(z,x);
%Determine auxiliary parameters
k=2*pi/L;
c=L/T;
%Determine velocity potential
v=-c*H*cosh(k*z).*cos(k*x)/2/sinh(k*eta0);
%Determine the water-depth (m)
eta=eta0+H/2*sin(k*x);
%Rescale from 0<z<eta0 to 0<z<eta
z=z.*eta/eta0;
%Display results
figure(1);clf;hold on;box on;axis equal
contour(x,z,v,20,'r')
plot(x(1,:),eta(1:,:), 'b')
xlabel('Horizontal distance (m)')
ylabel('Elevation (m)')
```

(b) The following MATLAB code will plot the particle pathways using Eqs. (5.31) and (5.32):

```
%Specify mean location of particles
x0=L/4;
z0=[0.1 0.3 0.5 0.9]*eta0;
%Develop 50 equally-spaced time points
across the entire wave-period.
t=linspace(0,T,50)';
%Evaluate xi and zeta
u=k*(x0-c*t);
xi=H*cosh(k*z0).*cos(u)/2./sinh(k*eta0);
zeta=H*sinh(k*z0).*sin(u)/2./sinh(k*eta0);
```

```
%Plot the particle pathways on top of the
%velocity potential contours
plot(xi+x0,zeta+z0,'k')
legend('Velocity potential contours',...
'Water depth','Particle paths')
```

The results to part (a) and (b) are shown in Fig. 5.5.

Worked Solution 5.2 (see Problem 5.2)

The following MATLAB code can be used to determine the wavelength, L , for a given still-water depth, η_0 , and a given deep-water wavelength, L_0 , from Eq. (5.43):

```
eta0=4; %Still-water depth (m)
L0=34.5; %Deep-water wavelength (m)
L=fzero(@(L) L-L0*tanh(2*pi*eta0/L),L0/2)
```

The corresponding wavelength is found to be 25.9 m.

Worked Solution 5.3 (see Problem 5.3)

(a) Let $\eta_0 = 20$ m, $H = 1.31$ m and $T = 7$ s. Considering Eq. (5.42), the deep-water wavelength, L_0 , can be obtained as follows:

$$L_0 = \frac{gT^2}{2\pi} = 76.50 \text{ m}$$

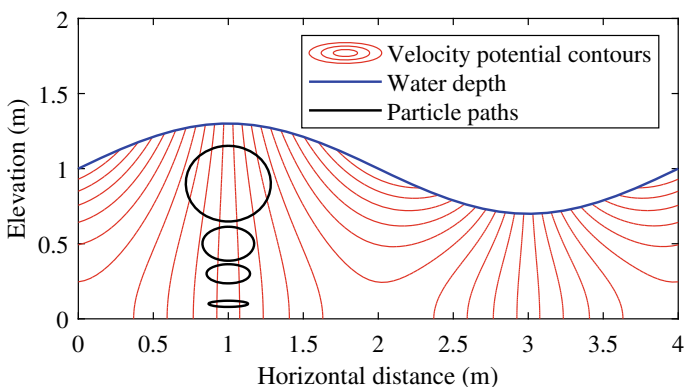


Fig. 5.5 Contour plot of velocity potential (obtained using Eq. (5.26)) and particle trajectories (obtained using Eqs. (5.31) and (5.32)) for Airy waves

Given $\eta_0/L_0 = 0.2614$, inspection of Table 5.1 reveals that $L/L_0 = 0.9409$ and therefore that the wavelength (where $\eta_0 = 20$ m), $L = 71.98$ m. Considering Eq. (5.46), the deep-water wave-height, H_0 , can be obtained from

$$H_0 = H \sqrt{\frac{L}{L_0} \left[1 + \frac{4\pi\eta_0}{L} \operatorname{csch} \left(\frac{4\pi\eta_0}{L} \right) \right]} = 1.399 \text{ m}$$

So the deep-water wavelength and wave-height are 76.5 m and 1.40 m, respectively.

(b) Let $\eta_0 = 4$ m, $L_0 = 76.50$ m and $H_0 = 1.399$ m. Given $\eta_0/L_0 = 0.05228$, inspection of Table 5.1 reveals that $L/L_0 = 0.5417$ and therefore that the wavelength (where $\eta_0 = 4$ m), $L = 41.44$ m. Considering Eq. (5.46), the wave-height, H , can be obtained from

$$H = H_0 \sqrt{\frac{L_0}{L} \left[1 + \frac{4\pi\eta_0}{L} \operatorname{csch} \left(\frac{4\pi\eta_0}{L} \right) \right]} = 1.421 \text{ m}$$

So at 4 m water depth, the wavelength and wave-height are 41.4 m and 1.42 m, respectively.

Worked Solution 5.4 (see Problem 5.4)

Let $\eta_0 = 8$ m, $U_{10} = 10 \text{ m s}^{-1}$, $F_W = 100,000$ m and $\tan \beta = 1/3$. From Eq. (5.50), $f_m = 0.1654$ Hz. From Eq. (5.51), $\alpha = 0.01006$. From Eq. (5.48), $T = 4.698$ s. From Eq. (5.49), $H_0 = 2.012$ m. From Eq. (5.42), $L_0 = 34.46$ m. Given that $\eta_0/L_0 = 0.2321$, Table 5.1 reveals that $L/L_0 = 0.9196$ and therefore that the wavelength, $L = 31.69$ m. From Eq. (5.46), $H = 1.865$ m. So the wavelength and wave-height at the breakwater location are 31.7 m and 1.87 m, respectively. From Eq. (5.52), $\xi_p = 1.433$, which is less than 2, therefore the waves are expected to break on the revetment.

Worked Solution 5.5 (see Problem 5.5)

(a) Let $\tan \beta = 1/4$, $H = 0.8$ m and $T = 10$ s. From Eq. (5.42), the deep-water wavelength, $L_0 = 156.1$ m. From Eq. (5.52), the Iribarren number, $\xi_p = 3.493$. Given that the slope is concrete, Table 5.2 gives that $\gamma_f = 1.0$. From Eq. (5.54), the wave run-up, $R_{u2} = 3.80$ m.

(b) Let $\tan \beta = 1/4$, $H = 0.8$ m and $T = 3$ s. From Eq. (5.42), the deep-water wavelength, $L_0 = 14.05$ m. From Eq. (5.52), the Iribarren number, $\xi_p = 1.048$. Given that the slope is concrete, Table 5.2 gives that $\gamma_f = 1.0$. From Eq. (5.54), the wave run-up, $R_{u2} = 1.68$ m.

Worked Solution 5.6 (see Problem 5.6)

Let $\eta_0 = 3.5$ m, $U_{10} = 13.89$ m s⁻¹ and $F_W = 100,000$ m. From Eq. (5.50), $f_m = 0.1479$ Hz. From Eq. (5.51), $\alpha = 0.01163$. From Eq. (5.48), $T = 5.253$ s. From Eq. (5.49), $H_0 = 2.704$ m. From Eq. (5.42), $L_0 = 43.09$ m. Given that $\eta_0/L_0 = 0.08123$, Table 5.1 reveals that $L/L_0 = 0.6534$ and therefore that the wavelength, $L = 28.15$ m. From Eq. (5.46), $H = 2.577$ m.

For wave-breaking, the Iribarren number, ξ_p , must be less than 2 (recall Eq. (5.53)). It follows from Eq. (5.52) that

$$\cot \beta > \sqrt{\frac{L_0}{4H}} = 2.045$$

where β is the angle of the sloped revetment to the horizontal.

For design purposes it is worth to round $\cot \beta$ up to the nearest half. Therefore we will choose that $\cot \beta = 2.5$. From Eq. (5.52), the Iribarren number, $\xi_p = 1.636$. From Table 5.2, it can be understood that the run-up will be minimised if we use two layers of armourstone such that $\gamma_f = 0.55$. From Eq. (5.54), it can then be determined that the wave run-up, $R_{u2} = 1.439$ m. For design purposes it is worth to round the crest-height up to the nearest 0.5 m. Therefore, we will choose the crest-height to be 1.5 m above still-water level.

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Shallow-Water Equations

6

Abstract

This chapter focuses on the derivation of shallow-water equations commonly used to describe water movement through flood plains and river channel networks. The Cauchy momentum equation is derived by combining a three-dimensional stress balance with Newton's second law. The Navier Stokes equations are developed by incorporating a viscosity relationship between deviatoric stress and fluid velocity. Shallow water equations are derived by vertically averaging the Navier Stokes equations using Leibniz's theorem for differentiation of an integral. Eddy viscosities are used to obtain simplified approximations for the associated internal deviatoric stress terms and differential advection terms. Wall shear stress is represented using a Darcy–Weisbach-type skin friction model. The Saint Venant equations are derived by assuming one-dimensional open channel flow. Three additional approximations are considered including the gradually varied flow equation (referred to as a quasi-steady approximation), the diffusion wave equation and the kinematic wave equation. The Ogata–Banks solution is presented as an analytical solution for the diffusion wave equation and used to explore some practical applications, presented through a problem sheet with worked solutions.

Notation

a	Acceleration vector [LT^{-2}].
a_x	Acceleration in the x -direction [LT^{-2}].
a_y	Acceleration in the y -direction [LT^{-2}].
a_z	Acceleration in the z -direction [LT^{-2}].
A	Area [L^2].
B	Breadth [L].
c	Wave speed [LT^{-1}].
f	Friction factor [-].
f_c	Coriolis parameter [T^{-1}].

F	Force vector [MLT^{-2}].
F_x	Force in the x -direction [MLT^{-2}].
F_y	Force in the y -direction [MLT^{-2}].
F_z	Force in the z -direction [MLT^{-2}].
g	Regional acceleration vector [LT^{-2}].
g	Gravitational acceleration [LT^{-2}].
g_x	Regional acceleration in the x -direction [LT^{-2}].
g_y	Regional acceleration in the y -direction [LT^{-2}].
g_z	Regional acceleration in the z -direction [LT^{-2}].
h	Water surface elevation [L].
$H(t)$	Heaviside step function [-].
K	Apparent diffusion coefficient [L^2T^{-1}].
m	Hydraulic radius [L].
n	Manning's coefficient [$\text{L}^{-\frac{1}{3}}\text{T}$].
p	Fluid pressure [$\text{ML}^{-1}\text{T}^{-2}$].
Pe	Peclet number [-].
Q	Flow rate [L^3T^{-1}].
Q_0	Boundary flow rate [L^3T^{-1}].
Q_I	Initial flow rate [L^3T^{-1}].
S_0	Bed slope [-].
S_f	Friction slope [-].
t	Time [T].
t_0	Duration of flow rate perturbation [T].
u	Fluid velocity vector [LT^{-1}].
u	Fluid velocity in the x -direction [LT^{-1}].
$\bar{u}$	Vertically averaged fluid velocity in the x -direction [LT^{-1}].
u'	Fluctuations of fluid velocity in the x -direction [LT^{-1}].
v	Fluid velocity in the y -direction [LT^{-1}].
$\bar{v}$	Vertically averaged fluid velocity in the y -direction [LT^{-1}].
v'	Fluctuations of fluid velocity in the y -direction [LT^{-1}].
w	Fluid velocity in the z -direction [LT^{-1}].
x	Horizontal distance in the x -direction [L].
y	Horizontal distance in the y -direction [L].
z	Elevation [L].
ζ	Elevation of the base of a water body [L].
η	Water depth [L].
κ	Volumetric viscosity [$\text{ML}^{-1}\text{T}^{-1}$].
λ	Lamé-type parameter [$\text{ML}^{-1}\text{T}^{-1}$].
μ	Kinematic viscosity [$\text{ML}^{-1}\text{T}^{-1}$].
ν_{Ex}	Eddy viscosity in the x -direction [L^2T^{-1}].
ν_{Ey}	Eddy viscosity in the y -direction [L^2T^{-1}].
ρ	Mass density of a fluid [ML^{-3}].
σ	Stress tensor [$\text{ML}^{-1}\text{T}^{-2}$].
σ_{xx}	Normal stress in the x -direction acting on a face normal to the x -direction [$\text{ML}^{-1}\text{T}^{-2}$].

σ_{xy}	Shear stress in the y -direction acting on a face normal to the x -direction [$ML^{-1}T^{-2}$].
σ_{xz}	Shear stress in the z -direction acting on a face normal to the x -direction [$ML^{-1}T^{-2}$].
σ_{yx}	Shear stress in the x -direction acting on a face normal to the y -direction [$ML^{-1}T^{-2}$].
σ_{yy}	Normal stress in the y -direction acting on a face normal to the y -direction [$ML^{-1}T^{-2}$].
σ_{yz}	Shear stress in the z -direction acting on a face normal to the y -direction [$ML^{-1}T^{-2}$].
σ_{zx}	Shear stress in the x -direction acting on a face normal to the z -direction [$ML^{-1}T^{-2}$].
σ_{zy}	Shear stress in the y -direction acting on a face normal to the z -direction [$ML^{-1}T^{-2}$].
σ_{zz}	Normal stress in the z -direction acting on a face normal to the z -direction [$ML^{-1}T^{-2}$].
τ	Dimensionless time [-].
$\boldsymbol{\tau}$	Deviatoric stress tensor [$ML^{-1}T^{-2}$].
τ_{xx}	Deviatoric stress in the x -direction acting on a face normal to the x -direction [$ML^{-1}T^{-2}$].
τ_{xy}	Deviatoric stress in the y -direction acting on a face normal to the x -direction [$ML^{-1}T^{-2}$].
τ_{xz}	Deviatoric stress in the z -direction acting on a face normal to the x -direction [$ML^{-1}T^{-2}$].
τ_{yx}	Deviatoric stress in the x -direction acting on a face normal to the y -direction [$ML^{-1}T^{-2}$].
τ_{yy}	Deviatoric stress in the y -direction acting on a face normal to the y -direction [$ML^{-1}T^{-2}$].
τ_{yz}	Deviatoric stress in the z -direction acting on a face normal to the y -direction [$ML^{-1}T^{-2}$].
τ_{zx}	Deviatoric stress in the x -direction acting on a face normal to the z -direction [$ML^{-1}T^{-2}$].
τ_{zy}	Deviatoric stress in the y -direction acting on a face normal to the z -direction [$ML^{-1}T^{-2}$].
τ_{zz}	Deviatoric stress in the z -direction acting on a face normal to the z -direction [$ML^{-1}T^{-2}$].
τ_{0x}	Frictional shear stress applied tangential to a lower water boundary in the x -direction [$ML^{-1}T^{-2}$].
τ_{0y}	Frictional shear stress applied tangential to a lower water boundary in the y -direction [$ML^{-1}T^{-2}$].
τ_{sx}	Frictional shear stress applied tangential to an upper water boundary in the x -direction [$ML^{-1}T^{-2}$].
τ_{sy}	Frictional shear stress applied tangential to an upper water boundary in the y -direction [$ML^{-1}T^{-2}$].

$\bar{\tau}_{xx}$	Vertically averaged deviatoric stress in the x -direction acting on a face normal to the x -direction $[\text{ML}^{-1}\text{T}^{-2}]$.
$\bar{\tau}_{xy}$	Vertically averaged deviatoric stress in the y -direction acting on a face normal to the x -direction $[\text{ML}^{-1}\text{T}^{-2}]$.
$\bar{\tau}_{yx}$	Vertically averaged deviatoric stress in the x -direction acting on a face normal to the y -direction $[\text{ML}^{-1}\text{T}^{-2}]$.
$\bar{\tau}_{yy}$	Vertically averaged deviatoric stress in the y -direction acting on a face normal to the y -direction $[\text{ML}^{-1}\text{T}^{-2}]$.
φ	Latitude $[-]$.
ω	Sidereal angular velocity $[\text{T}^{-1}]$.

6.1 Introduction

Many numerical modelling packages are available to simulate water movement through flood plains and river channel networks (e.g. [1–3]). Such models typically involve numerical solutions of shallow water equations [4]. These models play an important role in flood management [5], flood forecasting [6] and the development of flood risk maps [7].

This chapter is concerned with the derivation of shallow water equations. Newton's second law is applied to a three-dimensional control volume to derive the Cauchy momentum equation. The Cauchy momentum equation is combined with a generalised viscosity equation to derive the Navier Stokes equations. Shallow-water equations are obtained by assuming a hydrostatic pressure profile and integrating the Navier Stokes equations with respect to elevation.

The shallow-water equations are further simplified by assuming one-dimensional flow, giving rise to the Saint Venant equations. Additional assumptions associated with the friction slope then lead to the diffusion wave equation and the kinematic wave equation. Analytical solutions for the kinematic wave equation and the diffusion wave equation are presented in Chaps. 7 and 8, respectively. Numerical solutions for both the diffusion wave equation and kinematic wave equation are presented in Chap. 10.

6.2 The Cauchy Momentum Equation

Let σ $[\text{ML}^{-1}\text{T}^{-2}]$ be a matrix containing all the stresses acting on a point within a substance, i.e.

$$\sigma = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix}$$

There are two types of stress, normal stress and shear stress:

- σ_{xx} Normal stress in the x -direction acting on a face normal to the x -direction.
- σ_{xy} Shear stress in the y -direction acting on a face normal to the x -direction.
- σ_{xz} Shear stress in the z -direction acting on a face normal to the x -direction.
- σ_{yx} Shear stress in the x -direction acting on a face normal to the y -direction.
- σ_{yy} Normal stress in the y -direction acting on a face normal to the y -direction.
- σ_{yz} Shear stress in the z -direction acting on a face normal to the y -direction.
- σ_{zx} Shear stress in the x -direction acting on a face normal to the z -direction.
- σ_{zy} Shear stress in the y -direction acting on a face normal to the z -direction.
- σ_{zz} Normal stress in the z -direction acting on a face normal to the z -direction.

Now consider a control-volume of substance with dimensions, δx [L], δy [L] and δz [L], in the x , y and z directions, respectively. A corner of the control-volume (CV) is located at a reference point located at (x, y, z) and the corner of the CV furthest away from the reference point is located at $(x + \delta x, y + \delta y, z + \delta z)$.

First we will consider forces acting in the x direction. Let σ_{xx} [$\text{ML}^{-1}\text{T}^{-2}$], σ_{yx} [$\text{ML}^{-1}\text{T}^{-2}$] and σ_{zx} [$\text{ML}^{-1}\text{T}^{-2}$] be the stresses acting in the x direction on the CV faces that share the corner at (x, y, z) and are normal to the x , y and z directions, respectively. The stresses acting on the associated opposite faces are $\sigma_{xx} + \delta\sigma_{xx}$, $\sigma_{yx} + \delta\sigma_{yx}$ and $\sigma_{zx} + \delta\sigma_{zx}$, respectively. In addition to these stresses, the CV is also subject to a body force, $\delta x \delta y \delta z \rho g_x$, where ρ [ML^{-3}] is the density of the substance and g_x [LT^{-2}] is a regional acceleration in the x direction associated with gravity and/or Coriolis effects.

6.2.1 Net Forces in x , y and z Direction

Challenge 6.1 Determine an expression for the net force acting in the x -direction, F_x [MLT^{-2}].

The net force acting in the x -direction, F_x [MLT^{-2}], is found from

$$\begin{aligned}
 F_x &= -\delta y \delta z \sigma_{xx} - \delta x \delta z \sigma_{yx} - \delta x \delta y \sigma_{zx} + \delta y \delta z (\sigma_{xx} + \delta\sigma_{xx}) \\
 &\quad + \delta x \delta z (\sigma_{yx} + \delta\sigma_{yx}) + \delta x \delta y (\sigma_{zx} + \delta\sigma_{zx}) + \delta x \delta y \delta z \rho g_x \\
 &= \delta y \delta z \delta\sigma_{xx} + \delta x \delta z \delta\sigma_{yx} + \delta x \delta y \delta\sigma_{zx} + \delta x \delta y \delta z \rho g_x \\
 &= \delta x \delta y \delta z \left(\frac{\delta\sigma_{xx}}{\delta x} + \frac{\delta\sigma_{yx}}{\delta y} + \frac{\delta\sigma_{zx}}{\delta z} + \rho g_x \right)
 \end{aligned} \tag{6.1}$$

Challenge 6.2 Determine similar expressions for the net force acting in the y and z directions, F_y [MLT^{-2}] and F_z [MLT^{-2}], respectively.

Let σ_{xy} [$\text{ML}^{-1}\text{T}^{-2}$], σ_{yy} [$\text{ML}^{-1}\text{T}^{-2}$] and σ_{zy} [$\text{ML}^{-1}\text{T}^{-2}$] be the stresses acting in the y direction on the CV faces that share the corner at (x, y, z) and are normal to the x , y and z directions, respectively, and g_y [LT^{-2}] be the regional acceleration (associated with gravity and/or Coriolis effects) in the y direction. A corresponding expression for the net force acting in the y direction, F_y [MLT^{-2}], is

$$F_y = \delta x \delta y \delta z \left(\frac{\delta \sigma_{xy}}{\delta x} + \frac{\delta \sigma_{yy}}{\delta y} + \frac{\delta \sigma_{zy}}{\delta z} + \rho g_y \right) \quad (6.2)$$

Let σ_{xz} [$\text{ML}^{-1}\text{T}^{-2}$], σ_{yz} [$\text{ML}^{-1}\text{T}^{-2}$] and σ_{zz} [$\text{ML}^{-1}\text{T}^{-2}$] be the stresses acting in the z direction on the CV faces that share the corner at (x, y, z) and are normal to the x , y and z directions, respectively, and g_z [LT^{-2}] be the regional acceleration (associated with gravity and/or Coriolis effects) in the z direction. A corresponding expression for the net force acting in the z direction, F_z [MLT^{-2}], is

$$F_z = \delta x \delta y \delta z \left(\frac{\delta \sigma_{xz}}{\delta x} + \frac{\delta \sigma_{yz}}{\delta y} + \frac{\delta \sigma_{zz}}{\delta z} + \rho g_z \right). \quad (6.3)$$

6.2.2 Application of Newton's Second Law

Suppose that particles in the control-volume experience a local acceleration, $\mathbf{a}$ [LT^{-2}], where

$$\mathbf{a} = a_x \mathbf{i} + a_y \mathbf{j} + a_z \mathbf{k}$$

with a_x [LT^{-2}], a_y [LT^{-2}] and a_z [LT^{-2}] representing the local accelerations in the x , y and z directions, respectively.

Newton's second law gives that

$$\mathbf{F} = \delta x \delta y \delta z \rho \mathbf{a} \quad (6.4)$$

where

$$\mathbf{F} = F_x \mathbf{i} + F_y \mathbf{j} + F_z \mathbf{k}$$

Challenge 6.3 Derive an expression for $\mathbf{a}$ in terms of the stress tensor, $\boldsymbol{\sigma}$, and the regional acceleration vector $\mathbf{g}$.

Equating Eq. (6.4) with Eqs. (6.1), (6.2) and (6.3) leads to

$$\begin{aligned}\delta x \delta y \delta z \rho a_x &= \delta x \delta y \delta z \left(\frac{\delta \sigma_{xx}}{\delta x} + \frac{\delta \sigma_{yx}}{\delta y} + \frac{\delta \sigma_{zx}}{\delta z} + \rho g_x \right) \\ \delta x \delta y \delta z \rho a_y &= \delta x \delta y \delta z \left(\frac{\delta \sigma_{xy}}{\delta x} + \frac{\delta \sigma_{yy}}{\delta y} + \frac{\delta \sigma_{zy}}{\delta z} + \rho g_y \right) \\ \delta x \delta y \delta z \rho a_z &= \delta x \delta y \delta z \left(\frac{\delta \sigma_{xz}}{\delta x} + \frac{\delta \sigma_{yz}}{\delta y} + \frac{\delta \sigma_{zz}}{\delta z} + \rho g_z \right)\end{aligned}$$

which can be simplified to get:

$$\begin{aligned}\rho a_x &= \frac{\delta \sigma_{xx}}{\delta x} + \frac{\delta \sigma_{yx}}{\delta y} + \frac{\delta \sigma_{zx}}{\delta z} + \rho g_x \\ \rho a_y &= \frac{\delta \sigma_{xy}}{\delta x} + \frac{\delta \sigma_{yy}}{\delta y} + \frac{\delta \sigma_{zy}}{\delta z} + \rho g_y \\ \rho a_z &= \frac{\delta \sigma_{xz}}{\delta x} + \frac{\delta \sigma_{yz}}{\delta y} + \frac{\delta \sigma_{zz}}{\delta z} + \rho g_z\end{aligned}$$

At this stage it would be useful to exploit vector calculus notation so that we can introduce the stress tensor, $\boldsymbol{\sigma}$. To do this we need to make the CV infinitesimally small such that $\delta x \rightarrow 0$, $\delta y \rightarrow 0$ and $\delta z \rightarrow 0$. This is useful because

$$\lim_{\delta i \rightarrow 0} \frac{\delta \sigma_{ij}}{\delta i} = \frac{\partial \sigma_{ij}}{\partial i}$$

where $i = x, y, z$ and $j = x, y, z$.

In this way, it can be understood that:

$$\begin{aligned}\rho a_x &= \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} + \rho g_x \\ \rho a_y &= \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} + \rho g_y \\ \rho a_z &= \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} + \rho g_z\end{aligned}$$

Noting that

$$\nabla \cdot \boldsymbol{\sigma} = \begin{bmatrix} \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \\ \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \\ \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \end{bmatrix}$$

and

$$\mathbf{g} = g_x \mathbf{i} + g_y \mathbf{j} + g_z \mathbf{k}$$

it follows that [8, p. 80]

$$\rho \mathbf{a} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g} \quad (6.5)$$

which is commonly referred to as the Cauchy momentum equation.

6.3 Navier Stokes Equations

The Navier Stokes equations are a form of the Cauchy momentum equation used to describe the movement of fluids in terms of a fluid velocity vector, $\mathbf{u}$, where

$$\mathbf{u} = u\mathbf{i} + v\mathbf{j} + w\mathbf{k}$$

and u [LT^{-1}], v [LT^{-1}] and w [LT^{-1}] are the fluid velocities in the x , y and z direction, respectively.

In this context (assuming the z axis is normal to the Earth's surface)

$$\mathbf{a} \equiv \frac{d\mathbf{u}}{dt} = \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \quad (6.6)$$

$$\boldsymbol{\sigma} = \boldsymbol{\tau} - p\mathbf{I} \quad (6.7)$$

and

$$\mathbf{g} = f_c v \mathbf{i} - f_c u \mathbf{j} + g \mathbf{k} \quad (6.8)$$

where $\boldsymbol{\tau}$ [$\text{ML}^{-1}\text{T}^{-2}$] is referred to as the deviatoric stress tensor, p [$\text{ML}^{-1}\text{T}^{-2}$] is fluid pressure, f_c [T^{-1}] is the Coriolis parameter and g [LT^{-2}] is gravitational acceleration.

The Coriolis effect accounts for the fact that the spatial coordinate system is attached to the Earth, which is rotating around its axis. The Coriolis parameter, f_c , is found from [1, p. 77]

$$f_c = 2\omega \sin \varphi \quad (6.9)$$

where $\omega = 7.292 \times 10^{-5} \text{ s}^{-1}$ is the sidereal angular velocity of the Earth and φ is the latitude.

The deviatoric stress tensor can be related to the fluid velocity vector by the following generalised viscosity equation [8, p. 18]:

$$\boldsymbol{\tau} = \mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] + \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} \quad (6.10)$$

where μ [$\text{ML}^{-1}\text{T}^{-1}$] is the kinematic viscosity and λ [$\text{ML}^{-1}\text{T}^{-1}$] is a Lamé-type parameter, which in turn can be related to the so-called, volumetric viscosity, κ [$\text{ML}^{-1}\text{T}^{-1}$], by the expression

$$\lambda = \kappa - \frac{2\mu}{3}$$

Equation (6.10) is clearly analogous to Hooke's law with μ and κ being analogous to shear modulus and bulk modulus, respectively (e.g. [9, p. 109]). [8] argue that it is known from kinetic theory that κ is identically zero for monatomic gases at low viscosity. In the field of hydraulics, κ is also typically set to zero.

Challenge 6.4 Use the above set of equations to re-write the Cauchy momentum equation (Eq. (6.5)) in terms fluid velocity and fluid pressure.

Substituting Eqs. (6.6) and (6.7) into Eq. (6.5) leads to [8, p. 84]

$$\rho \frac{d\mathbf{u}}{dt} = \nabla \cdot \boldsymbol{\tau} - \nabla p + \rho \mathbf{g} \quad (6.11)$$

Substituting Eq. (6.10) then leads to

$$\rho \frac{d\mathbf{u}}{dt} = \nabla \cdot [\mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] + \lambda (\nabla \cdot \mathbf{u}) \mathbf{I}] - \nabla p + \rho \mathbf{g} \quad (6.12)$$

The above equation represents what is commonly referred to as the full Navier Stokes equations.

6.3.1 Constant Viscosity

Challenge 6.5 Assume that both μ and λ are constant and simplify Eq. (6.12) accordingly.

If we assume that μ and λ are uniform, Eq. (6.12) reduces to

$$\rho \frac{d\mathbf{u}}{dt} = \mu \nabla \cdot (\nabla \mathbf{u}) + \mu \nabla \cdot [(\nabla \mathbf{u})^T] + \lambda \nabla \cdot [(\nabla \cdot \mathbf{u}) \mathbf{I}] - \nabla p + \rho \mathbf{g}$$

Interestingly, it can be shown that:

$$\nabla \cdot (\nabla \mathbf{u}) = \nabla^2 \mathbf{u}$$

and

$$\nabla \cdot [(\nabla \mathbf{u})^T] = \nabla \cdot [(\nabla \cdot \mathbf{u}) \mathbf{I}] = \nabla (\nabla \cdot \mathbf{u})$$

It follows that

$$\rho \frac{d\mathbf{u}}{dt} = \mu \nabla^2 \mathbf{u} + (\mu + \lambda) \nabla (\nabla \cdot \mathbf{u}) - \nabla p + \rho \mathbf{g}. \quad (6.13)$$

6.3.2 Constant Density and Viscosity

Challenge 6.6 Now assume that ρ , μ and λ are constant and simplify Eq. (6.13) accordingly.

To understand the implications of setting ρ as constant, we need to revisit the mass conservation equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u})$$

When ρ is constant, the above equation reduces to the continuity equation

$$\nabla \cdot \mathbf{u} = 0 \quad (6.14)$$

It follows that Eq. (6.13) reduces to [8, p. 84]

$$\rho \frac{d\mathbf{u}}{dt} = \mu \nabla^2 \mathbf{u} - \nabla p + \rho \mathbf{g}. \quad (6.15)$$

6.4 Shallow-Water Equations

For studies of water movement in rivers, lakes and estuaries it is common to employ a two-dimensional vertically integrated set of equations. The resulting simplified equations are referred to as shallow-water equations [4].

Let $\zeta(x, y)$ [L] represent the elevation (above a given datum) of the base of a water body (e.g. a river bed) and $h(x, y, t)$ [L] represent the elevation of the overlying water surface. The corresponding water depth, $\eta = h - \zeta$. In this context, the following boundary conditions apply:

$$\begin{aligned}
 \frac{d\zeta}{dt} &= w, & z &= \zeta \\
 \tau_{0x} &= -\tau_{xx} \frac{\partial \zeta}{\partial x} - \tau_{yx} \frac{\partial \zeta}{\partial y} + \tau_{zx}, & z &= \zeta \\
 \tau_{0y} &= -\tau_{xy} \frac{\partial \zeta}{\partial x} - \tau_{yy} \frac{\partial \zeta}{\partial y} + \tau_{zy}, & z &= \zeta \\
 \frac{dh}{dt} &= w, & z &= h \\
 \tau_{sx} &= -\tau_{xx} \frac{\partial h}{\partial x} - \tau_{yx} \frac{\partial h}{\partial y} + \tau_{zx}, & z &= h \\
 \tau_{sy} &= -\tau_{xy} \frac{\partial h}{\partial x} - \tau_{yy} \frac{\partial h}{\partial y} + \tau_{zy}, & z &= h
 \end{aligned} \tag{6.16}$$

where τ_{0x} [$\text{ML}^{-1}\text{T}^{-2}$], τ_{sx} [$\text{ML}^{-1}\text{T}^{-2}$], τ_{0y} [$\text{ML}^{-1}\text{T}^{-2}$] and τ_{sy} [$\text{ML}^{-1}\text{T}^{-2}$] represent the frictional shear stresses applied tangential to the lower and upper water boundaries in the x and y directions, respectively.

Furthermore, it is assumed that fluid pressure is assumed hydrostatic in the vertical direction such that

$$p = \rho g(h - z), \quad z \in [\zeta, h] \tag{6.17}$$

Vertical integration of the continuity equation and the Navier Stokes equations is achieved using Leibniz's theorem for differentiation of an integral [10, p. 11]

$$\frac{d}{dc} \int_{\zeta}^h f(z, c) dz = \int_{\zeta}^h \frac{\partial f}{\partial c} dz + f(h, c) \frac{dh}{dc} - f(\zeta, c) \frac{d\zeta}{dc} \tag{6.18}$$

hereafter referred to as the Leibniz integral rule.

Following vertical integration, the resulting simplified equations will be written in terms of vertically averaged quantities such as

$$\bar{f}(x, y, t) = \frac{1}{\eta} \int_{\zeta}^h f(x, y, z, t) dz. \tag{6.19}$$

6.4.1 Continuity Equation

Challenge 6.7 Use the Leibniz integral rule to vertically integrate the continuity equation, Eq. (6.14), from ζ to h and invoke the relevant boundary conditions given by Eq. (6.16).

Integrating both sides of Eq. (6.14) with respect to z from ζ to h leads to

$$\int_{\zeta}^h \frac{\partial u}{\partial x} dz + \int_{\zeta}^h \frac{\partial v}{\partial y} dz + \int_{\zeta}^h \frac{\partial w}{\partial z} dz = 0 \quad (6.20)$$

From the Leibniz integral rule (Eq. (6.18)) we have that

$$\int_{\zeta}^h \frac{\partial u}{\partial x} dz = \frac{\partial(\eta \bar{u})}{\partial x} + [u]_{z=\zeta} \frac{\partial \zeta}{\partial x} - [u]_{z=h} \frac{dh}{dx} \quad (6.21)$$

and

$$\int_{\zeta}^h \frac{\partial v}{\partial y} dz = \frac{\partial(\eta \bar{v})}{\partial y} + [v]_{z=\zeta} \frac{\partial \zeta}{\partial y} - [v]_{z=h} \frac{dh}{dy} \quad (6.22)$$

where

$$\bar{u}(x, y, t) = \frac{1}{\eta} \int_{\zeta}^h u(x, y, z, t) dz$$

and

$$\bar{v}(x, y, t) = \frac{1}{\eta} \int_{\zeta}^h v(x, y, z, t) dz$$

Invoking the relevant boundary conditions in Eq. (6.16) it can be seen that

$$\int_{\zeta}^h \frac{\partial w}{\partial z} dz = [w]_{z=h} - [w]_{z=\zeta} = \frac{dh}{dt} - \frac{d\zeta}{dt}$$

Noting that

$$\frac{dh}{dt} = \frac{\partial h}{\partial t} + [u]_{z=h} \frac{\partial h}{\partial x} + [v]_{z=h} \frac{\partial h}{\partial y}$$

and

$$\frac{d\zeta}{dt} = \frac{\partial \zeta}{\partial t} + [u]_{z=\zeta} \frac{\partial \zeta}{\partial x} + [v]_{z=\zeta} \frac{\partial \zeta}{\partial y}$$

it follows that

$$\begin{aligned} \int_{\zeta}^h \frac{\partial w}{\partial z} dz &= \frac{\partial \eta}{\partial t} + [u]_{z=h} \frac{\partial h}{\partial x} + [v]_{z=h} \frac{\partial h}{\partial y} \\ &\quad - [u]_{z=\zeta} \frac{\partial \zeta}{\partial x} - [v]_{z=\zeta} \frac{\partial \zeta}{\partial y} \end{aligned} \quad (6.23)$$

Substituting Eqs. (6.21), (6.22) and (6.23) into Eq. (6.20) then leads to

$$\frac{\partial(\eta \bar{u})}{\partial x} + \frac{\partial(\eta \bar{v})}{\partial y} + \frac{\partial \eta}{\partial t} = 0. \quad (6.24)$$

6.4.2 Momentum Equations

Vertically integrated forms of the momentum equations are obtained by integrating both sides of Eq. (6.11), i.e.,

$$\int_{\zeta}^h \rho \frac{d\mathbf{u}}{dt} dz = \int_{\zeta}^h \nabla \cdot \boldsymbol{\tau} dz - \int_{\zeta}^h \nabla p dz + \int_{\zeta}^h \rho \mathbf{g} dz \quad (6.25)$$

Note that the vertical integration makes the third row of each vector redundant so only the first two rows are relevant.

6.4.2.1 Body Force Terms

Considering Eq. (6.8), vertical integration of the body force terms in Eq. (6.25) simply leads to:

$$\int_{\zeta}^h \rho f_c v dz = \rho f_c \eta \bar{v} \quad (6.26)$$

and

$$-\int_{\zeta}^h \rho f_c u dz = -\rho f_c \eta \bar{u}. \quad (6.27)$$

6.4.2.2 Pressure Gradient Terms

Challenge 6.8 Derive simplified expressions for the vertically integrated pressure gradient term in Eq. (6.25).

Applying the Leibniz integral rule to the first row of the integrated pressure gradient term in Eq. (6.25) leads to

$$\int_{\zeta}^h \frac{\partial p}{\partial x} dz = \frac{\partial}{\partial x} \left(\int_{\zeta}^h p dz \right) + [p]_{z=\zeta} \frac{\partial \zeta}{\partial x} - [p]_{z=h} \frac{\partial h}{\partial x}$$

Substituting Eq. (6.17) then yields

$$\begin{aligned} \int_{\zeta}^h \frac{\partial p}{\partial x} dz &= \rho g \left[\frac{\partial}{\partial x} \left(\int_{\zeta}^h (h - z) dz \right) + \eta \frac{\partial \zeta}{\partial x} \right] \\ &= \rho g \left[\frac{\partial}{\partial x} \left(\left[hz - \frac{z^2}{2} \right]_{\zeta}^h \right) + \eta \frac{\partial \zeta}{\partial x} \right] \\ &= \rho g \left[\frac{\partial}{\partial x} \left(h^2 - \frac{h^2}{2} - h\zeta + \frac{\zeta^2}{2} \right) + \eta \frac{\partial \zeta}{\partial x} \right] \\ &= \rho g \left[\frac{1}{2} \frac{\partial \eta^2}{\partial x} + \eta \frac{\partial \zeta}{\partial x} \right] \\ &= \rho g \eta \frac{\partial h}{\partial x} \end{aligned} \quad (6.28)$$

A corresponding expression for the second row of the integrated pressure gradient term takes the form

$$\int_{\zeta}^h \frac{\partial p}{\partial y} dz = \rho g \eta \frac{\partial h}{\partial y}. \quad (6.29)$$

6.4.2.3 Deviatoric Stress Divergence Terms

Challenge 6.9 Derive simplified expressions for the vertically integrated deviatoric stress divergence term in Eq. (6.25), and apply the boundary conditions in Eq. (6.16) where appropriate.

Applying the Leibniz integral rule to the first row of the $\nabla \cdot \boldsymbol{\tau}$ term in Eq. (6.25) leads to

$$\int_{\zeta}^h \nabla \cdot \boldsymbol{\tau} dz \cdot \mathbf{i} = \int_{\zeta}^h \frac{\partial \tau_{xx}}{\partial x} dz + \int_{\zeta}^h \frac{\partial \tau_{yx}}{\partial y} dz + \int_{\zeta}^h \frac{\partial \tau_{zx}}{\partial z} dz \quad (6.30)$$

From Eq. (6.18) we have that

$$\int_{\zeta}^h \frac{\partial \tau_{xx}}{\partial x} dz = \frac{\partial(\eta \bar{\tau}_{xx})}{\partial x} + [\tau_{xx}]_{z=\zeta} \frac{\partial \zeta}{\partial x} - [\tau_{xx}]_{z=h} \frac{dh}{dx} \quad (6.31)$$

and

$$\int_{\zeta}^h \frac{\partial \tau_{yx}}{\partial y} dz = \frac{\partial(\eta \bar{\tau}_{yx})}{\partial y} + [\tau_{yx}]_{z=\zeta} \frac{\partial \zeta}{\partial y} - [\tau_{yx}]_{z=h} \frac{dh}{dy} \quad (6.32)$$

where

$$\bar{\tau}_{xx}(x, y, t) = \frac{1}{\eta} \int_{\zeta}^h \tau_{xx}(x, y, z, t) dz$$

and

$$\bar{\tau}_{yx}(x, y, t) = \frac{1}{\eta} \int_{\zeta}^h \tau_{yx}(x, y, z, t) dz$$

Furthermore, it can be understood that

$$\int_{\zeta}^h \frac{\partial \tau_{zx}}{\partial z} dz = [\tau_{zx}]_{z=h} - [\tau_{zx}]_{z=\zeta} \quad (6.33)$$

Substituting Eqs. (6.31), (6.32) and (6.33) into Eq. (6.30) and invoking the relevant boundary conditions in Eq. (6.16) then leads to

$$\int_{\zeta}^h \nabla \cdot \boldsymbol{\tau} dz \cdot \mathbf{i} = \frac{\partial(\eta \bar{\tau}_{xx})}{\partial x} + \frac{\partial(\eta \bar{\tau}_{yx})}{\partial y} + \tau_{sx} - \tau_{0x} \quad (6.34)$$

A corresponding expression for the second row of the vertically integrated deviatoric stress divergence term takes the form

$$\int_{\zeta}^h \nabla \cdot \boldsymbol{\tau} dz \cdot \mathbf{j} = \frac{\partial(\eta \bar{\tau}_{xy})}{\partial x} + \frac{\partial(\eta \bar{\tau}_{yy})}{\partial y} + \tau_{sy} - \tau_{0y}. \quad (6.35)$$

6.4.2.4 The Acceleration Terms

Evaluating the vertically integrated acceleration terms in Eq. (6.25) requires a number of quite complicated steps. Consider first of all

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z}$$

Multiplying both sides of the continuity equation, Eq. (6.14), by u leads to

$$u \frac{\partial u}{\partial x} + u \frac{\partial v}{\partial y} + u \frac{\partial w}{\partial z} = 0$$

It follows that

$$\begin{aligned}\frac{du}{dt} &= \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} + u \frac{\partial v}{\partial x} + u \frac{\partial v}{\partial y} + u \frac{\partial w}{\partial z} \\ &= \frac{\partial u}{\partial t} + \frac{\partial(u^2)}{\partial x} + \frac{\partial(uv)}{\partial y} + \frac{\partial(uw)}{\partial z}\end{aligned}$$

The Leibniz integral rule (Eq. (6.18)) tells us that:

$$\begin{aligned}\int_{\zeta}^h \frac{\partial u}{\partial t} dz &= \frac{\partial(\eta \bar{u})}{\partial t} + [u]_{z=\zeta} \frac{\partial \zeta}{\partial t} - [u]_{z=h} \frac{\partial h}{\partial t} \\ \int_{\zeta}^h \frac{\partial(u^2)}{\partial x} dz &= \frac{\partial(\eta \overline{u^2})}{\partial x} + [u^2]_{z=\zeta} \frac{\partial \zeta}{\partial x} - [u^2]_{z=h} \frac{\partial h}{\partial x} \\ \int_{\zeta}^h \frac{\partial(uv)}{\partial y} dz &= \frac{\partial(\eta \overline{uv})}{\partial y} + [uv]_{z=\zeta} \frac{\partial \zeta}{\partial y} - [uv]_{z=h} \frac{\partial h}{\partial y} \\ \int_{\zeta}^h \frac{\partial(uw)}{\partial z} dz &= [uw]_{z=h} - [uw]_{z=\zeta}\end{aligned}$$

It follows that

$$\begin{aligned}\int_{\zeta}^h \frac{du}{dt} dz &= \frac{\partial(\eta \bar{u})}{\partial t} + \frac{\partial(\eta \overline{u^2})}{\partial x} + \frac{\partial(\eta \overline{uv})}{\partial y} \\ &\quad + \left[u \frac{\partial \zeta}{\partial t} + u^2 \frac{\partial \zeta}{\partial x} + uv \frac{\partial \zeta}{\partial y} - uw \right]_{z=\zeta} \\ &\quad - \left[u \frac{\partial h}{\partial t} + u^2 \frac{\partial h}{\partial x} + uv \frac{\partial h}{\partial y} - uw \right]_{z=h} \\ &= \frac{\partial(\eta \bar{u})}{\partial t} + \frac{\partial(\eta \overline{u^2})}{\partial x} + \frac{\partial(\eta \overline{uv})}{\partial y} \\ &\quad + \left[u \left(\frac{d\zeta}{dt} - w \right) \right]_{z=\zeta} - \left[u \left(\frac{dh}{dt} - w \right) \right]_{z=h}\end{aligned}\tag{6.36}$$

Applying the boundary conditions for w given in Eq. (6.16) then allows Eq. (6.36) to reduce to

$$\int_{\zeta}^h \frac{du}{dt} dz = \frac{\partial(\eta \bar{u})}{\partial t} + \frac{\partial(\eta \overline{u^2})}{\partial x} + \frac{\partial(\eta \overline{uv})}{\partial y}.\tag{6.37}$$

6.4.2.5 Differential Advection Terms

At this stage it would be useful to write the terms $\overline{u^2}$ and $\overline{uv}$ in terms of $\bar{u}$ and $\bar{v}$. Consider again the meaning of the overline operator defined by Eq. (6.19). Given that $\bar{u}$ and $\bar{v}$ are constant with z it follows that $\overline{u^2} = \bar{u}^2$ and $\overline{uv} = \bar{u} \bar{v}$. However, $\overline{u^2} \neq \bar{u}^2$ and $\overline{uv} \neq \bar{u} \bar{v}$.

The necessary separation can be achieved using the following decomposition

$$u = \bar{u} + u' \quad \text{and} \quad v = \bar{v} + v'$$

where u' and v' represent the fluctuations of u and v about $\bar{u}$ and $\bar{v}$, respectively. Importantly $\overline{u'} = \overline{v'} = 0$.

Note that

$$u^2 = (\bar{u} + u')^2 = \bar{u}^2 + 2u'\bar{u} + u'^2$$

and

$$uv = (\bar{u} + u')(\bar{v} + v') = \bar{u}\bar{v} + \bar{u}v' + u'\bar{v} + u'v'$$

It follows that

$$\overline{u^2} = \bar{u}^2 + \overline{u'^2} \quad (6.38)$$

and

$$\overline{uv} = \bar{u}\bar{v} + \overline{u'v'} \quad (6.39)$$

Substituting Eqs. (6.38) and (6.39) into Eq. (6.37) leads to

$$\int_{\zeta}^h \frac{du}{dt} dz = \frac{\partial(\eta\bar{u})}{\partial t} + \frac{\partial(\eta\bar{u}^2)}{\partial x} + \frac{\partial(\eta\bar{u}\bar{v})}{\partial y} + \frac{\partial(\eta\overline{u'^2})}{\partial x} + \frac{\partial(\eta\overline{u'v'})}{\partial y}$$

Application of the product rule then yields

$$\begin{aligned} \int_{\zeta}^h \frac{du}{dt} dz = & \bar{u} \left[\frac{\partial \eta}{\partial t} + \frac{\partial(\eta\bar{u})}{\partial x} + \frac{\partial(\eta\bar{v})}{\partial y} \right] \\ & + \eta \left[\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} \right] + \frac{\partial(\eta\overline{u'^2})}{\partial x} + \frac{\partial(\eta\overline{u'v'})}{\partial y} \end{aligned}$$

Given the vertically integrated continuity equation, Eq. (6.24), it follows that

$$\int_{\zeta}^h \frac{du}{dt} dz = \eta \left[\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} \right] + \frac{\partial(\eta\overline{u'^2})}{\partial x} + \frac{\partial(\eta\overline{u'v'})}{\partial y} \quad (6.40)$$

In a similar way it can be said that

$$\int_{\zeta}^h \frac{dv}{dt} dz = \eta \left[\frac{\partial \bar{v}}{\partial t} + \bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{v}}{\partial y} \right] + \frac{\partial(\eta\overline{u'v'})}{\partial x} + \frac{\partial(\eta\overline{v'^2})}{\partial y} \quad (6.41)$$

The last two terms on the right-hand-side of both Eqs. (6.40) and (6.41) are commonly referred to as differential advection terms.

6.4.2.6 Bringing Everything Together

Substituting Eqs. (6.26), (6.28), (6.34) and (6.40) into the first row of Eq. (6.25) leads to

$$\begin{aligned} & \rho \left[\eta \left(\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} \right) + \frac{\partial(\eta\overline{u'^2})}{\partial x} + \frac{\partial(\eta\overline{u'v'})}{\partial y} \right] \\ & = \frac{\partial(\eta\bar{\tau}_{xx})}{\partial x} + \frac{\partial(\eta\bar{\tau}_{yx})}{\partial y} + \tau_{sx} - \tau_{0x} - \rho g \eta \frac{\partial h}{\partial x} + \rho f_c \eta \bar{v} \end{aligned} \quad (6.42)$$

Substituting Eqs. (6.27), (6.29), (6.35) and (6.41) into the second row of Eq. (6.25) leads to

$$\begin{aligned} & \rho \left[\eta \left(\frac{\partial \bar{v}}{\partial t} + \bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{v}}{\partial y} \right) + \frac{\partial(\eta\overline{u'v'})}{\partial x} + \frac{\partial(\eta\overline{v'^2})}{\partial y} \right] \\ & = \frac{\partial(\eta\bar{\tau}_{xy})}{\partial x} + \frac{\partial(\eta\bar{\tau}_{yy})}{\partial y} + \tau_{sy} - \tau_{0y} - \rho g \eta \frac{\partial h}{\partial y} - \rho f_c \eta \bar{u} \end{aligned} \quad (6.43)$$

The internal deviatoric stress terms and the differential advection terms are commonly lumped together into a set of additional eddy viscosity terms through the following auxiliary equation:

$$\begin{bmatrix} \rho v_{Ex} & 0 \\ 0 & \rho v_{Ey} \end{bmatrix} \begin{bmatrix} \frac{\partial \bar{u}}{\partial x} & \frac{\partial \bar{v}}{\partial x} \\ \frac{\partial \bar{u}}{\partial y} & \frac{\partial \bar{v}}{\partial y} \end{bmatrix} = \begin{bmatrix} \bar{\tau}_{xx} & \bar{\tau}_{xy} \\ \bar{\tau}_{yx} & \bar{\tau}_{yy} \end{bmatrix} - \begin{bmatrix} \rho \overline{u'^2} & \rho \overline{u'v'} \\ \rho \overline{u'v'} & \rho \overline{v'^2} \end{bmatrix} \quad (6.44)$$

where v_{Ex} [$L^2 T^{-1}$] and v_{Ey} [$L^2 T^{-1}$] are the eddy viscosities in the x and y direction, respectively. It can then be stated that [1, p. 75]

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} = \frac{1}{\eta} \frac{\partial}{\partial x} \left(\eta v_{Ex} \frac{\partial \bar{u}}{\partial x} \right) + \frac{1}{\eta} \frac{\partial}{\partial y} \left(\eta v_{Ey} \frac{\partial \bar{u}}{\partial y} \right) + \frac{\tau_{sx} - \tau_{0x}}{\rho \eta} - g \frac{\partial h}{\partial x} + f_c \bar{v} \quad (6.45)$$

$$\frac{\partial \bar{v}}{\partial t} + \bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{v}}{\partial y} = \frac{1}{\eta} \frac{\partial}{\partial x} \left(\eta v_{Ex} \frac{\partial \bar{v}}{\partial x} \right) + \frac{1}{\eta} \frac{\partial}{\partial y} \left(\eta v_{Ey} \frac{\partial \bar{v}}{\partial y} \right) + \frac{\tau_{sy} - \tau_{0y}}{\rho \eta} - g \frac{\partial h}{\partial y} - f_c \bar{u} \quad (6.46)$$

The skin friction model in this context gives rise to

$$\tau_{0x} = \frac{f \rho |\bar{\mathbf{u}}| \bar{u}}{2} \quad (6.47)$$

$$\tau_{0y} = \frac{f \rho |\bar{\mathbf{u}}| \bar{v}}{2} \quad (6.48)$$

where f [-] is the friction factor associated with the Darcy–Weisbach equation and $|\bar{\mathbf{u}}| = (\bar{u}^2 + \bar{v}^2)^{\frac{1}{2}}$.

The water surface stresses, τ_{sx} and τ_{sy} , are largely attributed to wind-driven movement in the overlying air. Detailed guidance about how to determine τ_{sx} and τ_{sy} is provided by [1, p. 79].

6.5 Saint Venant Equations

For one-dimensional open channel flow, $\bar{v}$ is assumed to be negligibly small and the conservation and momentum equations reduce to the so-called Saint Venant equations:

$$\frac{\partial A}{\partial t} + \frac{\partial (A \bar{u})}{\partial x} = 0 \quad (6.49)$$

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left(A v_{Ex} \frac{\partial \bar{u}}{\partial x} \right) + \frac{B \tau_{sx} - P \tau_{0x}}{\rho A} - g \frac{\partial h}{\partial x} \quad (6.50)$$

where A [L^2] is the flowing cross-sectional area of the flowing channel, B [L] is the breadth of the channel at the water surface and P [L] is the wetted perimeter of the channel. The skin friction model in this context gives rise to

$$\tau_{0x} = \frac{f \rho |\bar{\mathbf{u}}| \bar{u}}{2} \quad (6.51)$$

A localised frictional slope, S_f [-], is often defined such that

$$0 = \frac{1}{A} \frac{\partial}{\partial x} \left(A v_{Ex} \frac{\partial \bar{u}}{\partial x} \right) + \frac{B \tau_{sx} - P \tau_{0x}}{\rho A} + g S_f \quad (6.52)$$

Four levels of approximation are often considered including [11, p. 205]:

1. Kinematic wave: $S_f = S_0$
2. Diffusion wave: $S_f = S_0 - \frac{\partial \eta}{\partial x}$
3. Quasi-steady: $S_f = S_0 - \frac{\partial \eta}{\partial x} - \frac{\bar{u}}{g} \frac{\partial \bar{u}}{\partial x}$
4. Fully dynamic: $S_f = S_0 - \frac{\partial \eta}{\partial x} - \frac{\bar{u}}{g} \frac{\partial \bar{u}}{\partial x} - \frac{1}{g} \frac{\partial \bar{u}}{\partial t}$

where $S_0 = -\frac{\partial \zeta}{\partial x}$ is the bed slope. Note that the quasi-steady approximation is identical to Eq. (3.2) in Sect. 3.2.

Also note that substituting Eq. (6.51) into Eq. (6.52) and assuming that v_{Ex} and τ_{sx} are negligible leads to the Darcy–Weisbach equation (see Sect. 2.4.2)

$$S_f = \frac{f |\bar{u}| \bar{u}}{2gm} \quad (6.53)$$

where m [L] is the hydraulic radius.

6.6 Diffusion Wave Equation

Substituting the diffusion wave approximation for S_f into Eq. (6.53) leads to

$$\frac{\partial \eta}{\partial x} = S_0 - \frac{f |\bar{u}| \bar{u}}{2gm} \quad (6.54)$$

Let $Q = A \bar{u}$ such that Eqs. (6.49) and (6.54) become

$$\frac{\partial A}{\partial t} = -\frac{\partial Q}{\partial x} \quad (6.55)$$

$$\frac{\partial \eta}{\partial x} = S_0 - \frac{f |Q| Q}{2gm A^2} \quad (6.56)$$

Partially differentiating both sides of Eq. (6.55) with respect to x leads to

$$\frac{\partial}{\partial t} \left[\frac{\partial A}{\partial x} \right] = -\frac{\partial^2 Q}{\partial x^2} \quad (6.57)$$

whilst applying the chain rule to Eq. (6.56) gives us

$$\frac{\partial A}{\partial x} = \frac{\partial A}{\partial \eta} \left[S_0 - \frac{f |Q| Q}{2gm A^2} \right] \quad (6.58)$$

Partially differentiating both sides of Eq. (6.58) with respect to t , then applying the product rule, then applying the chain rule and finally substituting Eq. (6.55), leads to

$$\begin{aligned}
 \frac{\partial}{\partial t} \left[\frac{\partial A}{\partial x} \right] &= \frac{\partial k_1}{\partial t} - \frac{\partial}{\partial t} (k_2 |Q|Q) \\
 &= \frac{\partial k_1}{\partial t} - |Q|Q \frac{\partial k_2}{\partial t} - k_2 \frac{\partial}{\partial t} (|Q|Q) \\
 &= \left(\frac{\partial k_1}{\partial A} - |Q|Q \frac{\partial k_2}{\partial A} \right) \frac{\partial A}{\partial t} - 2k_2 |Q| \frac{\partial Q}{\partial t} \\
 &= \left(|Q|Q \frac{\partial k_2}{\partial A} - \frac{\partial k_1}{\partial A} \right) \frac{\partial Q}{\partial x} - 2k_2 |Q| \frac{\partial Q}{\partial t}
 \end{aligned} \tag{6.59}$$

where

$$k_1 = \frac{\partial A}{\partial \eta} S_0 \quad \text{and} \quad k_2 = \frac{\partial A}{\partial \eta} \frac{f}{2gmA^2} \tag{6.60}$$

Equating Eqs. (6.57) and (6.59) then gives us

$$\left(|Q|Q \frac{\partial k_2}{\partial A} - \frac{\partial k_1}{\partial A} \right) \frac{\partial Q}{\partial x} - 2k_2 |Q| \frac{\partial Q}{\partial t} = -\frac{\partial^2 Q}{\partial x^2} \tag{6.61}$$

It follows that [11, p. 207]

$$\frac{\partial Q}{\partial t} = K \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} \tag{6.62}$$

where K [L^2T^{-1}] is the apparent diffusion coefficient found from

$$K = \frac{1}{2k_2 |Q|} \tag{6.63}$$

and c [LT^{-1}] is the wave speed found from

$$c = \frac{1}{2k_2 |Q|} \frac{\partial k_1}{\partial A} - \frac{Q}{2k_2} \frac{\partial k_2}{\partial A} \tag{6.64}$$

At a glance, it seems that K is inversely proportional to Q . However, substituting Eqs. (6.53) and (6.60) into Eq. (6.63) leads to [11, p. 207]

$$K = \frac{\partial \eta}{\partial A} \frac{Q}{2S_f}. \tag{6.65}$$

6.6.1 Wide Channel with Manning's Equation

Challenge 6.10 Derive simplified expressions for c and K assuming flow through a prismatic open channel with a broad rectangular cross-section and that Manning's equation applies. The final expressions should be purely in terms of $\bar{u}$, g , f and Fr .

Consider flow through a rectangular cross-section open channel of breadth, B [L]. The cross-sectional area, $A = B\eta$. Assuming the channel is broad (i.e., $B \gg \eta$), the hydraulic radius, $m = \eta$ and $\frac{\partial A}{\partial \eta} = B$. Assuming Manning's equation applies, $f = 2gn^2m^{-\frac{1}{3}}$ (see Sect. 2.5.3) where n [$L^{-\frac{1}{3}}T$] is Manning's coefficient. From Eq. (6.60), it can then be said that

$$k_1 = BS_0 \quad \text{and} \quad k_2 = \frac{n^2}{B\eta^{\frac{10}{3}}}$$

Substituting the above results into Eqs. (6.64) and (6.65) then leads to [11, p. 207]

$$c = \frac{5\bar{u}}{3} \quad (6.66)$$

and

$$K = \frac{Q}{2BS_f}. \quad (6.67)$$

6.6.2 Ogata–Banks Solution

For a semi-infinite channel with constant apparent diffusion coefficient, K , constant wave speed, c , a uniform initial flow rate, Q_I [L^3T^{-1}], and a constant boundary flow rate, Q_0 [L^3T^{-1}], [12] show that

$$\frac{Q(x, t) - Q_I}{Q_0 - Q_I} = F(x, t) \quad (6.68)$$

where

$$F(x, t) = \frac{H(t)}{2} \left[\exp\left(\frac{cx}{K}\right) \operatorname{erfc}\left(\frac{x + ct}{2\sqrt{Kt}}\right) + \operatorname{erfc}\left(\frac{x - ct}{2\sqrt{Kt}}\right) \right] \quad (6.69)$$

with $\operatorname{erfc}(x)$ being the complementary error function and $H(t)$ being the Heaviside step function

$$H(t) = \begin{cases} 0, & t \leq 1 \\ 1, & t > 1 \end{cases} \quad (6.70)$$

Equation (6.68) is often referred to as the Ogata–Banks solution. A detailed derivation of Eq. (6.68) is provided in Chap. 8.

6.6.3 Peclet Number

The Ogata–Banks solution can be simplified by substituting the dimensionless groups

$$\operatorname{Pe} = \frac{cx}{K} \quad \text{and} \quad \tau = \frac{ct}{x} \quad (6.71)$$

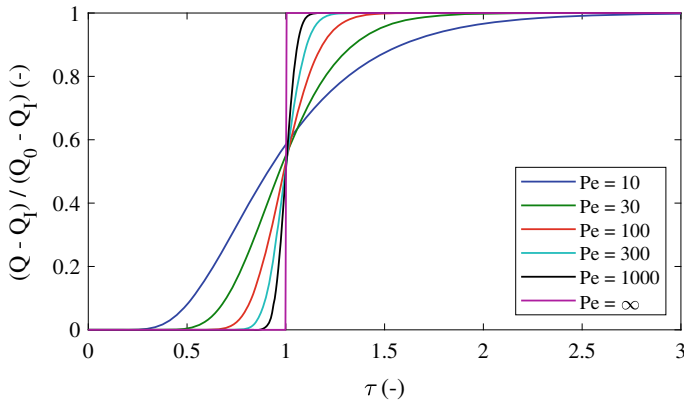


Fig. 6.1 Plots of dimensionless flow rate, $(Q - Q_I)/(Q_0 - Q_I)$, against dimensionless time, τ , for different Peclet numbers, Pe , using the Ogata–Banks solution, Eq. (6.72)

where Pe [-] is known as the Peclet number and τ [-] is a dimensionless time. In this way, Eq. (6.68) reduces to

$$\frac{Q - Q_I}{Q_0 - Q_I} = \frac{H(\tau)}{2} \left\{ e^{Pe} \operatorname{erfc} \left[\sqrt{\frac{Pe}{\tau}} \left(\frac{1 + \tau}{2} \right) \right] + \operatorname{erfc} \left[\sqrt{\frac{Pe}{\tau}} \left(\frac{1 - \tau}{2} \right) \right] \right\} \quad (6.72)$$

The Peclet number represents the ratio of advective transport rate to diffusive transport rate. High Peclet numbers imply an advective transport dominated system. Note that

$$\lim_{Pe \rightarrow \infty} \left\{ \frac{Q - Q_I}{Q_0 - Q_I} \right\} = H(\tau - 1) \quad (6.73)$$

Figure 6.1 shows plots of dimensionless flow rate against dimensionless time using Eq. (6.72). The plots represent how flow rate would increase with time at a fixed point in a channel. As the Peclet number increases the change becomes more sharp. The effect of the dispersion is to reduce the Peclet number and smooth out the front. From a flood protection perspective, low Peclet numbers are preferred because these lead to smoother changes.

6.6.4 Applying the Principle of Superposition

For constant K and c , Eq. (6.62) is a linear partial differential equation. In this context, the principle of superposition applies, which means the composite response of a system to a multitude of events can be obtained by summing the response of the system to each individual event. This idea can be used to modify Eq. (6.68) to account for scenarios where the boundary flow rate is raised to Q_0 for only a designated period of time, t_0 , [T].

6.6.4.1 Delayed Boundary Condition

Suppose that the boundary flow rate is raised from Q_I to Q_0 at $t = 0$. This implies that

$$Q(0, t) = (Q_0 - Q_I)H(t) + Q_I$$

and Eq. (6.68) would apply.

Now suppose that the boundary flow rate is raised from Q_I to Q_0 at $t = t_0$. In this case

$$Q(0, t) = (Q_0 - Q_I)H(t - t_0) + Q_I$$

and

$$Q(x, t) = (Q_0 - Q_I)F(x, t - t_0) + Q_I. \quad (6.74)$$

6.6.4.2 Pulsed Boundary Condition

Suppose that the boundary flow rate is raised from Q_I to Q_0 at $t = 0$ and then brought back down to Q_I at $t = t_0$. This implies that

$$Q(0, t) = (Q_0 - Q_I)[H(t) - H(t - t_0)] + Q_I$$

In this case, an analytical solution is obtained by subtracting the right-hand-side of Eq. (6.74) from the right-hand-side of Eq. (6.68) to get

$$Q(x, t) = (Q_0 - Q_I)[F(x, t) - F(x, t - t_0)] + Q_I. \quad (6.75)$$

6.6.5 Kinematic Wave Equation

For very steep friction slopes, K becomes negligibly small (consider Eq. (6.65)) and Eq. (6.62) reduces to

$$\frac{\partial Q}{\partial t} = -c(\bar{u}) \frac{\partial Q}{\partial x} \quad (6.76)$$

Multiplying both sides of Eq. (6.76) by $\frac{\partial \bar{u}}{\partial Q}$ leads to

$$\frac{\partial \bar{u}}{\partial t} = -c(\bar{u}) \frac{\partial \bar{u}}{\partial x} \quad (6.77)$$

which is typically referred to as the kinematic wave equation.

Steep friction slopes tend to come about in the presence of steep channel beds. Therefore the kinematic wave equation is often used to describe open channel flow and river flow in steep channel systems.

The kinematic wave equation is an example of a hyperbolic PDE. The best way to solve such equations is to use the method of characteristics, which is discussed in detail in Chap. 7.

6.7 Problem Sheet

Problem 6.1 (see Worked Solution 6.1)

A wide rectangular channel has a breadth of 150 m. Determine the Peclet number at 100 km downstream from a flow boundary for when:

- (a) the Manning coefficient is $0.05 \text{ m}^{-\frac{1}{3}} \text{ s}$, the flow rate is $150 \text{ m}^3 \text{ s}^{-1}$ and the friction slope is 0.001, 0.0005 and 0.0001.
- (b) the flow rate is $150 \text{ m}^3 \text{ s}^{-1}$ and the friction slope is 0.0005 and Manning coefficient is $0.03 \text{ m}^{-\frac{1}{3}} \text{ s}$, $0.05 \text{ m}^{-\frac{1}{3}} \text{ s}$ and $0.07 \text{ m}^{-\frac{1}{3}} \text{ s}$.
- (c) the Manning coefficient is $0.05 \text{ m}^{-\frac{1}{3}} \text{ s}$, the slope is 0.0005 and the flow rate is $100 \text{ m}^3 \text{ s}^{-1}$, $150 \text{ m}^3 \text{ s}^{-1}$ and $200 \text{ m}^3 \text{ s}^{-1}$.

Problem 6.2 (see Worked Solution 6.2)

The flow rate entering a river is suddenly increased from $60 \text{ m}^3 \text{ s}^{-1}$ to $750 \text{ m}^3 \text{ s}^{-1}$. The diffusion coefficient is $1000 \text{ m}^2 \text{ s}^{-1}$ and the wave speed is 1 m s^{-1} .

- (a) Plot flow rate against distance from the river inlet up to 400 km from the inlet, 20, 40, 60 and 80 h after the inlet flow rate is suddenly increased.
- (b) Use Eq. (6.74) to generate a set of plots identical to part (a) but assuming the inlet flow rate increase is delayed by 10 h. Note that you will still be plotting flow rates, 20, 40, 60 and 80 h after the hypothetical flow rate increase detailed in part (a).
- (c) Generate a set of plots identical to part (a) but assuming that the inlet flow rate is increased only for 10 h and then returns back to its initial value.

Problem 6.3 (see Worked Solution 6.3)

The flow rate entering a river is suddenly increased from $60 \text{ m}^3 \text{ s}^{-1}$ to $750 \text{ m}^3 \text{ s}^{-1}$ and then returned back to $60 \text{ m}^3 \text{ s}^{-1}$ after 10 h. The breadth of the river channel is 150 m. The Manning coefficient is $0.05 \text{ m}^{-\frac{1}{3}} \text{ s}$. This scenario is based on a case study described by [13, 14]. Plot flow rate against distance from the river inlet up to 400 km from the inlet, 20, 40, 60 and 80 h after the inlet flow rate is suddenly increased for when the friction slope is (a) 0.001, (b) 0.0005 and (c) 0.0001.

6.8 Worked Solutions

Worked Solution 6.1 (see Problem 6.1)

The Manning equation gives that

$$S_f = \frac{n^2 u^2}{m^{\frac{4}{3}}}$$

For a rectangular section

$$u = \frac{Q}{B\eta} \quad (6.78)$$

where B [L] is the breadth of the channel.

For a wide rectangular section, $m = \eta$ and therefore

$$\eta = \left(\frac{nQ}{B\sqrt{S_f}} \right)^{\frac{3}{5}} \quad (6.79)$$

It follows that K , η , u , c and Pe can be determined from Eqs. (6.67), (6.79), (6.78), (6.66) and (6.71), respectively.

(a) Let $B = 150$ m, $x = 100,000$ m, $n = 0.05$ m^{− $\frac{1}{3}$} s and $Q = 150$ m³s^{−1}. It follows that:

S_f (-)	0.001	0.0005	0.0001
K (m ² s ^{−1})	500	1000	5000
η (m)	1.316	1.621	2.627
u (m s ^{−1})	0.7597	0.6170	0.3807
c (m s ^{−1})	1.266	1.028	0.6346
Pe	253.2	102.8	12.69

Steeper friction slopes lead to lower diffusion coefficients and consequently higher Peclet numbers. It follows that steeper friction slopes lead to reduced attenuation of flood waves.

(b) Let $B = 150$ m, $x = 100,000$ m, $S_f = 0.0005$ and $Q = 150$ m³s^{−1}. It follows that:

n (m ^{−$\frac{1}{3}$} s)	0.03	0.05	0.07
K (m ² s ^{−1})	1000	1000	1000
η (m)	1.193	1.621	1.983
u (m s ^{−1})	0.8383	0.6170	0.5042
c (m s ^{−1})	1.397	1.028	0.8404
Pe	139.7	102.8	84.04

An increase in Manning's coefficient implies an increase in surface roughness. Surface roughness can be seen not to affect the diffusion coefficient. However, increased roughness leads to reduced fluid velocity, which in turn leads to reduced Peclet number. It follows that increased roughness leads to increased attenuation of flood waves.

(c) Let $B = 150$ m, $x = 100,000$ m, $n = 0.05 \text{ m}^{-\frac{1}{3}}\text{s}$ and $S_f = 0.0005$. It follows that:

$Q \text{ (m}^3\text{s}^{-1}\text{)}$	100	150	200
$K \text{ (m}^2\text{s}^{-1}\text{)}$	666.7	1000	1333
$\eta \text{ (m)}$	1.271	1.621	1.926
$u \text{ (m s}^{-1}\text{)}$	0.5247	0.6170	0.6923
$c \text{ (m s}^{-1}\text{)}$	0.8744	1.028	1.154
Pe	131.2	102.8	86.54

Increased flow rates lead to higher diffusion coefficients and consequently lower Peclet numbers. It follows that increased flow rates lead to increased attenuation of flood waves.

Worked Solution 6.2 (see Problem 6.2)

The MATLAB function `OgataBanks` given in Listing 6.1 provides an implementation of the Ogata–Banks solution as given by Eq. (6.69).

Listing 6.1 A MATLAB function for evaluating the Ogata–Banks solution as given by Eq. (6.69).

```
function F=OgataBanks(x,t,K,c)
%Implement Ogata-Banks solution
%x - Distance (m)
%t - Time (s)
%K - Apparent diffusion coefficient (m2/s)
%c - Wave speed (m/s)
%F - Normalised flow rate (-)
T1=exp(c.*x./K).*erfc((x+c.*t)/2./sqrt(K.*t));
%Note that the limit of T1 as x-> inf = 0
T1(isnan(T1)|isinf(T1))=0;
T2=erfc((x-c.*t)/2./sqrt(K.*t));
F=(t>1).*(T1+T2)/2;
```

Let $K = 1000 \text{ m}^2\text{s}^{-1}$, $c = 1 \text{ m s}^{-1}$ and $t_0 = 10 \text{ h}$.

- Use Eq. (6.68).
- Use Eq. (6.74).
- Use Eq. (6.75).

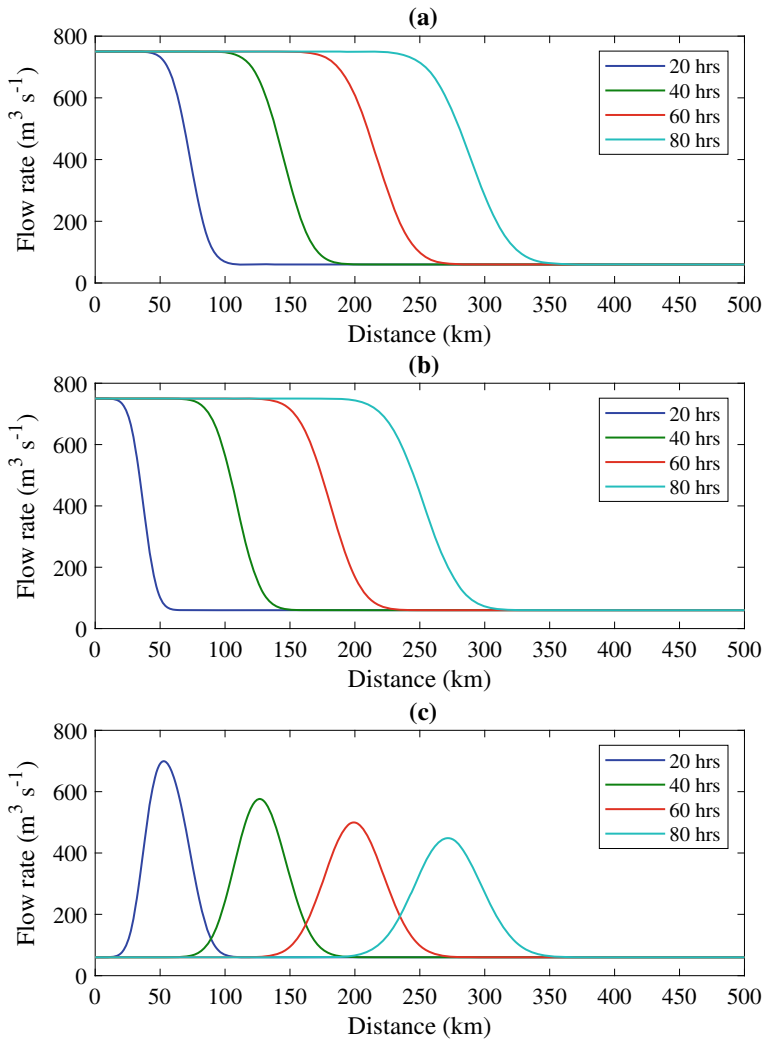


Fig. 6.2 Plots of flow rate against distance for different times. **a** Flow rate change starting at $t = 0$. **b** Flow rate change starting at $t = 10$ h. **c** Flow rate change occurring for $t \in [0, 10]$ h

The MATLAB code below utilizes the `OgataBanks` function (Listing 6.1) and plots the three profiles shown in Fig. 6.2.

```
K=1000; %Diffusion coefficient (m2/s)
c=1; %Wave speed (m/s)
x=linspace(0,500e3,500)'; %Distance (m)
t=[20 40 60 80]*60^2; %Time (s)
t0=10*60^2; %Pulse duration (s)
QI=60; %Initial flow rate (m3/s)
```

```

Q0=750; %Boundary flow rate (m3/s)
Q(:, :, 1)=(Q0-QI)*OgataBanks(x,t,K,c)+QI; %a)
Q(:, :, 2)=(Q0-QI)*OgataBanks(x,t-t0,K,c)+QI; %b)
Q(:, :, 3)=Q(:, :, 1)-Q(:, :, 2)+QI; %c)
figure(1);clf %Plot results
MyTitle='abc'; %Subplot titles
for k=1:3
subplot(3,1,k)
plot(x/1000,Q(:, :, k))
xlabel('Distance (km)')
ylabel('Flow rate (m^3 s^-1)')
legend('20 hrs', '40 hrs', '60 hrs', '80 hrs')
title([MyTitle(k) ''])
end

```

Worked Solution 6.3 (see Problem 6.3)

The relevant K and c values were previously derived for Problem 6.1a. The MATLAB code below utilizes the `OgataBanks` function from Listing 6.1 to obtain the presented in Fig. 6.3.

```

%Diffusion coefficient (m2/s)
K=reshape([500 1000 5000],1,1,3);
%Wave speed (m/s)
c=reshape([1.266 1.028 0.6346],1,1,3);
x=linspace(0,500e3,500)'; %Distance (m)
t=[20 40 60 80]*60^2; %Time (s)
t0=10*60^2; %Pulse duration (s)
QI=60; %Initial flow rate (m3/s)
Q0=750; %Boundary flow rate (m3/s)
Q=(Q0-QI)*(OgataBanks(x,t,K,c)...
-OgataBanks(x,t-t0,K,c))+QI;
figure(2);clf;hold on;box on %Plot results
plot(x/1000,Q(:, :, 1), '-') %a)
set(gca, 'ColorOrderIndex', 1)
plot(x/1000,Q(:, :, 2), '--') %b)
set(gca, 'ColorOrderIndex', 1)
plot(x/1000,Q(:, :, 3), '-.') %c)
xlabel('Distance (km)')
ylabel('Flow rate (m^3 s^-1)')
legend('20 hrs', '40 hrs', '60 hrs', '80 hrs')

```

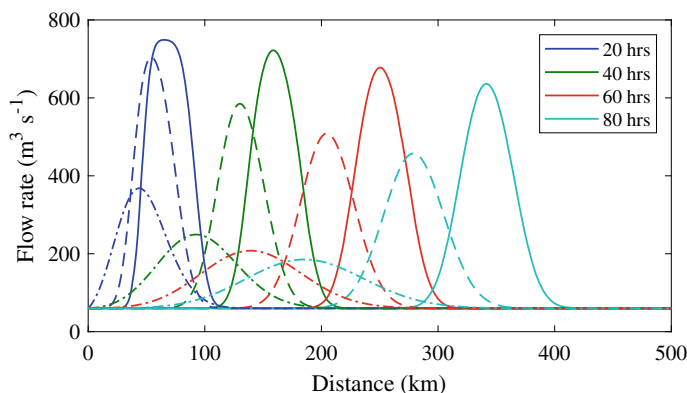


Fig. 6.3 Plots of flow rate against distance for different times and different friction slopes. The solid lines are for a friction slope of 0.001. The dashed lines are for a friction slope of 0.0005. The dash-dot lines are for a friction slope of 0.0001

As the friction slope is decreased, the diffusion coefficient is increased and the extent of flood wave attenuation is enhanced. This in turn has the effect of reducing the rate at which the flood wave moves and also reduces the flood wave magnitude.

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Method of Characteristics Solution for the Kinematic Wave Equation

7

Abstract

This chapter focuses on how to solve the kinematic wave equation using the method of characteristics. The concept of a characteristic curve is explained. Leibniz's theorem for differentiation of an integral is used to derive the Rankin Hugoniot jump condition for shock wave solutions. Rarefaction wave solutions are derived using a similarity transform. Plots of characteristic curves are used to derive a combined shock wave and rarefaction wave solution. Practical applications are presented through a problem sheet with worked solutions.

Notation

c	Wave speed [LT^{-1}].
t	Time [T].
u	Fluid velocity [LT^{-1}].
$\tilde{u}_I(x)$	Non-uniform initial fluid velocity distribution [LT^{-1}].
x	Horizontal distance in the x -direction [L].
x_I	Initial location of characteristic curve [L].
x_s	Location of a shock wave [L].
x_s^-	A location immediately upstream of a shock wave [L].
x_s^+	A location immediately downstream of a shock wave [L].
α	Similarity transform x -exponent [-].
β	Similarity transform t -exponent [-].
$\xi = x^\alpha t^\beta$	Similarity transform [$L^\alpha T^\beta$].
ϕ	Flux function [$L^2 T^{-2}$].
MoC	Method of characteristics.

7.1 Introduction

This chapter focuses on using the method of characteristics to derive analytical solutions for the kinematic wave equation (recall Sect. 6.6.5)

$$\frac{\partial u}{\partial t} + c(u) \frac{\partial u}{\partial x} = 0 \quad (7.1)$$

subject to the initial condition

$$u(x, 0) = \tilde{u}_I(x), \quad x \in [-\infty, \infty] \quad (7.2)$$

where u [LT^{-1}] is fluid velocity, t [T] is time, $c(u)$ [LT^{-1}] is wave speed, x [L] is distance and $\tilde{u}_I(x)$ is the initial fluid velocity distribution.

First we derive a similarity transform solution. We then rearrange Eq. (7.1) into a conservative form. Key concepts associated with method of characteristics are introduced, leading to a solution for constant wave speeds. The conservative form of Eq. (7.1) is used to derive the Rankine–Hugoniot jump condition for shock wave solutions. The similarity transform solution is used to derive rarefaction wave solutions. Finally it is explained how to derive composite solutions comprising a combination of shock waves and rarefaction waves.

7.2 Similarity Transform Solution

Challenge 7.1 Consider a similarity transform $\xi = x^\alpha t^\beta$. Determine α and β such that x and t are eliminated in Eq. (7.1), having been replaced by ξ .

Let $\xi = x^\alpha t^\beta$. Application of the chain-rule to Eq. (7.1) leads to

$$\frac{\partial \xi}{\partial t} \frac{\partial u}{\partial \xi} + c(u) \frac{\partial \xi}{\partial x} \frac{\partial u}{\partial \xi} = 0 \quad (7.3)$$

Noting that

$$\frac{\partial \xi}{\partial x} = \frac{\alpha \xi}{x} \quad \text{and} \quad \frac{\partial \xi}{\partial t} = \frac{\beta \xi}{t} \quad (7.4)$$

it follows that Eq. (7.3) reduces to

$$\frac{\alpha x}{\beta t} + c(u) = 0 \quad (7.5)$$

If we set $\alpha = 1$ and $\beta = -1$ then $\xi = \frac{x}{t}$ and

$$c(u) = \xi \quad (7.6)$$

In this way x and t are eliminated and Eq. (7.1) is shown to be potentially self-similar (depending on the nature of the initial condition and boundary condition).

Moreover, we have demonstrated that

$$c(u) = \frac{x}{t} \quad (7.7)$$

is a potential solution to Eq. (7.1).

7.3 Conservative Form

Challenge 7.2 Determine an expression for $c(u)$ in terms of a flux function, $\phi(u)$ [L^2T^{-2}], such that the conservation equation, $\frac{\partial u}{\partial t} + \frac{\partial \phi}{\partial x} = 0$, is satisfied.

Consider a conservation equation

$$\frac{\partial u}{\partial t} + \frac{\partial \phi}{\partial x} = 0 \quad (7.8)$$

where $\phi(u)$ [L^2T^{-2}] is a flux function.

Comparing Eqs. (7.1) and (7.8) reveals that

$$\frac{\partial \phi}{\partial x} = c(u) \frac{\partial u}{\partial x} \quad (7.9)$$

and so

$$c(u) = \frac{\partial \phi}{\partial u} \quad (7.10)$$

7.4 Method of Characteristics

A common approach to solving Eqs. (7.1) and (7.2) is to employ the method of characteristics (MoC). In this context, a characteristic curve represents a line (which can be straight or curved) on a plot of t against x where u is constant.

The total derivative of u with respect to t will therefore be zero on a characteristic curve:

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{dx}{dt} \frac{\partial u}{\partial x} = 0 \quad (7.11)$$

Comparison of Eq. (7.11) with Eq. (7.1) suggests that a characteristic curve, which satisfies Eq. (7.11), takes the form

$$\frac{dx}{dt} = c(u) \quad (7.12)$$

Let $x = x_I$ at $t = 0$. Note that $u(x_I, 0) = \tilde{u}_I(x_I)$. If u is constant along a characteristic curve, it follows that (on a characteristic curve)

$$u(x, t) = \tilde{u}_I(x_I) \quad (7.13)$$

and

$$\frac{dx}{dt} = c(\tilde{u}_I(x_I)) \quad (7.14)$$

Integrating Eq. (7.14) with respect to t then leads to [1, p. 24]

$$x = c(\tilde{u}_I(x_I))t + x_I \quad (7.15)$$

which represents the equation describing the geometry of all characteristic curves for all values of x_I .

7.4.1 Constant Wave Speed Solution

Challenge 7.3 Use MoC to derive an analytical solution for Eqs. (7.1) and (7.2) when c is constant.

From Eq. (7.13), we have $u(x, t) = \tilde{u}_I(x_I)$. From Eq. (7.15), we have $x_I = x - c(\tilde{u}_I(x_I))t$. It follows that

$$u(x, t) = \tilde{u}_I(x - c(\tilde{u}_I(x_I))t) \quad (7.16)$$

For constant c , it can be said that [2, p. 129]

$$u(x, t) = \tilde{u}_I(x - ct) \quad (7.17)$$

7.5 Shock Waves

Here we will consider the case where

$$c(u) = u \quad (7.18)$$

$$\tilde{u}_I(x) = \begin{cases} 1 & x \leq 0 \\ 0 & x > 0 \end{cases}. \quad (7.19)$$

Challenge 7.4 Sketch the characteristic curves describing the problem defined by Eqs. (7.1), (7.2), (7.18) and (7.19).

Substituting Eqs. (7.18) and (7.19) into Eq. (7.15) leads to

$$x = \begin{cases} t + x_I, & x_I \leq 0 \\ x_I, & x_I > 0 \end{cases} \quad (7.20)$$

A plot of the characteristics are shown in Fig. 7.1a. It can be seen that the xt -plane is covered by two sets of characteristics. The first set is associated with where $u = 0$ and are straight vertical lines. The second set is associated with where $u = 1$ and are straight diagonal lines. Where the two sets of characteristics intersect represents a so-called gradient catastrophe [2, p. 138].

Realistic solutions involve determining a line, $x_s(t)$, on the xt -plane where the two sets of characteristics terminate such that they no longer intersect. The discontinuity that takes place along this line is commonly referred to as a shock wave and gives rise to the analytical solution

$$u(x, t) = \begin{cases} 1, & x \leq x_s(t) \\ 0, & x > x_s(t) \end{cases} \quad (7.21)$$

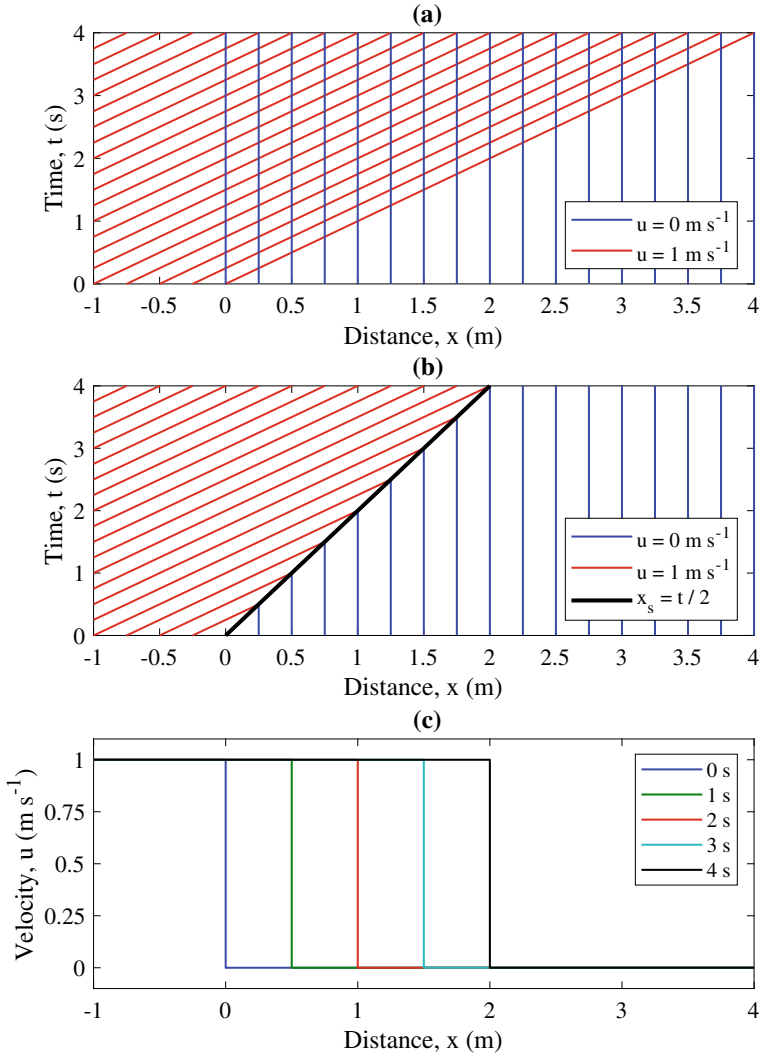


Fig. 7.1 Shock wave solution. **a** Shows the overlapping characteristics. **b** Shows the overlapping characteristics, truncated by a shock wave, $x_s(t)$. **c** Example velocity profiles from the analytical solution

The location of the shock wave, $x_s(t)$, can be determined using the Rankine–Hugoniot jump condition described below.

7.5.1 Rankine–Hugoniot Condition

Consider again the conservation equation, Eq. (7.8). Suppose a shock wave exists at $x = x_s(t)$. Let x_s^- and x_s^+ be locations immediately upstream and downstream of the shock front, respectively. The nature of this discontinuity is that $u(x_s^-, t) \neq u(x_s^+, t)$ and $\phi(x_s^-, t) \neq \phi(x_s^+, t)$.

Consider two points, a and b , chosen such that $a < x_s < b$. Integrating both sides of the conservation equation with respect to x in the region $x \in [a, b]$ leads to

$$\int_a^b \frac{\partial u}{\partial t} dx = - \int_a^b \frac{\partial \phi}{\partial x} dx \quad (7.22)$$

Leibniz's theorem for differentiation of an integral gives [3, p. 11]

$$\frac{d}{dt} \int_a^b u dx = \int_a^b \frac{\partial u}{\partial t} dx + u(b, t) \frac{db}{dt} - u(a, t) \frac{da}{dt} \quad (7.23)$$

Furthermore, we can state that

$$\int_a^b \frac{\partial \phi}{\partial x} dx = \phi(b, t) - \phi(a, t) \quad (7.24)$$

Substituting Eqs. (7.23) and (7.24) into Eq. (7.8) leads to

$$\frac{d}{dt} \int_a^b u dx + u(a, t) \frac{da}{dt} - u(b, t) \frac{db}{dt} = \phi(a, t) - \phi(b, t) \quad (7.25)$$

Letting $a \rightarrow x_s(t)$ and $b \rightarrow x_s(t)$ leads to

$$u(x_s^-, t) \frac{dx_s}{dt} - u(x_s^+, t) \frac{dx_s}{dt} = \phi(x_s^-, t) - \phi(x_s^+, t) \quad (7.26)$$

from which it follows that [2, p. 150]

$$\frac{dx_s}{dt} = \frac{\phi(x_s^+, t) - \phi(x_s^-, t)}{u(x_s^+, t) - u(x_s^-, t)} \quad (7.27)$$

which is referred to as the Rankine–Hugoniot jump condition [1, p. 31]. The location of the shock wave must be such that the Rankine–Hugoniot jump condition is satisfied.

7.5.2 Using the Rankine–Hugoniot Jump Condition to Locate a Shock Front

Challenge 7.5 Use the Rankine–Hugoniot jump condition to locate a shock front associated with the problem defined by Eqs. (7.1), (7.2), (7.18) and (7.19).

The location of a shock front associated with the problem defined by Eqs. (7.1), (7.2), (7.18) and (7.19) can be obtained using Eq. (7.27).

It can be seen from Eq.(7.21) that

$$u(x_s^-, t) = 1 \quad \text{and} \quad u(x_s^+, t) = 0$$

From Eqs. (7.10) and (7.18) we have that $\phi = \frac{u^2}{2}$. Therefore

$$\phi(x_s^-, t) = \frac{1}{2} \quad \text{and} \quad \phi(x_s^+, t) = 0$$

It follows from Eq. (7.27) that

$$\frac{dx_s}{dt} = \frac{1}{2}$$

Given the initial condition, Eq. (7.19), $x_s(t = 0) = 0$. It follows that

$$x_s = \frac{t}{2} \tag{7.28}$$

and therefore (recall Eq. (7.21)) [2, p. 151]

$$u(x, t) = \begin{cases} 1, & x \leq \frac{t}{2} \\ 0, & x > \frac{t}{2} \end{cases} \tag{7.29}$$

Figure 7.1b shows how the shock wave, defined by Eq. (7.28), divides up the overlapping characteristics shown in Fig. 7.1a. Some example velocity profiles resulting from Eq. (7.29) are shown in Fig. 7.1c.

7.6 Rarefaction Waves

Now consider the scenario where $c = u$ and

$$\tilde{u}_I(x) = \begin{cases} 0, & x \leq 0 \\ 1, & x > 0 \end{cases} \tag{7.30}$$

such that the characteristics curves are found from

$$x = \begin{cases} x_I, & x_I \leq 0 \\ t + x_I, & x_I > 0 \end{cases} \tag{7.31}$$

Plots of the resulting characteristic curves are shown in Fig. 7.2a.

7.6.1 Showing That a Shock Wave Does Not Work

Challenge 7.6 Try and find a shock wave solution for Eqs.(7.1), (7.2), (7.18) and (7.30).

First we will hypothesise that

$$u(x, t) = \begin{cases} 0, & x \leq x_s(t) \\ 1, & x > x_s(t) \end{cases}$$

It would follow that

$$\begin{aligned} u(x_s^-, t) &= 0, \quad u(x_s^+, t) = 1 \\ \phi(x_s^-, t) &= 0, \quad \phi(x_s^+, t) = \frac{1}{2} \end{aligned}$$

and, from the Rankine–Hugoniot jump condition (Eq. (7.27)),

$$\frac{dx_s}{dt} = -\frac{1}{2}$$

Letting $x_s = 0$ at $t = 0$ we then have

$$x_s = -\frac{t}{2}$$

which is obviously not possible because the fluid is moving in the positive direction.

The issue here is that the two sets of characteristic lines from Eq. (7.31) do not intersect each other (see Fig. 7.2a), which means that we would not expect a shock wave to develop. Instead, there is a wedged-shaped region, $x \in (0, t)$, free of characteristic curves.

7.6.2 Applying a Similarity Transform Solution

Note that the boundaries of the wedged-shaped region are described as follows:

$$\begin{aligned} u &= 0, \quad x = 0, \quad t \geq 0 \\ u &= 1, \quad x = t, \quad t \geq 0 \end{aligned} \tag{7.32}$$

The similarity transform solution we defined previously (recall Eq. (7.7)) provides an analytical solution that satisfies both the governing equation, Eq. (7.1), and, after setting $c = u$, the boundary conditions described by Eq. (7.32). Consequently, it can be further stated that

$$u = \frac{x}{t}, \quad x \in (0, t), \quad t \geq 0 \tag{7.33}$$

Equation (7.33) provides an additional “fan” of characteristic curves, $x = ut$, that fill the wedge-shape region in Eq. (7.31), i.e.,

$$x = \begin{cases} x_I, & x_I < 0 \\ ut, & x_I = 0 \\ t + x_I, & x_I > 0 \end{cases} \tag{7.34}$$

Such a fan of curves is referred to as a rarefaction wave [1, p. 30].

Utilizing this rarefaction wave to fill the wedged-shaped region, $x \in (0, t)$, leads to the analytical solution for the complete problem [2, p. 168]:

$$u(x, t) = \begin{cases} 0, & x \leq 0 \\ \frac{x}{t}, & 0 < x < t \\ 1, & x \geq t \end{cases} \tag{7.35}$$

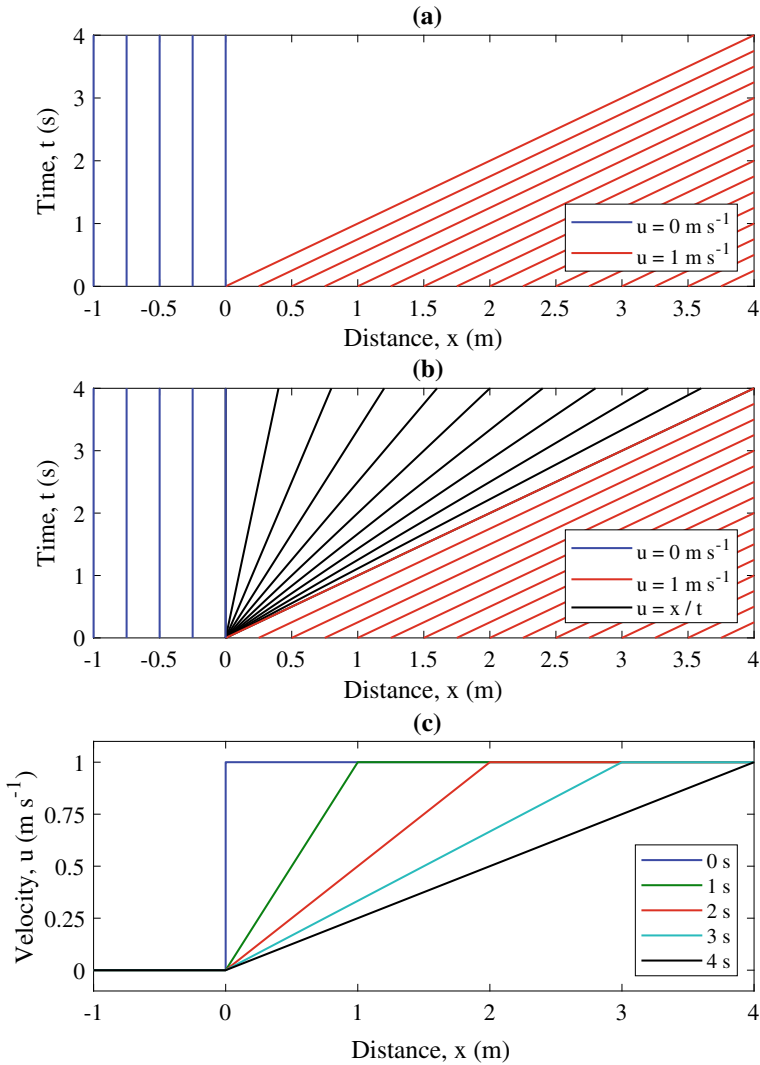


Fig. 7.2 Rarefaction wave solution. **a** Shows the wedge shaped region free of characteristics. **b** Shows the wedged shape region filled with a fan of characteristics, $x = ut$. **c** Example velocity profiles from the analytical solution

Figure 7.2b shows how the fan of characteristic curves fills the wedged-shape region, $x \in (0, t)$. Some example velocity profiles resulting from Eq. (7.35) are shown in Fig. 7.2c.

7.7 Combined Shock Wave and Rarefaction Wave

Now consider the situation where

$$\tilde{u}_I(x_I) = \begin{cases} 0, & x \leq 0 \\ 1, & 0 < x < 1 \\ 0, & x \geq 1 \end{cases} \quad (7.36)$$

Challenge 7.7 Sketch the characteristic curves describing the problem defined by Eqs. (7.1), (7.2), (7.18) and (7.36).

Substituting Eqs. (7.18) and (7.36) into Eq. (7.15) leads to

$$x = \begin{cases} x_I, & x_I \leq 0 \\ t + x_I, & 0 < x_I < 1 \\ x_I, & x_I \geq 1 \end{cases}$$

Figure 7.3a shows plots of the characteristic curves. Notice that there are two complications. Firstly there is a region, bounded by $x > t$ for $x \in (0, 1)$, that is free of characteristics (excluding the black lines attributed to $u = x/t$). Secondly, the diagonal characteristics (the red lines) overlap the vertical characteristics (the blue lines) for $x_I \geq 1$.

The region free of characteristics can be filled with a fan of characteristics associated with the similarity solution (Eq. (7.33)), which are shown as black diagonal lines on Fig. 7.3a. It follows that we can then say

$$x = \begin{cases} x_I, & x_I < 0 \\ ut, & x_I = 0 \\ t + x_I, & 0 < x_I < 1 \\ x_I, & x_I \geq 1 \end{cases}$$

However, there is now the additional problem that the fan of characteristics also intersect the vertical characteristics for $x_I \geq 1$ (see Fig. 7.3a). The two sets of overlapping characteristics give rise to gradient catastrophes and can therefore be represented as shock wave solutions.

Let $x_s(t)$ [L] be the location of a shock wave, defined by

$$x_s(t) = \begin{cases} x_{s1}(t), & t < t_c \\ x_{s2}(t), & t \geq t_c \end{cases} \quad (7.37)$$

where, with further reference to Fig. 7.3a, x_{s1} [L] represents the shock wave separating the blue lines ($x = x_I$) from the red lines ($x = t + x_I$), x_{s2} [L] represents the shock wave separating the blue lines ($x = x_I$) from the black lines ($x = ut$) and t_c represents a critical time, beyond which the red lines ($x = t + x_I$) no longer intersect the $x_{s1}(t)$ line.

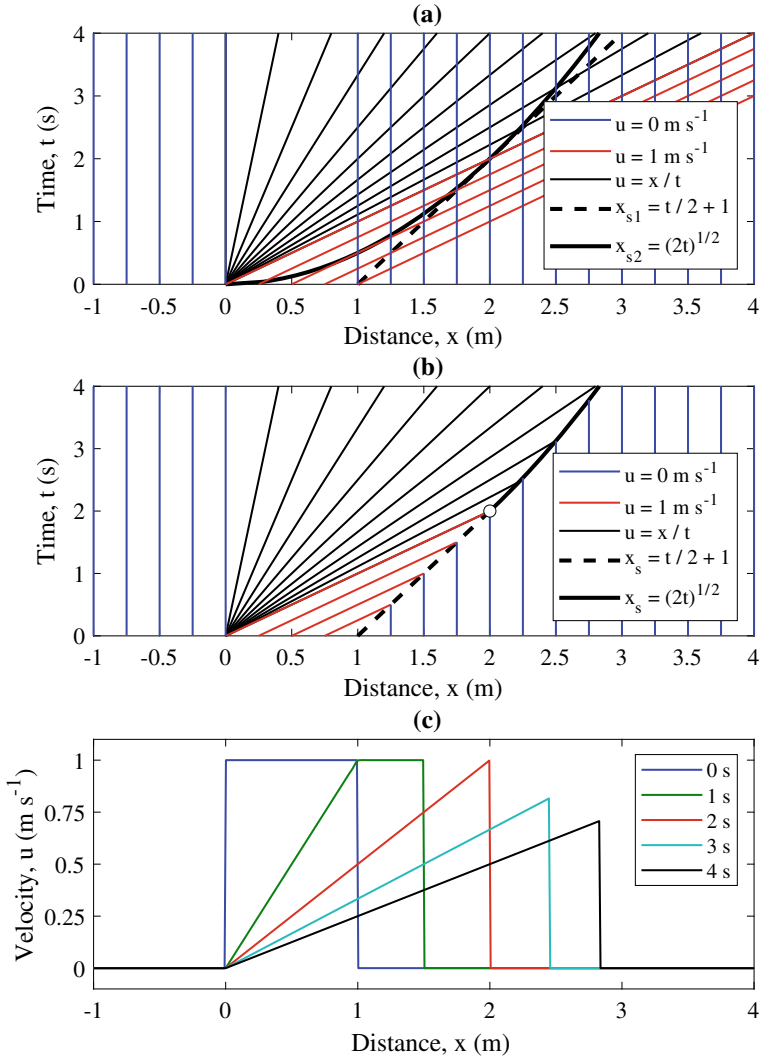


Fig. 7.3 Combined rarefaction and shock wave solution. **a** Shows various overlapping sets of characteristic curves along with the functional form of two shock waves. **b** Shows how the characteristic curves are truncated by the shock waves. **c** Example velocity profiles from the analytical solution

Given our experience from deriving Eqs. (7.29) and (7.35), we can say

$$u(x, t) = \begin{cases} 0, & x \leq 0 \\ \frac{x}{t}, & 0 < x < t \\ 1, & t \leq x < x_{s1}(t) \\ 0, & x \geq x_{s1}(t) \end{cases}, \quad t < t_c \quad (7.38)$$

and

$$u(x, t) = \begin{cases} 0, & x \leq 0 \\ \frac{x}{t}, & 0 < x < x_{s2}(t) \\ 0, & x \geq x_{s2}(t) \end{cases}, \quad t \geq t_c. \quad (7.39)$$

Challenge 7.8 Determine an equation for the location of the shock wave, $x_{s1}(t)$.

Considering the Rankine–Hugoniot jump condition (Eq. (7.27)) with Eq. (7.38)

$$\begin{aligned} u(x_{s1}^-, t) &= 1, & u(x_{s1}^+, t) &= 0 \\ \phi(x_{s1}^-, t) &= \frac{1}{2}, & \phi(x_{s1}^+, t) &= 0 \end{aligned}$$

and so

$$\frac{dx_{s1}}{dt} = \frac{1}{2}$$

Looking at the initial condition, Eq. (7.36), it can be seen that the shock wave starts at $x = 1$. It can therefore be understood that $x_{s1} = 1$ at $t = 0$ and consequently

$$x_{s1} = \frac{t}{2} + 1. \quad (7.40)$$

Challenge 7.9 Determine the value of the critical time, t_c .

The critical time, t_c , occurs when $x_{s1}(t)$ intersects the upper most red line ($x = t + x_I$) on Fig. 7.3a, which is where $x_I = 0$. Equating Eq. (7.40) with $x = t$ and setting $t = t_c$ leads to

$$t_c = \frac{t_c}{2} + 1$$

and so $t_c = 2$.

Challenge 7.10 Determine an equation for the location of the shock wave, $x_{s2}(t)$.

Considering the Rankine–Hugoniot jump condition (Eq. (7.27)) with Eq. (7.39)

$$\begin{aligned} u(x_{s2}^-, t) &= \frac{x_{s2}}{t}, \quad u(x_{s2}^+, t) = 0 \\ \phi(x_{s2}^-, t) &= \frac{x_{s2}^2}{2t^2}, \quad \phi(x_{s2}^+, t) = 0 \end{aligned}$$

and so

$$\frac{dx_{s2}}{dt} = \frac{x_{s2}}{2t}$$

Separating variables and integrating both sides with respect to t leads to

$$\ln x_{s2} = \frac{1}{2} \ln t + C \quad (7.41)$$

where C is an integration constant.

We know that Eq. (7.41) should intersect Eq. (7.40) at $t = 2$ for the shock wave to be continuous. Noting that $x_{s1}(t = 2) = 2$ we can also say that $x_{s2} = 2$ at $t = 2$. It follows that

$$C = \frac{1}{2} \ln 2$$

and

$$x_{s2} = \sqrt{2t} \quad (7.42)$$

The resulting analytical solution for u is therefore [2, p. 178]

$$u(x, t) = \begin{cases} 0, & x \leq 0 \\ \frac{x}{t}, & 0 < x < t \\ 1, & t \leq x < \frac{t}{2} + 1 \\ 0, & x \geq \frac{t}{2} + 1 \end{cases}, \quad t < 2 \quad (7.43)$$

and

$$u(x, t) = \begin{cases} 0, & x \leq 0 \\ \frac{x}{t}, & 0 < x < \sqrt{2t} \\ 0, & x \geq \sqrt{2t} \end{cases}, \quad t \geq 2 \quad (7.44)$$

Figure 7.3b shows how the overlapping lines are truncated by the composite shock path defined by Eq. (7.37). Some example velocity profiles resulting from Eqs. (7.43) and (7.44) are shown in Fig. 7.3c.

7.8 Problem Sheet

Problem 7.1 (see Worked Solution 7.1)

- (a) Determine an analytical solution for Eqs. (7.1) and (7.2) when c is constant and

$$\tilde{u}_I(x) = \begin{cases} u_I, & x \leq 0 \\ u_0, & 0 < x < x_0 \\ u_I, & x \geq x_0 \end{cases} \quad (7.45)$$

(b) Use the analytical solution derived above to plot u as a function of x for $t = 0, 20, 40, 60$ and 80 h assuming $c = 1 \text{ m s}^{-1}$, $u_I = 0.4$, $u_0 = 1.2 \text{ m s}^{-1}$ and $x_0 = 50$ km.

Problem 7.2 (see Worked Solution 7.2)

(a) Derive an analytical solution for Eqs. (7.1) and (7.2) when

$$c = \frac{5u}{3} \quad (7.46)$$

and

$$\tilde{u}_I(x) = \begin{cases} u_0, & x \leq 0 \\ u_I, & x > 0 \end{cases} \quad (7.47)$$

where u_0 [LT^{-1}] represents the velocity at an inlet boundary and u_I [LT^{-1}] represents the initial velocity.

(b) Use the analytical solution derived above to plot u as a function of x after 20 h assuming $u_0 = 1.2 \text{ m s}^{-1}$ with $u_I = 2.4, 2, 1.6, 1.2, 0.8, 0.4$ and 0 m s^{-1} .

Problem 7.3 (see Worked Solution 7.3)

(a) Use dimensionless transformations to modify the analytical solution given by Eqs. (7.43) and (7.44) such that c is defined by Eq. (7.46) and

$$\tilde{u}_I(x) = \begin{cases} u_0, & x \in [0, x_0] \\ 0, & x \notin [0, x_0] \end{cases} \quad (7.48)$$

(b) Use the analytical solution derived above to plot u as a function of x after 0, 5, 10, 20 and 40 h assuming $u_0 = 1.2 \text{ m s}^{-1}$ and $x_0 = 50$ km.

7.9 Worked Solutions

Worked Solution 7.1 (see Problem 7.1)

(a) Given that c is constant we can use Eq. (7.17), which states that

$$u(x, t) = \tilde{u}_I(x - ct)$$

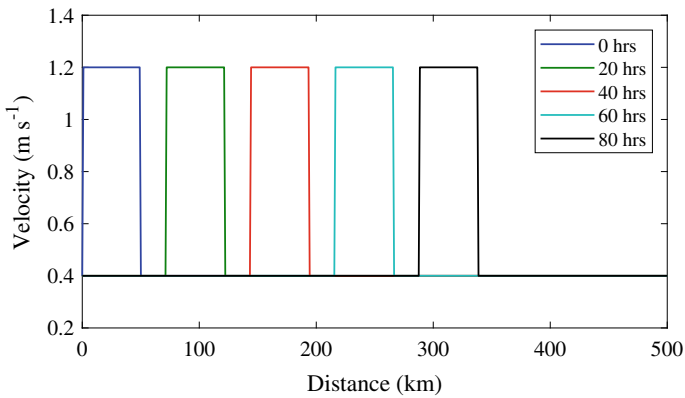


Fig. 7.4 Plots of velocity against distance for a pulse wave with a constant wave speed at different times, as indicated by the legend

Substituting Eq. (7.45) then leads to

$$u(x, t) = \begin{cases} u_I, & x - ct \leq 0 \\ u_0, & 0 < x - ct < x_0 \\ u_I, & x - ct \geq x_0 \end{cases} \quad (7.49)$$

(b) The following MATLAB code will perform the task of concern:

```
x= linspace(0,500e3,500)'; %Space points (m)
t=[0 20 40 60 80]*60^2; %Time points (s)
c=1; %Wave speed (m/s)
uI=0.4; %Minimum velocity (m/s)
u0=1.2; %Maximum velocity (m/s)
x0=50e3; %Spatial extent of velocity wave (m)
%Analytical solution
u=(u0-uI)*(x-c*t>0&x-c*t<x0)+uI;
figure(1);clf;box on %Plot results
plot(x/1000,u)
xlabel('Distance (km)')
ylabel('Velocity (m s^-1)')
legend('0 hrs', '20 hrs', '40 hrs', '60 hrs', '80 hrs')
```

The relevant results are shown in Fig. 7.4.

Worked Solution 7.2 (see Problem 7.2)

(a) The first step is derive equations for the characteristic curves. Substituting Eqs. (7.46) and (7.47) into Eq. (7.15) leads to

$$x = \begin{cases} \frac{5u_0 t}{3} + x_0, & x_0 \leq 0 \\ \frac{5u_I t}{3} + x_0, & x_0 > 0 \end{cases} \quad (7.50)$$

When $u_0 > u_I$, the characteristic curves, Eq.(7.50), will have an overlap region, similar to as in Fig. 7.1a, suggesting that the problem will lead to a shock wave solution, similar to when we looked at Eq.(7.19). Considering Eq.(7.21), it follows that

$$u(x, t) = \begin{cases} u_0, & x \leq x_s(t) \\ u_I, & x > x_s(t) \end{cases}, \quad u_0 > u_I \quad (7.51)$$

where x_s represents the location of the shock wave.

An equation for x_s can be obtained by applying the Rankine–Hugoniot condition, Eq.(7.27). It can be seen from Eq.(7.51) that

$$u(x_s^-, t) = u_0 \quad \text{and} \quad u(x_s^+, t) = u_I$$

From Eqs.(7.10) and (7.46) we have that $\phi = \frac{5u^2}{6}$. Therefore

$$\phi(x_s^-, t) = \frac{5u_0^2}{6} \quad \text{and} \quad \phi(x_s^+, t) = \frac{5u_I^2}{6}$$

It follows from Eq.(7.27) that

$$\frac{dx_s}{dt} = \frac{5}{6}(u_0 + u_I)$$

Given the initial condition, Eq.(7.47), $x_s(t = 0) = 0$. It follows that

$$x_s = \frac{5}{6}(u_0 + u_I)t$$

and therefore (recall Eq.(7.51))

$$u(x, t) = \begin{cases} u_0, & x \leq \frac{5}{6}(u_0 + u_I)t \\ u_I, & x > \frac{5}{6}(u_0 + u_I)t \end{cases}, \quad u_0 > u_I \quad (7.52)$$

When $u_0 < u_I$, the characteristic curves, Eq.(7.50), will have a wedge shaped region, free of characteristic curves, similar to as in Fig. 7.2a, suggesting that the problem will lead to a rarefaction wave solution, similar to when we looked at Eq.(7.30). Considering Eq.(7.50) again, the wedge shaped region, to be filled with an associated “fan” of characteristics, is described by (similar to Eq.(7.32))

$$\begin{aligned} u &= u_0, & x &= \frac{5u_0 t}{3}, & t &\geq 0 \\ u &= u_I, & x &= \frac{5u_I t}{3}, & t &\geq 0 \end{aligned} \quad (7.53)$$

The similarity transform solution we defined previously (recall Eq.(7.7)) provides a rarefaction wave solution that satisfies both the governing equation, Eq.(7.1), and, after setting $c = \frac{5u}{3}$, the boundary conditions described by Eq.(7.53). Consequently, it can be further stated that

$$u = \frac{3x}{5t}, \quad x \in \left(\frac{5u_0 t}{3}, \frac{5u_I t}{3} \right), \quad t \geq 0 \quad (7.54)$$

Utilizing this rarefaction wave to fill the wedged-shaped region, $x \in \left(\frac{5u_0t}{3}, \frac{5u_I t}{3}\right)$, leads to the analytical solution for the complete problem:

$$u(x, t) = \begin{cases} u_0, & x \leq \frac{5u_0t}{3} \\ \frac{3x}{5t}, & \frac{5u_0t}{3} < x < \frac{5u_I t}{3} \\ u_I, & x \geq \frac{5u_I t}{3} \end{cases}, \quad u_0 < u_I \quad (7.55)$$

(b) A MATLAB function for evaluating Eqs. (7.52) and (7.55) is given in Listing 7.1.

Listing 7.1 A MATLAB function for evaluating the method of characteristics solution given by Eqs. (7.52) and (7.55).

```
function u=MoCsolaFun(x,t,uI,u0)
%Analytical solution for kinematic wave equation
%with u(x,0)=u0 for x<=0 and u(x,0)=uI elsewhere
%u - Fluid velocity (m/s)
%x - Distance (m)
%t - Time (s)
%uI - Initial velocity (m/s)
%u0 - Boundary velocity (m/s)
if u0>uI
u=(u0-uI)*(x<=5/6*(u0+uI)*t)+uI;
else
u=3/5*x./t;
u(x<=5/3*u0*t)=u0;
u(x>=5/3*uI*t)=uI;
end
```

The MATLAB code listed below utilizes the MoCsolaFun function from Listing 7.1 to generate the results shown in Fig. 7.5.

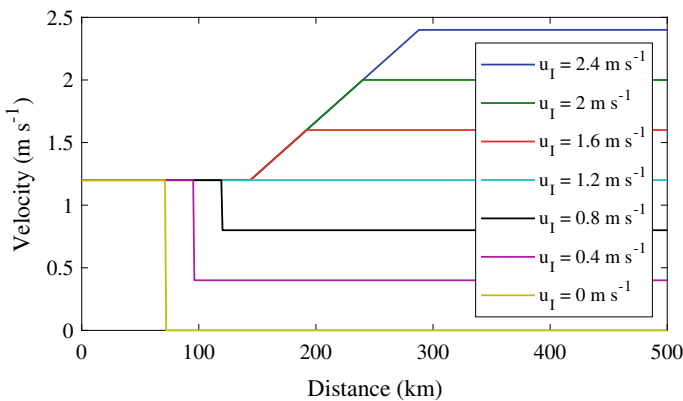


Fig. 7.5 Plots of velocity against distance after 20h according to the kinematic wave equation (i.e., with $c = \frac{5u}{3}$), for a constant inlet velocity of 1.2 m s^{-1} and a uniform initial velocity, u_I , as indicated in the legend

```

x=linspace(0,500e3,500)'; %Space points (m)
t=20*60^2; %Time (s)
uI=[2.4:-0.4:0]; %Initial velocities (m/s)
u0=1.2; %Boundary velocity (m/s)
figure(2);clf;box on;hold on %Make figure
for k=1:numel(uI)
%Analytical solution
u=MoCsolAFun(x,t,uI(k),u0);
plot(x/1000,u) %Plot results
%Add to legend
MYlegend{k}=['u_I = ' num2str(uI(k))' m s^-1'];
end
xlabel('Distance (km)')
ylabel('Velocity (m s^-1)')
legend(MYlegend,'location','southeast')

```

It can be seen that when $u_I < u_0$, there is a shock wave present. This is because water particles upstream of the shock wave are moving faster than water particles downstream of the shock. In contrast when $u_I > u_0$, there is a rarefaction wave instead. This is because water particles upstream of the rarefaction wave are moving slower than water particles downstream of the change. Study Fig. 7.2c to see how the rarefaction wave develops with time.

Worked Solution 7.3 (see Problem 7.3)

(a) In this case

$$\frac{\partial u}{\partial t} + \frac{5u}{3} \frac{\partial u}{\partial x} = 0$$

and

$$u(x, 0) = \begin{cases} u_0, & x \in [0, x_0] \\ 0, & x \notin [0, x_0] \end{cases}$$

To utilize the analytical solution given by Eqs. (7.43) and (7.44), we need to modify the above problem such that it looks more like when Eq. (7.36) with $c = u$. To this end we will apply the dimensionless transformations

$$u_D = \frac{u}{u_0} \quad \text{and} \quad x_D = \frac{x}{x_0} \quad (7.56)$$

such that

$$\frac{\partial u_D}{\partial t} + \frac{5u_0 u_D}{3x_0} \frac{\partial u_D}{\partial x_D} = 0$$

and

$$u_D(x, 0) = \begin{cases} 1, & x_D \in [0, 1] \\ 0, & x_D \notin [0, 1] \end{cases}$$

It follows that a sensible dimensionless transformation for time is

$$t_D = \frac{5u_0 t}{3x_0} \quad (7.57)$$

such that

$$\frac{\partial u_D}{\partial t_D} + u_D \frac{\partial u_D}{\partial x_D} = 0$$

Considering again Eqs. (7.43) and (7.44) then reveals that

$$u_D(x_D, t_D) = \begin{cases} 0, & x_D \leq 0 \\ \frac{x_D}{t_D}, & 0 < x_D < t_D \\ 1, & t_D \leq x_D < \frac{t_D}{2} + 1 \\ 0, & x_D \geq \frac{t_D}{2} + 1 \end{cases}, \quad t_D < 2 \quad (7.58)$$

and

$$u_D(x_D, t_D) = \begin{cases} 0, & x_D \leq 0 \\ \frac{x_D}{t_D}, & 0 < x_D < \sqrt{2t_D}, \quad t_D \geq 2 \\ 0, & x_D \geq \sqrt{2t_D} \end{cases} \quad (7.59)$$

(b) A MATLAB function for evaluating Eqs. (7.58) and (7.59) is given in Listing 7.2.

Listing 7.2 A MATLAB function for evaluating the method of characteristics solution given by Eqs. (7.58) and (7.59).

```
function u=MoCsolBFun(x,t,u0,x0)
%Analytical solution for kinematic wave equation
%with u(x,0)=u0 for 0<x<xI and u(x,0)=0 elsewhere
%u - Fluid velocity (m/s)
%x - Distance (m)
%t - Time (s)
%u0 - Maximum velocity (m/s)
%x0 - Spatial extent of velocity wave (m)
xD=x/x0; %Dimensionless transform
tD=5*u0*t/3/x0; %Dimensionless transform
uD=xD./tD;
uD(xD<0,:)=0;
uD(xD>tD&tD<2)=1;
uD(xD>tD/2+1&tD<2)=0;
uD(xD>sqrt(2*tD)&tD>=2)=0;
u=u0*uD; %Reverse dimensionless transform
```

The MATLAB code listed below utilizes the MoCsolBFun function from Listing 7.2 to generate the results shown in Fig. 7.6.

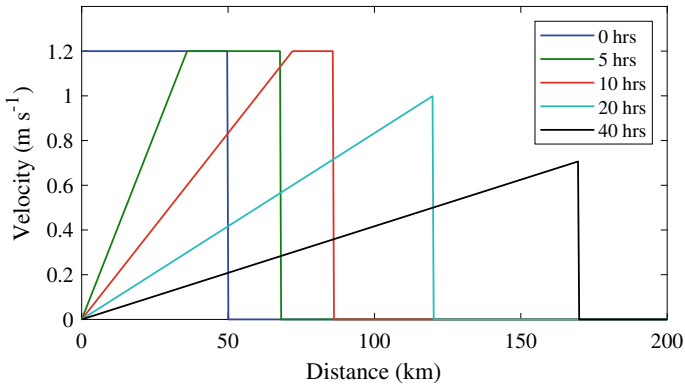


Fig. 7.6 Plots of velocity against distance according to the kinematic wave equation (i.e., with $c = \frac{5u}{3}$) for different times as indicated in the legend

```
x=linspace(0,200e3,500)'; %Space points (m)
t=[0 5 10 20 40]*60^2; %Time points (s)
u0=1.2; %Maximum velocity (m/s)
x0=50e3; %Spatial extent of velocity wave (m)
%Analytical solution
u=MoCsolBFun(x,t,u0,x0);
figure(3);clf;box on %Plot results
plot(x/1000,u)
xlabel('Distance (km)')
ylabel('Velocity (m s⁻¹)')
legend('0 hrs','5 hrs','10 hrs','20 hrs','40 hrs')
```

References

1. R.J. LeVeque, *Numerical Methods for Conservation Laws*, 2nd edn. (Birkhauser Verlag, 1992)
2. R. Knobel, *An Introduction to the Mathematical Theory of Waves*, vol. 3 (American Mathematical Society, 2000)
3. M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Tenth Printing (National Bureau of Standards Applied Mathematics, 1972)

Convolution Solution for the Diffusion Wave Equation

8

Abstract

This chapter explains how to use Laplace transforms to derive analytical solutions for a one-dimensional diffusion wave equation with an additional decay term and a time-varying boundary condition. A dependant variable transform is designed to reduce the diffusion wave and decay equation to a simple diffusion equation. The Laplace transform is used to reduce the resulting partial differential equation to a linear, second-order, ordinary differential equation. An analytical solution is developed in the Laplace transform domain and inverted back to the time domain using a table of Laplace transforms. A constant flow rate boundary is applied, leading to an analytical solution in terms of complementary error functions. When the decay term can be ignored, this latter equation reduces to the Ogata-Banks solution. An instantaneous water release boundary condition is applied, leading to an impulse response function made up of exponential functions. The analytical solution for an arbitrary time-varying boundary condition is found by convolving a boundary condition function with the aforementioned impulse response function. Practical applications are presented through a problem sheet with worked solutions.

Notation

c	Wave speed [LT^{-1}].
$\hat{f}(s)$	The Laplace transform of a function, $f(t)$ [-].
$G(x, t)$	Impulse response function [-].
$H(t)$	Heaviside step function [-].
K	Apparent diffusion coefficient [L^2T^{-1}].
Q	Flow rate [L^3T^{-1}].
$\bar{Q}_0$	Constant boundary flow rate [L^3T^{-1}].
$\bar{Q}_0(t)$	Variable boundary flow rate [L^3T^{-1}].
Q_I	Uniform initial flow rate [L^3T^{-1}].

s	Laplace transform variable [T^{-1}].
t	Time [T].
U	Dimensionless dependent variable transform [-].
V_0	Volume of water instantaneously released at a boundary [L^3].
x	Horizontal distance in the x -direction [L].
α	Transform coefficient [L^{-1}].
β	Transform coefficient [T^{-1}].
$\delta(T)$	Dirac delta function [T^{-1}].
κ	Decay coefficient [T^{-1}].
τ	Auxiliary time [T].

8.1 Introduction

This chapter focuses on the derivation of an analytical solution for the diffusion wave equation (recall Sect. 6.6) with an additional decay term. The Ogata-Banks solution [1], discussed previously in Sect. 6.6.2, represents a special case where there is a constant flow rate boundary condition and zero decay.

An analytical solution for a constant flow rate boundary is obtained using Laplace transforms. The resulting equation is differentiated with respect to time to obtain an analytical solution describing an instantaneous water release. This latter solution is used within a convolution integral to obtain analytical solutions for time-varying flow rate boundaries.

8.1.1 Governing Equations

Consider a one-dimensional diffusion wave equation with an additional decay term

$$\frac{\partial Q}{\partial t} = K \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} - \kappa \cdot (Q - Q_I) \quad (8.1)$$

subjected to the following constraints:

$$\begin{aligned} Q &= Q_I, & x &> 0, & t &= 0 \\ Q &= \tilde{Q}_0(t), & x &= 0, & t &\geq 0 \\ Q &= Q_I, & x &\rightarrow \infty, & t &> 0 \end{aligned} \quad (8.2)$$

where Q [L^3T^{-1}] is flow rate, K [L^2T^{-1}] is the apparent diffusion coefficient, c [LT^{-1}] is the wave speed, κ [T^{-1}] is a decay coefficient, which can be used to account for losses of flow rate due to sedimentation (e.g. [2]), Q_I [L^3T^{-1}] is a uniform initial flow rate and $\tilde{Q}_0(t)$ is a time-varying flow rate applied at the inlet boundary.

8.2 Constant Flow Rate Boundary

First we will consider the case where

$$\tilde{Q}_0(t) = (Q_0 - Q_I)H(t) + Q_I \quad (8.3)$$

with Q_0 [L^3T^{-1}] being a constant flow rate applied at the inlet boundary and $H(t)$ being the Heaviside step function

$$H(t) = \begin{cases} 0, & t \leq 0 \\ 1, & t > 0 \end{cases} \quad (8.4)$$

8.2.1 Reduction to a Diffusion Equation

The above problem is greatly simplified by making the following dependent variable transform

$$Q(x, t) = (Q_0 - Q_I)U(x, t)e^{\alpha x - \beta t} + Q_I \quad (8.5)$$

where $U(x, t)$ is the new dependent variable and α and β are coefficients yet to be defined.

Challenge 8.1 Substitute Eq. (8.5) into Eq. (8.1) and derive expressions for α and β such that Eq. (8.1) reduces to a simple diffusion equation (i.e., with no advection term or decay term).

Partial differentiation of Eq. (8.5) with respect to t gives

$$\frac{\partial Q}{\partial t} = (Q_0 - Q_I) \left[-\beta U(x, t) + \frac{\partial U}{\partial t} \right] e^{\alpha x - \beta t} \quad (8.6)$$

Partial differentiation of Eq. (8.5) with respect to x gives

$$\frac{\partial Q}{\partial x} = (Q_0 - Q_I) \left[\alpha U(x, t) + \frac{\partial U}{\partial x} \right] e^{\alpha x - \beta t} \quad (8.7)$$

Partial differentiation of Eq. (8.7) with respect to x gives

$$\frac{\partial^2 Q}{\partial x^2} = (Q_0 - Q_I) \left[\alpha^2 U(x, t) + 2\alpha \frac{\partial U}{\partial x} + \frac{\partial^2 U}{\partial x^2} \right] e^{\alpha x - \beta t} \quad (8.8)$$

Substituting Eqs. (8.5) to (8.8) into Eq. (8.1) leads to

$$\frac{\partial U}{\partial t} = K \frac{\partial^2 U}{\partial x^2} - (c - 2\alpha K) \frac{\partial U}{\partial x} - (\kappa + \alpha c - K\alpha^2 - \beta) U$$

which further reduces to a simple diffusion equation

$$\frac{\partial U}{\partial t} = K \frac{\partial^2 U}{\partial x^2} \quad (8.9)$$

when

$$\alpha = \frac{c}{2K} \quad \text{and} \quad \beta = \frac{c^2}{4K} + \kappa \quad (8.10)$$

Meanwhile, the initial and boundary conditions, given in Eq. (8.2), transform to

$$\begin{aligned} U &= 0, & x > 0, & \quad t = 0 \\ U &= H(t)e^{\beta t}, & x = 0, & \quad t > 0 \\ U &= 0, & x \rightarrow \infty, & \quad t > 0 \end{aligned} \quad (8.11)$$

8.2.2 Solution by Laplace Transform

The simplified boundary value problem described by Eqs. (8.9) and (8.11) is best solved by Laplace transform due to the time varying boundary condition in Eq. (8.11). A particularly useful aspect is that the Laplace transform, reduces a partial differential equation in time and space to an ordinary differential equation in space.

Let $\hat{f}(s)$ be the Laplace transform of $f(t)$, i.e. [3, p. 162],

$$\hat{f}(s) = \int_0^\infty f(t)e^{-st} dt \quad (8.12)$$

where s is the Laplace transform variable. Relevant inverse Laplace transforms for solving this problem are provided in Table 8.1.

Challenge 8.2 Use the Laplace transform to derive an analytical solution for the boundary value problem, described by Eqs. (8.9) and (8.11), in terms of a convolution integral.

Applying the Laplace transform to Eqs. (8.9) and (8.11) leads to [3, p. 214]

$$s\hat{U} = K \frac{\partial^2 \hat{U}}{\partial x^2} \quad (8.13)$$

Table 8.1 A selection of inverse Laplace transforms from [4, pp. 1020–1026]. Note that $\delta(t)$ and $H(t)$ denote the Dirac delta function and Heaviside step function, respectively

	$\hat{f}(s)$	$f(t)$
(i)	1	$\delta(t)$
(ii)	$\frac{1}{s}$	1
(iii)	$s\hat{f}(s) - f(0)$	$\frac{df}{dt}$
(iv)	$e^{-as}\hat{f}(s)$	$f(t-a)H(t-a)$
(v)	$\frac{1}{s+a}$	e^{-at}
(vi)	$e^{-a\sqrt{s}}$	$\frac{a}{2\sqrt{\pi t^3}} \exp\left(-\frac{a^2}{4t}\right)$
(vii)	$\hat{f}(s)\hat{g}(s)$	$\int_0^t f(t-\tau)g(\tau)d\tau$

and

$$\begin{aligned}\hat{U} &= \frac{1}{s-\beta}, \quad x = 0 \\ \hat{U} &= 0, \quad x \rightarrow \infty\end{aligned}\quad (8.14)$$

Recall that the general solution of an ordinary differential equation of the form

$$a \frac{d^2 y}{dx^2} + b \frac{dy}{dx} + cy = 0 \quad (8.15)$$

is [5, p. 1093]

$$y(x) = A_1 \exp \left[\left(\frac{-b + \sqrt{b^2 - 4ac}}{2a} \right) x \right] + A_2 \exp \left[\left(\frac{-b - \sqrt{b^2 - 4ac}}{2a} \right) x \right] \quad (8.16)$$

where A_1 and A_2 are unknown constants defined by any associated boundary conditions.

The general solution for Eq. (8.13) is therefore

$$\hat{U}(x, s) = A_1 \exp \left[\left(\frac{s}{K} \right)^{1/2} x \right] + A_2 \exp \left[- \left(\frac{s}{K} \right)^{1/2} x \right]$$

and application of the boundary conditions in Eq. (8.14) leads to

$$\hat{U}(x, s) = \frac{1}{s - \beta} \exp \left[- \left(\frac{s}{K} \right)^{1/2} x \right]$$

Considering Table 8.1, let us set $\hat{U}(x, s) = \hat{f}(s)\hat{g}(x, s)$ where

$$\hat{f}(s) = \frac{1}{s - \beta} \quad \text{and} \quad \hat{g}(x, s) = \exp \left[- \left(\frac{s}{K} \right)^{1/2} x \right]$$

An analytical solution for $U(x, t)$ can therefore be written as a convolution integral in the form

$$U(x, t) = \int_0^t f(t - \tau) g(x, \tau) d\tau \quad (8.17)$$

where

$$f(t) = e^{\beta t} \quad \text{and} \quad g(x, t) = \frac{x}{2\sqrt{\pi K t^3}} \exp \left(-\frac{x^2}{4Kt} \right)$$

8.2.3 Writing in Terms of Error Functions

Substituting the expressions for $f(t)$ and $g(x, t)$ into Eq. (8.17) and factorising out the constants leads to

$$U(x, t) = \frac{x e^{\beta t}}{2\sqrt{\pi K}} \int_0^t \frac{1}{\sqrt{\tau^3}} \exp \left(-\beta \tau - \frac{x^2}{4K\tau} \right) d\tau \quad (8.18)$$

A relevant integral identity is [4, p. 304]

$$\int \exp \left(-a^2 x^2 - \frac{b^2}{x^2} \right) dx = \frac{\sqrt{\pi}}{4a} \left[e^{2ab} \operatorname{erf} \left(ax + \frac{b}{x} \right) + e^{-2ab} \operatorname{erf} \left(ax - \frac{b}{x} \right) \right] \quad (8.19)$$

where $\text{erf}(x)$ denotes the error function defined by

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-z^2} dz \quad (8.20)$$

To make Eq. (8.18) look more like Eq. (8.19) we need to make the substitutions $\zeta^{-2} = \tau$ and $\xi^{-2} = t$ such that

$$U(x, t) = \frac{x e^{\beta t}}{\sqrt{\pi K}} \int_{\xi}^{\infty} \exp\left(-\frac{x^2 \zeta^2}{4K} - \frac{\beta}{\zeta^2}\right) d\zeta \quad (8.21)$$

Comparing Eqs. (8.19) and (8.21) then leads to

$$\begin{aligned} U(x, t) = \frac{e^{\beta t}}{2} & \left[\exp\left(\sqrt{\frac{\beta x^2}{K}}\right) \text{erf}\left(\sqrt{\frac{x^2 \zeta^2}{4K}} + \sqrt{\frac{\beta}{\zeta^2}}\right) \right. \\ & \left. + \exp\left(-\sqrt{\frac{\beta x^2}{K}}\right) \text{erf}\left(\sqrt{\frac{x^2 \zeta^2}{4K}} - \sqrt{\frac{\beta}{\zeta^2}}\right) \right]_{\xi}^{\infty} \end{aligned}$$

Noting that $\text{erf}(\infty) = 1$ it follows that

$$\begin{aligned} U(x, t) = \frac{e^{\beta t}}{2} & \left[\exp\left(\sqrt{\frac{\beta x^2}{K}}\right) \text{erfc}\left(\sqrt{\frac{x^2 \xi^2}{4K}} + \sqrt{\frac{\beta}{\xi^2}}\right) \right. \\ & \left. + \exp\left(-\sqrt{\frac{\beta x^2}{K}}\right) \text{erfc}\left(\sqrt{\frac{x^2 \xi^2}{4K}} - \sqrt{\frac{\beta}{\xi^2}}\right) \right] \end{aligned}$$

where $\text{erfc}(x) = 1 - \text{erf}(x)$ is the complementary error function.

Reversing the substitutions of U and ξ then leads to [6]

$$\begin{aligned} \frac{Q(x, t) - Q_I}{Q_0 - Q_I} = \frac{1}{2} & \left[\exp\left(\alpha x + \sqrt{\frac{\beta x^2}{K}}\right) \text{erfc}\left(\sqrt{\frac{x^2}{4Kt}} + \sqrt{\beta t}\right) \right. \\ & \left. + \exp\left(\alpha x - \sqrt{\frac{\beta x^2}{K}}\right) \text{erfc}\left(\sqrt{\frac{x^2}{4Kt}} - \sqrt{\beta t}\right) \right] \quad (8.22) \end{aligned}$$

where α and β are as defined in Eq. (8.10).

8.2.4 Limiting Cases

When there is no decay, we have $\kappa = 0$, $\alpha = \frac{c}{2K}$ and $\beta = \frac{c^2}{4K}$, which leads to

$$\lim_{\kappa \rightarrow 0} \left\{ \frac{Q(x, t) - Q_I}{Q_0 - Q_I} \right\} = \frac{1}{2} \left[\exp\left(\frac{cx}{K}\right) \text{erfc}\left(\frac{x + ct}{2\sqrt{Kt}}\right) + \text{erfc}\left(\frac{x - ct}{2\sqrt{Kt}}\right) \right] \quad (8.23)$$

The above equation is commonly referred to as the Ogata-Banks solution after [1].

When there is no advection, we have $c = 0$, $\alpha = 0$ and $\beta = \kappa$ such that

$$\lim_{c \rightarrow 0} \left\{ \frac{Q(x, t) - Q_I}{Q_0 - Q_I} \right\} = \frac{1}{2} \left[\exp \left(\sqrt{\frac{\kappa x^2}{K}} \right) \operatorname{erfc} \left(\sqrt{\frac{x^2}{4Kt}} + \sqrt{\kappa t} \right) + \exp \left(-\sqrt{\frac{\kappa x^2}{K}} \right) \operatorname{erfc} \left(\sqrt{\frac{x^2}{4Kt}} - \sqrt{\kappa t} \right) \right] \quad (8.24)$$

which is often used to look at the diffusion and decay of radionuclides.

When there is no advection and no decay we have the complementary error function solution of the basic diffusion problem

$$\lim_{\substack{\kappa \rightarrow 0 \\ c \rightarrow 0}} \left\{ \frac{Q(x, t) - Q_I}{Q_0 - Q_I} \right\} = \operatorname{erfc} \left(\frac{x}{2\sqrt{Kt}} \right) \quad (8.25)$$

8.3 Instantaneous Water Release

The analytical solution given by Eq. (8.22) assumes a constant value boundary condition (recall Eq. (8.3)). An alternative and useful boundary condition includes

$$\tilde{Q}_0(t) = V_0 \delta(t) + Q_I \quad (8.26)$$

where V_0 [L^3] represents a volume of water that is instantaneously released at the boundary and $\delta(t)$ denotes the Dirac delta function, defined by

$$\delta(t) = \begin{cases} \infty, & t = 0 \\ 0, & t \neq 0 \end{cases} \quad (8.27)$$

Note that

$$\frac{dH(t)}{dt} = \delta(t) \quad (8.28)$$

Comparing Eqs. (8.3) and (8.26), it follows that Eq. (8.22) can be modified to account for Eq. (8.26) by differentiating with respect to t and setting $Q_0 - Q_I = V_0$.

Challenge 8.3 Modify Eq. (8.22) such that it conforms to the boundary condition prescribed by Eq. (8.26).

Differentiation of Eq. (8.22) is made easier by making the substitutions:

$$F_1 = \operatorname{erfc}(z_1) = 1 - \operatorname{erf}(z_1) \quad (8.29)$$

$$F_2 = \operatorname{erfc}(z_2) = 1 - \operatorname{erf}(z_2) \quad (8.30)$$

$$z_1 = \sqrt{\frac{x^2}{4Kt}} + \sqrt{\beta t} \quad (8.31)$$

$$z_2 = \sqrt{\frac{x^2}{4Kt}} - \sqrt{\beta t} \quad (8.32)$$

such that Eq. (8.22) reduces to

$$\frac{Q(x, t) - Q_I}{Q_0 - Q_I} = \frac{e^{\alpha x}}{2} \left[\exp \left(\sqrt{\frac{\beta x^2}{K}} \right) F_1 + \exp \left(-\sqrt{\frac{\beta x^2}{K}} \right) F_2 \right] \quad (8.33)$$

Following the discussion above, it follows that

$$\frac{Q(x, t) - Q_I}{V_0} = \frac{e^{\alpha x}}{2} \left[\exp \left(\sqrt{\frac{\beta x^2}{K}} \right) \frac{\partial F_1}{\partial t} + \exp \left(-\sqrt{\frac{\beta x^2}{K}} \right) \frac{\partial F_2}{\partial t} \right] \quad (8.34)$$

provides an analytical solution for $Q(x, t)$ that satisfies the instantaneous input boundary condition, Eq. (8.26).

Using the chain rule, it can be said that:

$$\frac{\partial F_1}{\partial t} = \frac{\partial z_1}{\partial t} \frac{\partial F_1}{\partial z_1} \quad (8.35)$$

$$\frac{\partial F_2}{\partial t} = \frac{\partial z_2}{\partial t} \frac{\partial F_2}{\partial z_2} \quad (8.36)$$

From Eqs. (8.31) and (8.32) it can be seen that

$$\frac{\partial z_1}{\partial t} = -\frac{z_2}{2t} \quad (8.37)$$

$$\frac{\partial z_2}{\partial t} = -\frac{z_1}{2t} \quad (8.38)$$

From Eqs. (8.20), (8.29) and (8.30) we have

$$\frac{\partial F_1}{\partial z_1} = -\frac{2}{\sqrt{\pi}} e^{-z_1^2} \quad (8.39)$$

$$\frac{\partial F_2}{\partial z_2} = -\frac{2}{\sqrt{\pi}} e^{-z_2^2} \quad (8.40)$$

Substituting Eqs. (8.37) and (8.39) into Eqs. (8.35) and Eqs. (8.38) and (8.40) into Eq. (8.36) leads to

$$\frac{\partial F_1}{\partial t} = \frac{z_2}{\sqrt{\pi t}} e^{-z_1^2} \quad (8.41)$$

$$\frac{\partial F_2}{\partial t} = \frac{z_1}{\sqrt{\pi t}} e^{-z_2^2} \quad (8.42)$$

Substituting Eqs. (8.41) and (8.42) into Eq. (8.34) yields

$$Q(x, t) = V_0 G(x, t) + Q_I \quad (8.43)$$

where

$$G(x, t) = \frac{e^{\alpha x}}{2\sqrt{\pi t}} \left[z_2 \exp \left(\sqrt{\frac{\beta x^2}{K}} - z_1^2 \right) + z_1 \exp \left(-\sqrt{\frac{\beta x^2}{K}} - z_2^2 \right) \right] \quad (8.44)$$

which is sometimes referred to as an impulse response function.

8.4 Time-Varying Flow Rate Boundary

Here we will derive an analytical solution for the more general problem defined by Eqs. (8.1) and (8.2). The first step involves deriving an analytical solution in the Laplace transform domain. This is then inverted back to the time domain using a convolution integral, which contains a kernel function that turns out to be the impulse response function associated with our previous analytical solution concerning an instantaneous water release (i.e., Eq. (8.44)).

8.4.1 Laplace Transform Solution

Challenge 8.4 Apply the Laplace transform to Eqs. (8.1) and (8.2).

Applying the Laplace transform to the Eqs. (8.1) and (8.2) leads to:

$$s\hat{Q} - Q_I = K \frac{d^2 \hat{Q}}{dx^2} - c \frac{d\hat{Q}}{dx} - \kappa \cdot \left(\hat{Q} - \frac{Q_I}{s} \right) \quad (8.45)$$

and

$$\begin{aligned} \hat{Q} &= \hat{Q}_0, \quad x = 0 \\ \hat{Q} &= \frac{Q_I}{s}, \quad x \rightarrow \infty \end{aligned} \quad (8.46)$$

Challenge 8.5 Derive an analytical solution, in the Laplace transform domain, for Eqs. (8.45) and (8.46).

Equation (8.45) can be rearranged to get

$$K \frac{d^2 \hat{Q}}{dx^2} - c \frac{d\hat{Q}}{dx} - (s + \kappa) \cdot \left(\hat{Q} - \frac{Q_I}{s} \right) = 0 \quad (8.47)$$

According to Eqs. (8.15) and (8.16), the general solution to Eq. (8.47) is

$$\hat{Q} - \frac{Q_I}{s} = B_1 \exp \left[\left(\frac{c + \sqrt{c^2 + 4K(s + \kappa)}}{2K} \right) x \right] + B_2 \exp \left[\left(\frac{c - \sqrt{c^2 + 4K(s + \kappa)}}{2K} \right) x \right]$$

Given the far-field boundary condition in Eq. (8.46), it can be understood that $B_1 = 0$. Given the near-field boundary condition in Eq. (8.46), it can be understood that $B_2 = \hat{Q}_0 - \frac{Q_I}{s}$. It follows that

$$\hat{Q} - \frac{Q_I}{s} = \left(\hat{Q}_0 - \frac{Q_I}{s} \right) \exp \left[\left(\frac{c - \sqrt{c^2 + 4K(s + \kappa)}}{2K} \right) x \right] \quad (8.48)$$

8.4.2 Writing in Terms of a Convolution Integral

Let

$$\hat{G}(x, s) = \exp \left[\left(\frac{c - \sqrt{c^2 + 4K(s + \kappa)}}{2K} \right) x \right] \quad (8.49)$$

such that

$$\hat{Q}(x, s) - \frac{Q_I}{s} = \left(\hat{Q}_0 - \frac{Q_I}{s} \right) \hat{G}(x, s) \quad (8.50)$$

Considering the inverse Laplace transform of $\hat{f}(s)\hat{g}(s)$ in Table 8.1, it follows that

$$Q(x, t) = \int_0^t [\tilde{Q}_0(t - \tau) - Q_I] G(x, \tau) d\tau + Q_I \quad (8.51)$$

where $G(x, t)$ is the inverse Laplace transform of $\hat{G}(x, s)$.

8.4.3 Consideration of the Instantaneous Water Release Solution

The impulse response function, $G(x, t)$, can be found by considering Eq. (8.51) in the context of the instantaneous water release boundary condition given in Eq. (8.26).

Let $\tilde{Q}_0(t - \tau) = V_0\delta(t - \tau) + Q_I$ such that

$$Q(x, t) = V_0 \int_0^t \delta(t - \tau) G(x, \tau) d\tau + Q_I \quad (8.52)$$

Given Eq. (8.27), we have that $\delta(t - \tau) = 0$ for $\tau \neq t$. Given Eq. (8.28), we have that $\int_0^t \delta(t - \tau) d\tau = 1$. Consequently it can be said that

$$\int_0^t \delta(t - \tau) G(x, \tau) d\tau = G(x, t) \quad (8.53)$$

and therefore

$$Q(x, t) = V_0 G(x, t) + Q_I \quad (8.54)$$

Comparing Eqs. (8.54) and (8.43), it can then be understood that $G(x, t)$ is the function previously defined by Eq. (8.44).

8.5 Problem Sheet

Problem 8.1 (see Worked Solution 8.1)

A river flows from a dammed reservoir at a steady rate of $60 \text{ m}^3 \text{ s}^{-1}$. The river is characterised by an apparent diffusion coefficient of $1000 \text{ m}^2 \text{ s}^{-1}$ and a wave speed of 1 m s^{-1} . The dam fails, instantaneously releasing an additional 40 million m^3 water. This scenario is based on a case study described by [2] and [7].

- Generate plots of expected river flow rate against time at 70, 140, 210 and 280 km downstream of the dam failure, assuming the reservoir water is sediment free.
- In practice, water released from the reservoir will be high in suspended sediments. Take into account loss of flow rate due to sedimentation by repeating the exercise in part (a) assuming $\kappa = 0.1 \text{ day}^{-1}$ and then again with $\kappa = 0.3 \text{ day}^{-1}$.

Problem 8.2 (see Worked Solution 8.2)

Consider a river where $K = 1000 \text{ m}^2 \text{ s}^{-1}$, $c = 1 \text{ m s}^{-1}$ and $\kappa = 0.3 \text{ day}^{-1}$. The river initially has a uniform flow rate of $60 \text{ m}^3 \text{ s}^{-1}$. The flow rate at the inlet is then suddenly increased and maintained at a constant value of $750 \text{ m}^3 \text{ s}^{-1}$.

- Use the impulse response function, Eq. (8.44), in conjunction with the convolution integral, Eq. (8.51), to obtain a plot of flow rate against time for a location 50 km downstream of the inlet. Hint: use MATLAB's `conv` function.
- Obtain a plot of flow rate against time for a location 50 km downstream of the inlet using Eq. (8.22) and compare your results with those from part (a).

Problem 8.3 (see Worked Solution 8.3)

Consider a river where $K = 1000 \text{ m}^2 \text{ s}^{-1}$, $c = 1 \text{ m s}^{-1}$ and $\kappa = 0 \text{ day}^{-1}$. The river initially has a uniform initial flow rate of $60 \text{ m}^3 \text{ s}^{-1}$. The inlet river flow rate follows the following time-series:

t (hours)	0	5	10	15	20	25	100
$\bar{Q}_0$ ($\text{m}^3 \text{ s}^{-1}$)	60	1000	100	100	1200	200	200

Assume that the inlet flow rate varies linearly with time in between the times listed above and use convolution to develop plots of flow rate against time at 70, 140 km and 210 km downstream of the inlet.

8.6 Worked Solutions

Worked Solution 8.1 (see Problem 8.1)

For this problem, we can use the analytical solution describing an instantaneous water release given by Eq. (8.43). A MATLAB function for evaluating Eq. (8.43) is given in Listing 8.1.

Listing 8.1 A MATLAB function for evaluating the analytical solution describing an instantaneous water release given by Eq. (8.43)

```
function Q=ImpulseFun(x,t,V0,QI,K,c,k)
%Analytical solution for advection dispersion
%equation with decay subject to an instantaneous
%release of water
%Q - Flow rate (m3/s)
%x - Distance from inlet (m)
%t - Time (s)
%V0 - Volume of water released (m3)
%QI - Uniform initial flow rate (m3/s)
%K - Apparent diffusion coefficient (m2/s)
%c - Wave speed (m/s)
%k - Decay rate (1/s)
a=c/2./K;
b=c.^2/4./K+k;
z1=sqrt(x.^2/4./K./t)+sqrt(b.*t);
z2=sqrt(x.^2/4./K./t)-sqrt(b.*t);
F1=z2.*exp(sqrt(b.*x.^2./K)-z1.^2);
F2=z1.*exp(-sqrt(b.*x.^2./K)-z2.^2);
G=exp(a.*x)/2/sqrt(pi)./t.*(F1+F2);
G(isnan(G))=0; %Nan values are actually zero
Q=V0*G+QI;
```

The MATLAB code below utilizes the ImpulseFun function, given in Listing 8.1, to generate the results shown in Fig. 8.1.

```
K=1000; %Diffusion coefficient (m2/s)
c=1; %Wave speed (m/s)
%Decay coefficient (1/s)
k=reshape([0 0.1 0.3]/24/60^2,1,1,3);
QI=60; %Initial flow rate (m3/s)
V0=40e6; %Released water volume (m3)
x=[70 140 210 280]'*1e3; %Distance (m)
t=linspace(0,100*60^2,200); %Time (s)
%Determine flow rates
Q=ImpulseFun(x,t,V0,QI,K,c,k);
```

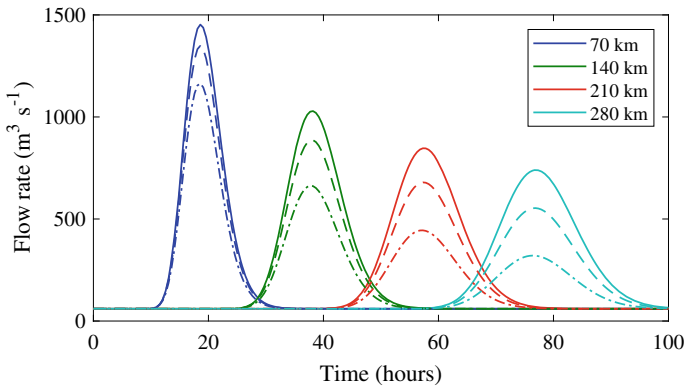


Fig. 8.1 Plots of flow rate against time for different locations downstream of a dam failure. The solid, dashed and dash-dot lines represent results from simulations with decay rates, $\kappa = 0, 0.1$ and 0.3 day^{-1} , respectively

```
figure(1);clf;hold on;box on %Plot results
plot(t/60^2,Q(:,:,1))
set(gca,'ColorOrderIndex',1)
plot(t/60^2,Q(:,:,2),'--')
set(gca,'ColorOrderIndex',1)
plot(t/60^2,Q(:,:,3),'-.')
xlabel('Time (hours)')
ylabel('Flow rate (m^3 s^-1)')
legend('70 km','140 km','210 km','280 km')
```

Although the water release is represented as an instantaneous process (recall Eq. (8.26)), the diffusion process leads to the flood wave becoming increasingly attenuated with increasing distance from the source (see Fig. 8.1). The effect of sediment removal is represented through the decay coefficient. Increasing the decay coefficient (compare the solid and dash-dot lines) leads to a reduction in flow rate, which becomes more pronounced with increasing distance from the source.

Worked Solution 8.2 (see Problem 8.2)

(a) This problem can be solved using the aforementioned `ImpulseFun` function (see Listing 8.1), in conjunction with MATLAB's `conv` function. We will choose to solve for 200 uniformly distributed times ranging from zero to 30 days. The inlet flow rate, $\tilde{Q}_0(t)$, therefore needs to be specified as an array of 200 values, all equal to $750 \text{ m}^3 \text{ s}^{-1}$. A corresponding set of impulse response function values, from $G(t)$, can be obtained using `ImpulseFun` with $V_0 = 1$ and $Q_I = 0$.

The convolution is achieved by inputting both $\tilde{Q}_0(t)$ and $G(t)$ into `conv` and multiplying the result by the uniform time interval between each time point studied;

this latter step is needed because `conv` automatically treats the time-intervals as each being one unit. Finally we need to exclude values generated beyond the specified 200 values because the additional results generated by `conv` are based on the impulse function continuing with no additional input from $\tilde{Q}_0(t)$. The instructions listed can be implemented using the MATLAB code detailed below:

```
function ConvolutionTest
K=1000; %Diffusion coefficient (m2/s)
c=1; %Wave speed (m/s)
k=0.3/24/60^2; %Decay rate (1/s)
QI=60; %Initial flow rate (m3/s)
Q0=750; %Boundary flow rate (m3/s)
x=50e3; %Distance (m)
N=200; %Number of time increments
t=linspace(0,30*60^2,N); %Time (s)
%Define inlet flow rate
Q0tilde=Q0*ones(size(t));
G=ImpulseFun(x,t,1,0,K,c,k); %Impulse function
%Apply Convolution
Q=conv(Q0tilde-QI,G)*(t(2)-t(1))+QI;
Q=Q(1:numel(t)); %Truncate impulse tail
figure(2); clf %Plot data
subplot(2,1,1);hold on;box on
plot(t/60^2,G*60^2,'k')
xlabel('Time (hours)')
ylabel('Impulse function (hour^-1)')
title('a')
subplot(2,1,2);hold on;box on
plot(t/60^2,Q,'g','linewidth',3)
xlabel('Time (hours)')
ylabel('Flow rate (m^3 s^-1)')
title('b')
```

(b) The convolution solution described in part (a) represents an approximate solution for the problem where $\tilde{Q}_0(t)$ is continuously held at a value Q_0 . The exact solution for this scenario is provided by Eq. (8.22), which can be evaluated using the `OgataBanksDecay` function given in Listing 8.2. Note that the `OgataBanksDecay` function extends the `OgataBanks` function (given in Listing 6.1) by accounting for decay.

Listing 8.2 A MATLAB function for evaluating the analytical solution for a constant flow rate boundary condition given by Eq. (8.22)

```
function Q=OgataBanksDecay(x,t,Q0,QI,K,c,k)
%Analytical solution for advection dispersion
%equation with decay subjected to a constant
%inlet flow rate
%Q - Flow rate (m3/s)
```

```

%x - Distance from inlet (m)
%t - Time (s)
%Q0 - Inlet flow rate (m3/s)
%QI - Uniform initial flow rate (m3/s)
%K - Apparent diffusion coefficient (m2/s)
%c - Wave speed (m/s)
%k - Decay rate (1/s)
a=c/2./K;
b=c.^2/4./K+k;
T1a=exp(a.*x+sqrt(b.*x.^2./K));
T1b=erfc(sqrt(x.^2/4./K./t)+sqrt(b.*t));
T1=T1a.*T1b;
T2a=exp(a.*x-sqrt(b.*x.^2./K));
T2b=erfc(sqrt(x.^2/4./K./t)-sqrt(b.*t));
T2=T2a.*T2b;
%Note that the limit of T1 as x-> inf = 0
T1(isnan(T1)|isinf(T1))=0;
Q=(Q0-QI)*(T1+T2)/2+QI;

```

The following MATLAB code can be appended to the function, ConvolutionTest listed in part (a), such that the OgataBanksDecay function (given in Listing 8.2) is called and the results are plotted alongside the convolution solution for comparison:

```

%Exact solution
Qexact=OgataBanksDecay(x,t,Q0,QI,K,c,k);
subplot(2,1,2)
plot(t/60^2,Qexact,'k')
legend('Convolution','Exact')

```

The results to part (a) and (b) are shown in Fig. 8.2b. A plot of the impulse response function is shown in Fig. 8.2a for reference. It can be seen that the convolution solution provides a good approximation to the exact solution. However, the accuracy of the convolution solution is dependent on the number of time increments used. The convolution solution becomes more accurate as the time-interval between increments is reduced.

Worked Solution 8.3 (see Problem 8.3)

This problem can be solved in a similar way to how we dealt with Problem 8.2a above. Here we will use 500 uniformly distributed time increments ranging from zero to 100 days. We will then use MATLAB's `interp1` function to linearly interpolate the $\tilde{Q}_0(t)$ values listed in the table provided in Problem 8.3. Following on from this, the array of values for $\tilde{Q}_0(t)$ can be convolved with an array of impulse response function values obtained from the `ImpulseFun` function (Listing 8.1), using MATLAB's `conv` function. A relevant MATLAB code is listed below:

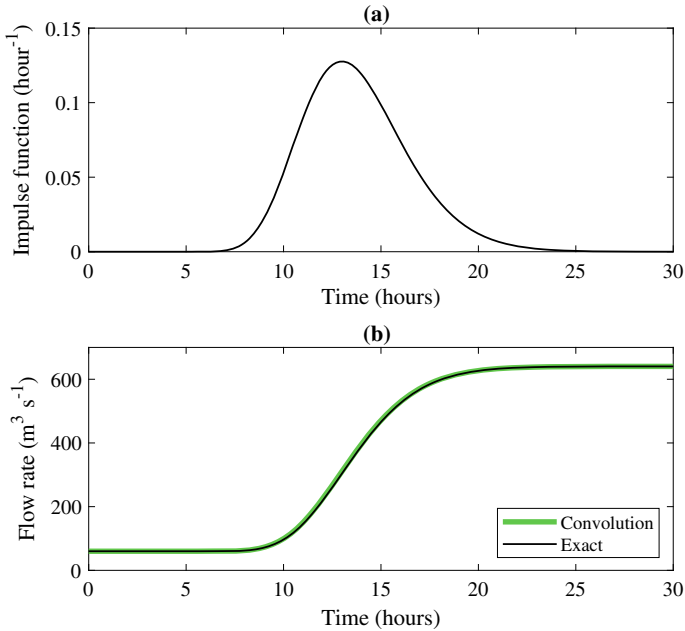


Fig. 8.2 **a** The impulse response function, $G(t)$, according to Eq. (8.44). **b** Plot of flow rate against time assuming a constant flow rate at the inlet. The green line is obtained by convolution using Eq. (8.21). The black line is from the exact solution given by Eq. (8.22)

```
K=1000; %Diffusion coefficient (m2/s)
c=1; %Wave speed (m/s)
k=0; %Decay rate (1/s)
QI=60; %Initial flow rate (m3/s)
x=[70 140 210]'*1e3; %Distance (m)
N=500; %Number of time increments
t=linspace(0,100*60^2,N); %Time (s)
%Define inlet flow rate
tPT=[0 5 10 15 20 25 100]*60^2;
Q0PT=[60 1000 100 100 1200 200 200];
%Interpolate Q0 to time grid
Q0tilde=interp1(tPT,Q0PT,t);
G=ImpulseFun(x,t,1,0,K,c,k); %Impulse function
for n=1:numel(x) %Apply Convolution
    Q(n,:)=conv(Q0tilde-QI,G(n,:))*(t(2)-t(1))+QI;
end
Q=Q(:,1:numel(t)); %Truncate impulse tail
figure(3);clf;hold on;box on %Plot data
plot(t/60^2,[Q0tilde;Q])
xlabel('Time (hours)')
```

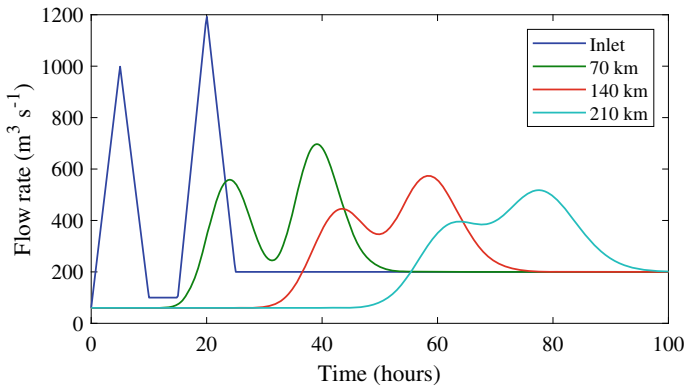


Fig. 8.3 Plot of flow rate against time for a river inlet along with additional locations downstream from the inlet, as indicated in the legend. The inlet flow rate is as specified in Problem 8.3

```
ylabel('Flow rate (m3 s-1)')
legend('Inlet', '70 km', '140 km', '210 km')
```

The results are shown in Fig. 8.3. Note how the two spikes in flow rate become increasingly smooth with distance from the inlet due to the attenuating effect of the diffusion process.

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Chemical and Heat Transport

9

Abstract

The diffusion wave equation is more commonly referred to as the advection dispersion equation. This chapter looks at how the advection dispersion equation with decay can be used to look at chemical and heat transport in porous media. The concepts of total and kinematic porosity are explained. A range of relevant transport processes are introduced including adsorption, microbial degradation, radioactive decay, molecular diffusion, hydrodynamic dispersion and heat conduction. It is explained how these processes can be incorporated into analytical solutions previously developed in Chap. 8. Simplified analytical solutions are also derived for when diffusion, dispersion and conduction can be ignored. Indicative parameter values for each of these processes are provided for a wide range of different scenarios. A selection of relevant practical applications are presented through a problem sheet with worked solutions.

Notation

A_T	Total cross-sectional area of a porous medium [L^2].
A_V	Cross-sectional area of voids in a plane of porous medium [L^2].
c_p	Specific heat capacity [$L^2T^{-2}\Theta^{-1}$].
c_{pf}	Specific heat capacity of a fluid [$L^2T^{-2}\Theta^{-1}$].
c_{pg}	Specific heat capacity of a solid matrix defining a porous medium [$L^2T^{-2}\Theta^{-1}$].
C	Dissolved phase solute concentration [ML^{-3}].
$\tilde{C}_0(t)$	Variable boundary solute concentration [ML^{-3}].
C_0	Constant boundary solute concentration [ML^{-3}].
$\tilde{C}_I(x)$	Non-uniform initial solute concentration distribution [ML^{-3}].
C_I	Uniform initial solute concentration [ML^{-3}].
D_0	Diffusion coefficient of a solute in free water [L^2T^{-1}].
$\mathbf{D_E}$	Effective diffusion coefficient tensor [L^2T^{-1}].

D_E	Effective diffusion coefficient [L^2T^{-1}].
$\mathbf{D_d}$	Hydrodynamic dispersion coefficient tensor [L^2T^{-1}].
D_L	Longitudinal dispersion coefficient [L^2T^{-1}].
f_{oc}	Mass fraction of soil that comprises organic carbon [-].
$H(t)$	Heaviside step function [-].
$\mathbf{J_a}$	Mass flux vector for solute due to advection [$ML^{-2}T^{-1}$].
$\mathbf{J_d}$	Mass flux vector for solute due to hydrodynamic dispersion [$ML^{-2}T^{-1}$].
$\mathbf{J_D}$	Mass flux vector for solute due to diffusion [$ML^{-2}T^{-1}$].
k	Thermal conductivity [$MLT^{-3}\Theta^{-1}$].
k_E	Effective thermal conductivity of a combined fluid and porous medium mixture [$MLT^{-3}\Theta^{-1}$].
k_f	Effective thermal conductivity of a fluid [$MLT^{-3}\Theta^{-1}$].
k_g	Effective thermal conductivity of a mineral grain [$MLT^{-3}\Theta^{-1}$].
K_d	Linear equilibrium adsorption coefficient [$M^{-1}L^3$].
K_{oc}	Linear equilibrium adsorption coefficient for a contaminant with organic carbon [$M^{-1}L^3$].
L	Length [L].
m	Total mass of a given substance per unit volume of porous media [ML^{-3}].
Q	Flow rate [L^3T^{-1}].
r	Total decay rate of a chemical per unit volume of porous medium [$ML^{-3}T^{-1}$].
R	Retardation factor [-].
S	Adsorbed phase concentration [-].
t	Time [T].
$t_{\frac{1}{2}}$	Half-life [T].
T	Temperature [Θ].
$\mathbf{u}$	Fluid velocity vector [LT^{-1}].
u	Fluid velocity in the x -direction [LT^{-1}].
V_V	Volume of voids [L^3].
V_T	Total volume [L^3].
x	Distance [L].
α_L	Longitudinal dispersivity [L].
η	Empirical tortuosity exponent [-].
κ	Overall decay coefficient [T^{-1}].
λ_f	Decay coefficient for a substance in a dissolved phase [T^{-1}].
λ_s	Decay coefficient for a substance in an adsorbed phase [T^{-1}].
ρ	Mass density [ML^{-3}].
ρ_f	Mass density of fluid [ML^{-3}].
ρ_g	Mass density of solid grains [ML^{-3}].
ϕ	Porosity [-].
ϕ_k	Kinematic porosity [-].

9.1 Introduction

This chapter demonstrates how we can use the analytical solution for the diffusion wave equation, derived in Chap. 8, to describe chemical transport and heat transport in porous media. In the context of chemical transport, the diffusion wave equation is commonly referred to as the advection dispersion equation. Porous media are solid substances containing a distributed and connected set of voids, referred to as pore-space. Here we will assume that the pore-space is completely filled with a single fluid, ordinarily water.

A range of relevant chemical and heat transport processes are sequentially introduced including advection, adsorption, decay, diffusion, hydrodynamic dispersion and heat conduction. Practical examples are presented related to hydrocarbon contaminant transport, radionuclide transport and heat conduction.

9.2 Units for Aqueous Concentrations

The presence of dissolved substances in solvents is generally accounted for using solute concentration, C [ML^{-3}], which represents the mass of a dissolved substance present within a unit volume of fluid. Typical units include mg l^{-1} or $\mu\text{g l}^{-1}$. For example, a benzene concentration of 15 mg l^{-1} implies that there is 15 mg of benzene present for every litre of solvent.

Where water is the solvent, $1 \text{ mg l}^{-1} = 1 \text{ ppm}$ where ppm stands for parts per million. Similarly $1 \mu\text{g l}^{-1} = 1 \text{ ppb}$ where ppb stands for parts per billion. This is because one litre of water has a mass of one kg.

9.3 Total and Kinematic Porosity

The total porosity of a substance, ϕ [-], is defined by

$$\phi = \frac{V_V}{V_T} \quad (9.1)$$

where V_V [L^3] is the volume of voids contained within the substance and V_T [L^3] is the total volume of the substance.

Consider fluid moving through a porous block. Let u [LT^{-1}] be the mean velocity in the x -direction of fluid particles in the pore-space. Now consider a plane normal to the x -direction of area, A_T [L^2]. Let Q [ML^{-3}] be the total flow rate of water through this plane. It can be deduced that $Q < Au$ because not all of A_T is pore-space. Let A_V be the area within A_T that intersects the pore-space. In fact $Q = A_V u$.

The kinematic porosity of a substance, ϕ_K [-], is defined by

$$\phi_k = \frac{A_V}{A_T} \quad (9.2)$$

It follows that $Q = A_T \phi_k u$. Note that ϕ_k is directional and should be represented as a tensor. However, in practice ϕ_k is generally unknown and is assumed to be equal to ϕ , which is a scalar quantity. Hence it is commonly assumed that

$$Q = A_T \phi u \quad (9.3)$$

9.4 Advection

The transport of a dissolved substance by moving fluid particles is referred to as advection. The mass flux of solute due to advection, $\mathbf{J}_a$ [$\text{ML}^{-2}\text{T}^{-1}$], is found from

$$\mathbf{J}_a = \phi \mathbf{u} C \quad (9.4)$$

where $\mathbf{u}$ [LT^{-1}] represents the fluid velocity in the pores. The additional ϕ term is required to represent the fact that only a fraction of a given cross-sectional area of a porous medium contains pores and therefore contributes to fluid movement (recall Sect. 9.3).

9.4.1 Pure Advection with Initial Condition

Let m [ML^{-3}] be the total mass of a given substance per unit volume of porous media. Suppose that advection is the only mechanism leading to changes in m . Mass conservation dictates that

$$\frac{\partial m}{\partial t} = -\nabla \cdot \mathbf{J}_a \quad (9.5)$$

For steady state and one-dimensional flow in a homogeneous porous medium this reduces to

$$\frac{\partial m}{\partial t} = -\phi u \frac{\partial C}{\partial x} \quad (9.6)$$

For a non-sorbing substance, $m = \phi C$, therefore Eq. (9.6) reduces to.

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = 0 \quad (9.7)$$

For the initial condition

$$C(x, 0) = \tilde{C}_I(x) \quad (9.8)$$

the following method of characteristics solution can be found (recall Sect. 7.4.1)

$$C(x, t) = \tilde{C}_I(x - ut). \quad (9.9)$$

9.4.2 Pure Advection with Boundary Condition

Alternatively, we may want to consider the boundary condition

$$C(0, t) = \tilde{C}_0(t) \quad (9.10)$$

In this case it is helpful to rearrange Eq. (9.7) to get

$$\frac{\partial C}{\partial x} + \frac{1}{u} \frac{\partial C}{\partial t} = 0 \quad (9.11)$$

Comparing Eqs. (9.10) and (9.11) with Eqs. (9.7) and (9.8) whilst considering Eq. (9.9) suggests that the method of characteristics solution for Eq. (9.7) subjected to the boundary condition given by Eq. (9.10) is

$$C(x, t) = \tilde{C}_0 \left(t - \frac{x}{u} \right) \quad (9.12)$$

The dashed lines in Fig. 9.1a show results from Eq. (9.12) for when

$$\tilde{C}_0(t) = C_0 H(t) \quad (9.13)$$

where C_0 [ML^{-3}] is some constant concentration value and $H(t)$ is the Heaviside step function

$$H(t) = \begin{cases} 0, & t \leq 0 \\ 1, & t > 0 \end{cases} \quad (9.14)$$

It can be seen, in Fig. 9.1a, that advection leads to a pure translation of the Heaviside step function, with a sharp concentration front moving into the porous medium at a constant rate of u . The location of the concentration front at any time is exactly ut .

9.5 Adsorption

Soluble substances present within a porous medium can reside as a mobile dissolved phase in the pore fluid or as an immobile adsorbed phase, stuck to the solid walls surrounding the pores. Adsorption is a process by which dissolved chemicals become adhered to interfacing solid surfaces.

The dissolved phase is accounted for through the solute concentration, C [ML^{-3}]. The adsorbed phase is accounted for through the adsorbed concentration, S [-], which represents the mass of adsorbed substance present within a unit mass of solid material that makes up the porous medium of concern.

The total mass of a given substance per unit volume of porous media, in this context, is found from

$$m = \phi C + (1 - \phi) \rho_g S \quad (9.15)$$

where ρ_g [ML^{-3}] is the mass density of the solid grains that make up the porous medium of concern.

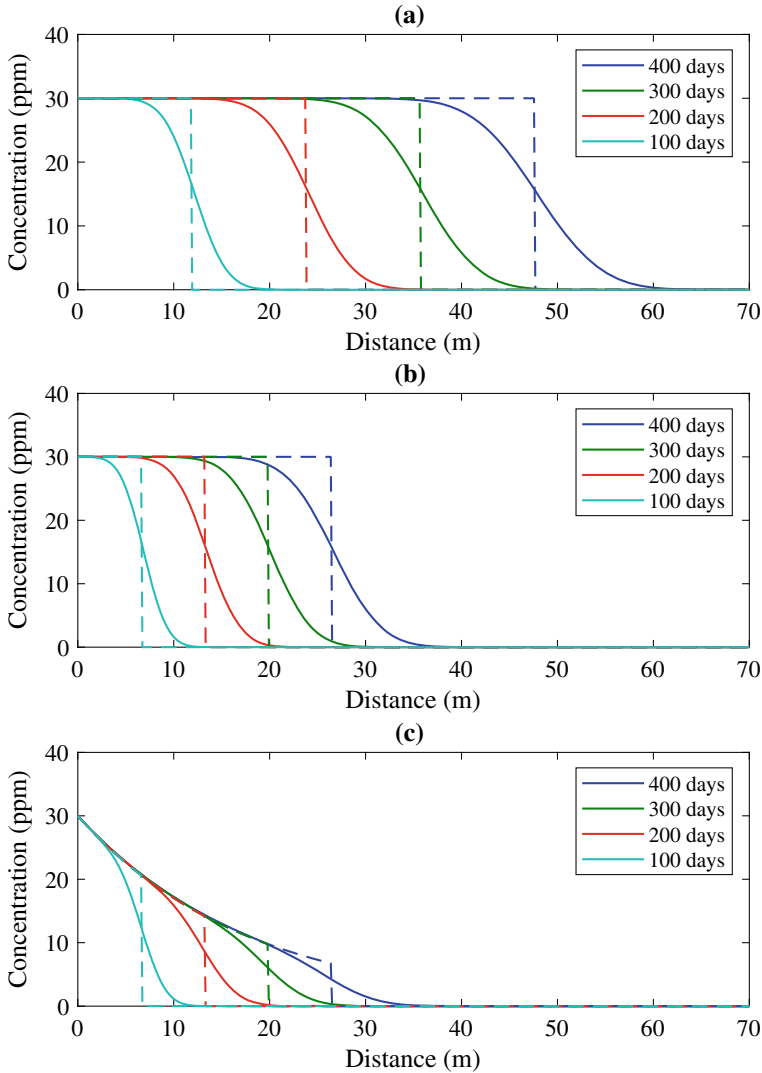


Fig. 9.1 Solute concentration profiles at different times considering various processes. The dashed line results are from Eq. (9.37) for negligible dispersion. The solid line results from Eq. (8.22), which accounts for dispersion. **a** Considers a conservative solute. **b** Considers an adsorbing solute. **c** Considers an adsorbing solute that also decays

The adsorbed phase concentration is often assumed to be in equilibrium with the dissolved phase concentration. The following linear relationship is often applied

$$S = K_d C \quad (9.16)$$

where K_d [M^{-1}L^3] is the linear equilibrium adsorption coefficient.

Substituting Eq. (9.16) into Eq. (9.15) leads to

$$m = \phi RC \quad (9.17)$$

where

$$R = 1 + \frac{(1 - \phi)\rho_g K_d}{\phi}. \quad (9.18)$$

9.5.1 Pure Advection with Adsorption

Substituting Eq. (9.17) into Eq. (9.6) yields

$$R \frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} \quad (9.19)$$

Comparing Eqs. (9.7) and (9.19) whilst considering Eq. (9.12), it can be understood that a method of characteristics solution that incorporates the boundary condition, Eq. (9.10), in the presence of adsorption, takes the form

$$C(x, t) = \tilde{C}_0 \left(t - \frac{Rx}{u} \right) \quad (9.20)$$

Comparing Eqs. (9.12) and (9.20) it can be seen that the effect of the adsorption is to slow the movement of the solute down by a factor, R . Hence R is often referred to as a retardation factor.

The dashed lines in Fig. 9.1b show results from Eq. (9.20) for when $\tilde{C}_0(t)$ is defined by Eq. (9.13). Comparing Fig. 9.1a, b, it can be seen that the adsorption slows the progression of the concentration front associated with the Heaviside step function by the retardation factor, R . The location of the concentration front at any time, in this case, is exactly $\frac{ut}{R}$.

9.5.2 Linear Equilibrium Adsorption Partition Coefficients

In the context of adsorption, it is useful to classify dissolved contaminants in terms of cations, anions and uncharged organics. Adsorbents within rocks and soils include layer silicate clays (LSC), metal-(oxyhydr)oxides (MOO) and soil organic matter (SOM) [1].

LSC are primarily negatively charged and therefore act as strong adsorbents for cations. MOO are variably charged and are likely to be positively charged at low pH and negatively charged at high pH. Therefore, MOO act as an adsorbent for anions at low pH and cations at high pH. SOM tend to act as a strong adsorbent to other dissolved organic compounds.

Table 9.1 Linear equilibrium adsorption coefficients (from [2, pp. 30, 33 and 57]) and radioactive half-lives (from [3, p. 361]) for selected radionuclides and selected porous media

Radionuclide	Linear adsorption coefficient, K_d (cm^3g^{-1})			Half-life, $t_{1/2}$ (years)
	Bentonite	Opalinus clay	Sandy limestone	
Chlorine-36	0.0	0.0	0.0	3.01×10^5
Iodine-131	0.0	0.0	0.0	0.0220
Caesium-137	29.3	2040	433	30.0
Polonium-210	1200	528	112	0.379

Table 9.2 Linear equilibrium adsorption coefficients in organic carbon, K_{oc} , (from [4, pp. 29 and 102]) and both aerobic and anaerobic degradation half-lives (from [4, pp. 43 and 130]) for selected hydrocarbons

Hydrocarbon	Linear adsorption coefficient	Half-life, $t_{1/2}$ (days)	
	K_{oc} (cm^3g^{-1})	Aerobic	Anaerobic
Napthalene	1290	2.20	765
Benzene	134	7.22	103
Toluene	178	3.47	11.7

Two classes of contaminants of particular interest to environmental engineers include radionuclides from pollution due to radioactive waste and hydrocarbons due to pollution related to handling of oil and gas.

Linear equilibrium adsorption coefficients for a selection of radionuclides within a selection of relevant porous media are shown in Table 9.1. Chlorine-36 and Iodine-131 commonly manifest as anions and therefore have close to zero K_d values. Caesium-137 and Polonium-210 are ordinarily present as cations and therefore have much higher K_d values. To some extent, K_d values for cations tend to increase with clay-content in the host mineral although this is not always the case. Predicting K_d values is generally very difficult. Nevertheless, Table 9.1 provides some useful data which we can use to work through the problem sheet at the end of this chapter.

Linear equilibrium adsorption coefficients for hydrocarbons are normally estimated from

$$K_d = f_{oc} K_{oc} \quad (9.21)$$

where f_{oc} [–] is the mass fraction of soil that comprises organic carbon and K_{oc} [M^{-1}L^3] is the linear equilibrium adsorption coefficient for a contaminant with organic carbon.

Linear equilibrium adsorption coefficients in organic carbon, K_{oc} , for a selection of hydrocarbons are shown in Table 9.2. The K_d value for Napthalene is 10 times more than that for Benzene and Toluene suggesting that these latter two contaminant will migrate 10 times faster in a given soil.

9.6 Decay

Chemical substances often degrade over time due to chemical reactions or radioactive decay. These processes are frequently treated as linear kinetic processes. The total decay rate of a chemical per unit volume of porous medium, r [$\text{ML}^{-3}\text{T}^{-1}$], is then described by

$$r = \phi\lambda_f C + (1 - \phi)\rho_g\lambda_s S \quad (9.22)$$

where λ_f [T^{-1}] and λ_s [T^{-1}] represent the decay coefficients for the dissolved and adsorbed phases, respectively.

Substituting the linear equilibrium adsorption equation, Eq. (9.16), into Eq. (9.22) leads to

$$r = \phi [\lambda_f + (R - 1)\lambda_s] C \quad (9.23)$$

where R is the retardation factor defined in Eq. (9.18).

Radioactive decay is an atomic process and independent of the adsorption process. Therefore it is commonly assumed that $\lambda_s = \lambda_f$ for radionuclide contamination scenarios.

The degradation of hydrocarbons is generally due to microbial processes. Microbes require hydrocarbons to be in a dissolved form in order to absorb them within their cellular structures. Consequently the degradation of adsorbed hydrocarbons is very slow. It is therefore common to assume that $\lambda_s = 0$ for hydrocarbon contamination scenarios.

9.6.1 Decay Coefficients and Half-Lives

For a static decaying dissolved substance residing in the absence of an adsorbent

$$\frac{\partial C}{\partial t} = -\lambda_f C \quad (9.24)$$

Challenge 9.1 Derive an analytical solution for Eq. (9.24) assuming $C = C_I$ when $t = 0$.

Separating variables and integrating both sides with respect to t , i.e.,

$$\int \frac{1}{C} \frac{\partial C}{\partial t} dt = \int -\lambda_f dt$$

leads to

$$\ln C = -\lambda_f t + A_1 \quad (9.25)$$

where A_1 is an integration constant.

Letting $C = C_I$ when $t = 0$ leads to $A_1 = \ln C_I$, which, on substitution into Eq. (9.25), gives us

$$C = C_I \exp(-\lambda_f t) \quad (9.26)$$

Challenge 9.2 Determine the time at which the solute concentration in Eq. (9.26) is reduced to half of the initial condition.

Let $t_{\frac{1}{2}}$ be the time at which $C = \frac{C_I}{2}$. From Eq. (9.26) we have

$$\frac{C_I}{2} = C_I \exp(-\lambda_f t_{\frac{1}{2}})$$

from which it follows that

$$t_{\frac{1}{2}} = \frac{\ln 2}{\lambda_f} \quad (9.27)$$

The $t_{\frac{1}{2}}$ term is often referred to as the half-life. Half-lives for radioactive decay of selected radionuclides are presented in Table 9.1. Half-lives for the aerobic and anaerobic degradation of selected hydrocarbons are presented in Table 9.2. Note that anaerobic half-lives tend to be longer than their aerobic counterparts because aerobic respiration is generally a much faster process.

Given Eq. (9.27), the decay coefficient, λ , can be obtained for a given half-life from

$$\lambda_f = \frac{\ln 2}{t_{\frac{1}{2}}} \quad (9.28)$$

9.6.2 Pure Advection with Adsorption and Decay

The mass conservation statement in Eq. (9.6) can be extended to include decay as follow

$$\frac{\partial m}{\partial t} = -\phi u \frac{\partial C}{\partial x} - r \quad (9.29)$$

Substituting Eqs. (9.17) and (9.23) into Eq. (9.29) leads to

$$R \frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} - [\lambda_f + (R - 1)\lambda_s] C \quad (9.30)$$

The above problem is greatly simplified by making the following dependent variable transform

$$C(x, t) = G(x, t) e^{-\kappa t} \quad (9.31)$$

where $G(x, t)$ is the new dependent variable and κ is a coefficient yet to be defined.

Challenge 9.3 Substitute Eq. (9.31) into Eq. (9.30) and derive an expression for κ such that Eq. (9.30) reduces to a simple advection equation (i.e., with no decay term).

Partial differentiation of Eq. (9.31) with respect to t gives

$$\frac{\partial C}{\partial t} = \left[-\kappa G(x, t) + \frac{\partial G}{\partial t} \right] e^{-\kappa t} \quad (9.32)$$

Substituting Eqs. (9.31) and (9.32) into Eq. (9.30) leads to

$$R \frac{\partial G}{\partial t} = -u \frac{\partial G}{\partial x} - [\lambda_f + (R - 1)\lambda_s - R\kappa] G$$

which further reduces to the simple advection equation

$$R \frac{\partial G}{\partial t} = -u \frac{\partial G}{\partial x} \quad (9.33)$$

when

$$\kappa = \frac{\lambda_f + (R - 1)\lambda_s}{R} \quad (9.34)$$

Challenge 9.4 Derive a method of characteristics solution for Eq. (9.33) that incorporates the boundary condition specified in Eq. (9.10) and write the final answer in terms of $C(x, t)$.

Applying the transform, Eq. (9.31), to the boundary condition, Eq. (9.10), leads to

$$G(0, t) = \tilde{C}_0(t) e^{\kappa t} \quad (9.35)$$

Comparing Eqs. (9.7) and (9.33) whilst considering Eq. (9.12), it can be understood that a method of characteristics solution that incorporates the boundary condition, Eq. (9.10), in the presence of adsorption and decay, takes the form

$$G(x, t) = \tilde{C}_0 \left(t - \frac{Rx}{u} \right) \exp \left[\kappa \left(t - \frac{Rx}{u} \right) \right] \quad (9.36)$$

Reversing the transform in Eq. (9.31) then leads to

$$C(x, t) = \tilde{C}_0 \left(t - \frac{Rx}{u} \right) \exp \left(-\frac{R\kappa x}{u} \right) \quad (9.37)$$

9.6.3 Radioactive Decay Versus Microbial Degradation

For radioactive decay

$$\lim_{\lambda_s \rightarrow \lambda_f} \kappa = \lambda_f \quad (9.38)$$

For microbial degradation of hydrocarbons

$$\lim_{\lambda_s \rightarrow 0} \kappa = \frac{\lambda_f}{R} \quad (9.39)$$

Considering Eq. (9.37), it can therefore be understood that the amount of microbial degradation that takes place before a solute reaches a given point, x , is independent

of how much the solute is retarded by adsorption. This is because degradation only applies to the dissolved phase.

The dashed lines in Fig. 9.1c show results from Eq. (9.37) for when $\tilde{C}_0(t)$ is defined by Eq. (9.13). Comparing Fig. 9.1b, c, it can be seen that the decay has no effect on the location of the concentration front. Instead, the decay reduces the concentration magnitude exponentially with distance. The concentration magnitude at any point upstream of the solute front is constant with time and exactly determined from

$$C\left(x < \frac{ut}{R}, t\right) = C_0 \exp\left(-\frac{R\kappa x}{u}\right) \quad (9.40)$$

9.7 Molecular Diffusion

The dissolved phase will also be transported by molecular diffusion, which is a random process whereby solutes move from high concentration to low concentration. The mass flux of solute due to diffusion, $\mathbf{J}_D$ [$\text{ML}^{-2}\text{T}^{-1}$], is described by Fick's first law

$$\mathbf{J}_D = -\mathbf{D}_E \nabla C \quad (9.41)$$

where $\mathbf{D}_E$ [L^2T^{-1}] is known as the effective diffusion coefficient tensor, which is a combined property of the solute, the solvent and the porous medium of concern.

The effective diffusion coefficient of a solute in a porous medium, D_E , will be smaller than the diffusion coefficient of the same solute in free solvent, D_0 , due to the tortuosity of diffusion pathways within the porous structure. Effective diffusion coefficients are often estimated using power law functions of porosity, of the form $D_E = D_0 \phi^\eta$ where η [-] is an empirical exponent typically equal to around two [5]. However, anion solutes tend to be excluded from negatively charged pores and hence their effective diffusion coefficients are often much smaller than those for cation counterparts [6]. Some example values are presented in Table 9.3.

9.8 Hydrodynamic Dispersion

The movement of fluid particles is a chaotic process and leads to additional dispersion of the solute. Typically this is represented as an additional diffusion flux, $\mathbf{J}_d$ [$\text{ML}^{-2}\text{T}^{-1}$], described by

$$\mathbf{J}_d = -\phi \mathbf{D}_d \nabla C \quad (9.42)$$

where $\mathbf{D}_d$ [L^2T^{-1}] is referred to as the hydrodynamic dispersion coefficient tensor.

When considering one dimensional dispersion

$$J_d = -\phi D_L \frac{\partial C}{\partial x}$$

Table 9.3 Porosities and effective diffusion coefficients for selected radionuclides and selected porous media (from [6, pp. 65, 68 and 73])

Radionuclide	Free water diffusion coefficient, D_0 ($\text{m}^2 \text{s}^{-1}$)	Effective diffusion coefficient, D_E ($\text{m}^2 \text{s}^{-1}$)		
		Bentonite	Opalinus clay	Sandy limestone
Porosity, ϕ (-)		0.36	0.11	0.10
Chlorine-36	2.0×10^{-9}	2.0×10^{-12}	2.4×10^{-12}	2.0×10^{-12}
Iodine-131	2.0×10^{-9}	2.0×10^{-12}	2.4×10^{-12}	2.0×10^{-12}
Caesium-137	2.0×10^{-9}	8.3×10^{-10}	1.7×10^{-10}	3.8×10^{-11}
Polonium-210	7.5×10^{-10}	6.8×10^{-11}	4.9×10^{-12}	4.0×10^{-12}

where D_L [L^2T^{-1}] is referred to as the longitudinal dispersion coefficient.

Dispersion coefficients are functions of fluid velocity. The higher the fluid velocity the more dispersion is expected to occur. A commonly applied relationship is

$$D_L = \alpha_L |u| \quad (9.43)$$

where α_L [L] is referred to as the longitudinal dispersivity.

Longitudinal dispersivities have been determined for a wide variety of rock types and spatial scales using a range of different methods including laboratory scale core experiments and field scale tracer tests. It is generally found that dispersivity increases with scale [7]. [8] developed the following empirical relationship

$$\alpha_L = a_1 L^{a_2} \quad (9.44)$$

where L [L] is the length of porous medium under consideration and a_1 and a_2 are the empirical coefficients given in Table 9.4.

For static fluids, $D_L = 0$, and molecular diffusion will be the dominant process. However, for moving fluids, the dispersion coefficient, D_L , is typically orders of magnitude larger than the free water diffusion coefficient, D_0 , and molecular diffusion can often be neglected.

The solid lines in Fig. 9.1 show results from a set of associated models that account for dispersion. The effect of dispersion is to smooth out the concentration

Table 9.4 Empirical parameters obtained by [8] for the dispersivity function given in Eq. (9.44) assuming both α_L and L are in metres

Lithology	a_1	a_2
Sandstones	0.01	0.92
Carbonates	0.80	0.40
Basalts	0.15	0.61
Granites	0.21	0.51

fronts (compare the solid lines with the dashed lines). Some solute travels faster than with pure advection because some of the pathways are shorter than the mean pathway length. Some solute travels slower than with pure advection because some of the pathways are longer than the mean pathway length.

9.9 Advection, Dispersion and Decay

Considering all of the processes described above, mass conservation dictates that

$$\frac{\partial m}{\partial t} = -\nabla \cdot (\mathbf{J}_d + \mathbf{J}_D + \mathbf{J}_a) - r \quad (9.45)$$

Substituting Eqs. (9.17), (9.4), (9.41), (9.42) and (9.23) into Eq. (9.45) leads to

$$\begin{aligned} \frac{\partial}{\partial t}[(\phi + (1 - \phi)\rho_g K_d)C] = \nabla \cdot [(\phi \mathbf{D}_d + \mathbf{D}_E)\nabla C - \phi \mathbf{u}C] \\ - [\phi \lambda_f + (1 - \phi)\rho_g K_d \lambda_s]C \end{aligned} \quad (9.46)$$

Assuming all properties except for C are constant and considering only one-dimensional solute transport, Eq. (9.46) reduces to

$$\frac{\partial C}{\partial t} = \left(\frac{\phi D_L + D_E}{\phi R} \right) \frac{\partial^2 C}{\partial x^2} - \frac{u}{R} \frac{\partial C}{\partial x} - \kappa C \quad (9.47)$$

By setting $\phi = 1$, Eq. (9.47) reduces to a form that can be applied to describe solute transport in a pipe or channel where porous media is not relevant.

Comparing Eq. (8.1) with Eq. (9.47), it can be understood that the analytical solution given in Eq. (8.22) can be used for chemical transport problems in porous media by setting

$$Q = C, \quad Q_0 = C_0, \quad Q_l = 0 \quad (9.48)$$

and

$$K = \frac{\phi D_L + D_E}{\phi R}, \quad c = \frac{u}{R}, \quad \kappa = \frac{\lambda_f + (R - 1)\lambda_s}{R} \quad (9.49)$$

Indeed, the results shown as solid lines in Fig. 9.1 were obtained using Eq. (8.22).

9.10 Heat Transport in Porous Media

An analogous equation to Eq. (9.47) for heat transport takes the form (similar to [9, p. 28])

$$[\phi \rho_f c_{pf} + (1 - \phi)\rho_g c_{pg}] \frac{\partial T}{\partial t} = (\phi \rho_f c_{pf} D_L + k_E) \frac{\partial^2 T}{\partial x^2} - \phi \rho_f c_{pf} u \frac{\partial T}{\partial x} \quad (9.50)$$

where ρ_f [ML⁻³] is the mass density of the fluid, c_{pf} [L²T⁻²Θ⁻¹] is the specific heat capacity of the fluid, c_{pg} [L²T⁻²Θ⁻¹] is the specific heat capacity of the solid

Table 9.5 Densities, ρ , specific heat capacities, c_p , and thermal conductivities, k , for selected materials. ¹Values obtained from [10]. ²Values obtained from [11]

Substance	ρ (kg m ⁻³)	c_p (J kg ⁻¹ K ⁻¹)	k (W m ⁻¹ K ⁻¹)
Gold ¹	19300	145	310
Mild steel ¹	7850	450	50
Concrete ¹	2400	1100	1.25
Ice ¹	920	2100	2.3
Quartz ²	2660	800	8.8
Clay minerals ²	2650	900	2.92
Organic matter ²	1300	1920	0.25
Water ²	1000	4180	0.57
Air ²	1.2	1010	0.025

matrix that defines the porous medium, T [°] is temperature and k_E [MLT⁻³°⁻¹] is the effective thermal conductivity of the combined fluid and porous medium mixture.

A number of empirical functions have been developed to determine k_E from the thermal conductivities of the fluid and mineral grain, k_f [MLT⁻³°⁻¹] and k_g [MLT⁻³°⁻¹], respectively. A simple approach considered suitable for most practical purposes is to assume [9, p. 28]

$$k_E = k_g^{1-\phi} k_f^\phi \quad (9.51)$$

Heat conduction properties for a range of different substances are presented in Table 9.5. By setting $\phi = 1$, Eq. (9.50) reduces to a form that can be applied to describe heat transport in a pipe or channel where porous media is not relevant.

Comparing Eq. (8.1) with Eq. (9.50), it can be understood that the analytical solution given by Eq. (8.22) can be used for heat transport problems in porous media by setting

$$Q = T, \quad Q_0 = T_0, \quad Q_I = T_I \quad (9.52)$$

and

$$K = \frac{\phi \rho_f c_{pf} D_L + k_E}{\phi \rho_f c_{pf} + (1-\phi) \rho_g c_{pg}}, \quad c = \frac{\phi \rho_f c_{pf} u}{\phi \rho_f c_{pf} + (1-\phi) \rho_g c_{pg}}, \quad \kappa = 0 \quad (9.53)$$

where T_0 [°] and T_I [°] are boundary and initial temperatures, respectively.

9.11 Problem Sheet

Problem 9.1 (see Worked Solution 9.1)

A hydrocarbon storage tank leaks into a water reservoir with a hydraulic connection to a surrounding aquifer. Elevated benzene concentrations are detected in an inactive

groundwater production well located 40 m from the reservoir, 600 days after the leak is believed to have commenced. Water ordinarily moves through the aquifer at a rate of $0.025 \text{ m}^3 \text{ day}^{-1} \text{ m}^{-2}$. The aquifer material comprises a silty sand with an organic carbon mass fraction of 0.06% and a mineral grain mass density of 2660 kg m^{-3} .

- (a) Determine the porosity of the aquifer assuming that both diffusion and dispersion are negligible.
- (b) Determine the time at which you would expect naphthalene to also be detected in the observation well.
- (c) The resulting benzene concentrations in the reservoir and the production well are 30.0 ppm and 3.3 ppm, respectively. Assuming that the water in the observation well is purely derived from the reservoir, determine the half-life of benzene in the aquifer.

Problem 9.2 (see Worked Solution 9.2)

Consider a situation where the ground is a uniform temperature of -1°C and the air above the land surface is suddenly raised to a constant value of $+1^\circ\text{C}$. The ground is comprised of sand (i.e., quartz) with a porosity of 0.3 and that the pores are completely filled with air.

- (a) Assume that heat transport within the sand is purely driven by conduction and plot temperature as a function of depth after 3, 10, 30, 100 and 300 minutes after the surface temperature change.
- (b) Plot temperature as a function of depth after 100 minutes assuming the sand pores are filled with air, with water and then with ice.

Problem 9.3 (see Worked Solution 9.3)

High level radioactive waste is stored in an underground tunnel back filled with bentonite clay. With time, the tunnel and surrounding rocks become saturated with water. Trace levels of radionuclides leak from canisters maintaining constant solute concentrations immediately adjacent to the bentonite backfill at a level of 100 ppb for each radionuclide present. The water in the system is static such that solute migration through the bentonite can only take place by molecular diffusion.

- (a) Determine stable isotope (i.e., ignoring radioactive decay) concentrations, after 10,000 years of diffusion, as a function of distance into the bentonite backfill for chlorine, iodine, caesium and polonium (this is purely academic because polonium has no stable form).
- (b) Determine corresponding radionuclide concentrations, after 10,000 years of diffusion and decay, for chlorine-36, iodine-131, caesium-137 and polonium-210.

Problem 9.4 (see Worked Solution 9.4)

Water moves through a confined aquifer with a pore-water velocity of 0.24 m day^{-1} . The salinity of the water is initially 450 ppm. The salinity at the inlet of the aquifer is suddenly raised to 550 ppm. The subsequent rise in salinity is monitored in an observation well located 150 m downstream of the inlet.

(a) Determine the dispersion coefficient and Peclet number (recall Eq. (6.71)) assuming the lithology to be (i) sandstone, (ii) carbonate, (iii) basalt and (iv) granite.

(b) Generate plots of expected observation well salinity against time using properties for the four aforementioned properties. Assume that adsorption and decay are negligible in this case.

9.12 Worked Solutions**Worked Solution 9.1** (see Problem 9.1)

(a) Given that diffusion and dispersion are considered negligible, we can use Eq. (9.37), which tells us that the first arrival time, t_0 , is found from

$$t_0 = \frac{Rx}{u} \quad (9.54)$$

where R is the retardation factor, x is the distance between the reservoir and the production well and u is the pore-water velocity.

From Eqs. (9.18) and (9.21), we know that

$$R = 1 + \frac{(1 - \phi)\rho_g f_{oc} K_{oc}}{\phi} \quad (9.55)$$

where ρ_g is the mineral grain mass density, f_{oc} is the organic carbon mass fraction and K_{oc} is the adsorption coefficient for a contaminant with organic carbon.

From Eq. (9.3), we know that

$$u = \frac{Q}{\phi A_T} \quad (9.56)$$

where Q is the flow rate in the aquifer, ϕ is the porosity and A_T is the flowing cross-sectional area of the aquifer.

Substituting the Eqs. (9.55) and (9.56) into Eq. (9.54) and solving for ϕ leads to

$$\phi = \frac{\frac{qt_0}{x} - \rho_g f_{oc} K_{oc}}{1 - \rho_g f_{oc} K_{oc}} \quad (9.57)$$

where $q = \frac{Q}{A_T}$.

From the information provided we have that $x = 40$ m, $t_0 = 600$ days, $q = 0.025$ m³ day⁻¹ m⁻², $f_{oc} = 0.0006$ and $\rho_g = 2600$ kg m⁻³. From Table 9.2 we have that, for benzene, $K_{oc} = 0.134$ m³ kg⁻¹. It follows that $\phi = 0.2050$.

(b) The first arrival time for an alternative substance can be obtained by solving Eq. (9.57) for t_0 to get

$$t_0 = \frac{x[\phi + (1 - \phi)\rho_g f_{oc} K_{oc}]}{q}$$

From Table 9.2 we have that, for naphthalene, $K_{oc} = 1.290$ m³ kg⁻¹. It follows that the first arrival time for naphthalene would be 2950 days.

(c) Substituting Eqs. (9.3), (9.28), (9.39) into (9.40) leads to

$$C = C_0 \exp\left(-\frac{\phi x \ln 2}{q t_{\frac{1}{2}}}\right)$$

where C_0 and C now represents the benzene concentrations in the reservoir and the well, respectively and $t_{\frac{1}{2}}$ represents the half-life of benzene.

Solving for $t_{\frac{1}{2}}$ leads to

$$t_{\frac{1}{2}} = \frac{\phi x \ln 2}{q \ln\left(\frac{C_0}{C}\right)}$$

and setting $C_0 = 30.0$ ppm and $C = 3.3$ ppm gives us that $t_{\frac{1}{2}} = 103$ days.

Worked Solution 9.2 (see Problem 9.2)

(a) The temperature distribution can be determined using Eq. (8.25) with the auxiliary equations, Eqs. (9.52) and (9.53), and with k_E determined from Eq. (9.51). Relevant parameter values are given in Table 9.5. The MATLAB code below utilizes the OgataBanksDecay function (Listing 8.2) to produce the desired results:

```
T0=1; %Boundary temperature (deg C)
TI=-1; %Initial temperature (deg C)
phi=0.3; %Porosity (-)
rhog=2660; %Grain density (kg/m3)
cpg=800; %Grain heat capacity (J/kg/K)
kg=8.8; %Grain conductivity (W/m/K)
rhof=1.2; %Fluid density (kg/m3)
cpf=1010; %Fluid heat capacity (J/kg/K)
kf=0.025; %Fluid conductivity (W/m/K)
%Determine effective thermal conductivity
kE=kg^(1-phi)*kf^phi;
%Determine apparent diffusion coefficient
K=kE/(phi*rhof*cpf+(1-phi)*rhog*cpg);
```

```
%Specify times in seconds
t=[3 10 30 100 300]*60;
%Define depths to solve for in m
x=linspace(0,0.6,200)';
%Determine temperature distribution
T=OgataBanksDecay(x,t,T0,TI,K,0,0);
figure(1);clf %Plot results
subplot(1,2,1)
plot(T,x*100)
set(gca,'ydir','reverse')
xlabel('Temperature in air filled sand (^oC)')
ylabel('Depth (cm)')
legend('3 min','10 min','30 min','100 min',...
'300 min','location','southeast')
title('a')
```

(b) The following MATLAB code can be appended to provide the results to compare the presence of air, water and ice:

```
%Fluid properties:
rhof=[1.2 1000 920]; %Density (kg/m3)
cpf=[1010 4180 2100]; %Heat capacity (J/kg/K)
kf=[0.025 0.57 2.3]; %Conductivity (W/m/K)
%Determine effective thermal conductivity
kE=kg^(1-phi)*kf.^phi;
%Determine apparent diffusion coefficient
K=kE./(phi*rhof.*cpf+(1-phi)*rhog.*cpg);
%Specify time in seconds
t=100*60;
%Determine temperature distribution
T=OgataBanksDecay(x,t,T0,TI,K,0,0);
subplot(1,2,2) %Plot results
plot(T,x*100)
set(gca,'ydir','reverse')
xlabel('Temperature after 100 min (^oC)')
ylabel('Depth (cm)')
legend('Sand and air','Sand and water',...
'Sand and ice','location','southeast')
title('b')
```

The results to (a) and (b) are shown in Figs. 9.2a and b, respectively. For part (a) it can be seen that temperature front diffuses into the sand with time on a logarithmic time-scale. For part (b) it can be seen that heat diffuses into sand fastest for sand and ice and slowest for sand and air. This is due to the differences in the apparent diffusion coefficient, K , for the three fluids.

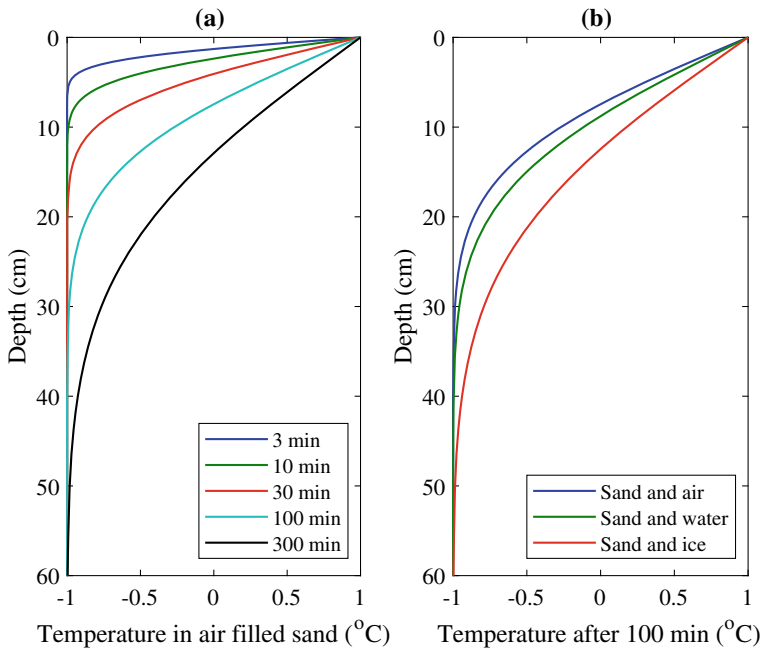


Fig. 9.2 Heat conduction from a fixed temperature ground surface. **a** Shows temperature profiles after different times for heat conduction through air filled sand. **b** Shows temperature profiles after 100 min for different media as indicated in the legend

Worked Solution 9.3 (see Problem 9.3)

(a) Because decay is negligible, the concentration distribution can be determined using Eq. (8.25) with the auxiliary equations, Eqs. (9.48) and (9.49). Relevant parameter values are given in Tables 9.1 and 9.3. The mineral grain density of bentonite can be taken to be that of clay minerals given in Table (9.5). The MATLAB code below utilizes the OgataBanksDecay function (Listing 8.2) to produce the desired results:

```
C0=100; %Boundary concentration (ppb)
CI=0; %Initial concentration (ppb)
phi=0.36; %Porosity (-)
rhog=2650; %Mineral grain density (kg/m3)
x=logspace(-4,2,200)'; %Distance to solve for (m)
t=10000*365*24*60^2; %Specify time (s)
%Effective diffusion coefficient (m2/s)
De=[2e-12 2e-12 8.3e-10 6.8e-11];
%Linear equilibrium adsorption coefficient (m3/kg)
Kd=[0 0 29.3 1200]/1000;
```

```
%Apparent diffusion coefficient
K=De./(phi+(1-phi).*rhog.*Kd);
%Determine stable isotope concentrations
Ca=OgataBanksDecay(x,t,C0,CI,K,0,0);
figure(2);clf %Plot results
subplot(2,1,1)
semilogx(x,Ca)
axis([1e-4 1e2 0 100])
legend('Chlorine','Iodine','Caesium','Polonium')
xlabel('Distance (m)')
ylabel('Concentration (ppb)')
title('a')
```

(b) For this case, the concentration distribution can be determined using Eq. (8.24) with the auxiliary equations, Eqs. (9.48) and (9.49), with λ_f determined from Eqs. (9.38) and (9.28) and with half-lives taken from Table 9.1. The desired results are obtained by appending the MATLAB code below:

```
%Radionuclide half-lives (s)
thalf=[3.01e5 0.022 30 0.379]*365*24*60^2;
%Determine decay rates
k=log(2)./thalf;
%Determine unstable isotope concentrations
Cb=OgataBanksDecay(x,t,C0,CI,K,0,k);
subplot(2,1,2) %Plot results
semilogx(x,Cb)
axis([1e-4 1e2 0 100])
legend('Chlorine-36','Iodine-131',...
'Caesium-137','Polonium-210')
xlabel('Distance (m)')
ylabel('Concentration (ppb)')
title('b')
```

The results to (a) and (b) are shown in Fig. 9.3a, b, respectively. From part (a) it can be seen that the penetration depths after 10,000 years, for the different radionuclides, are less than 10 m for all stable isotopes and less than 50 cm for polonium. The small distance travelled is due to the slowness of the molecular diffusion process. The variation in penetration depth for the different stable isotopes is mostly due to their different adsorption coefficients, K_d .

From part (b) it can be seen that penetration depths for radionuclides such as Iodine-131 and Polonium-210 are much less than that for Chlorine-36 because of a combination of higher K_d values and short half-lives. Note that radionuclides continue decay regardless of their adsorption status.

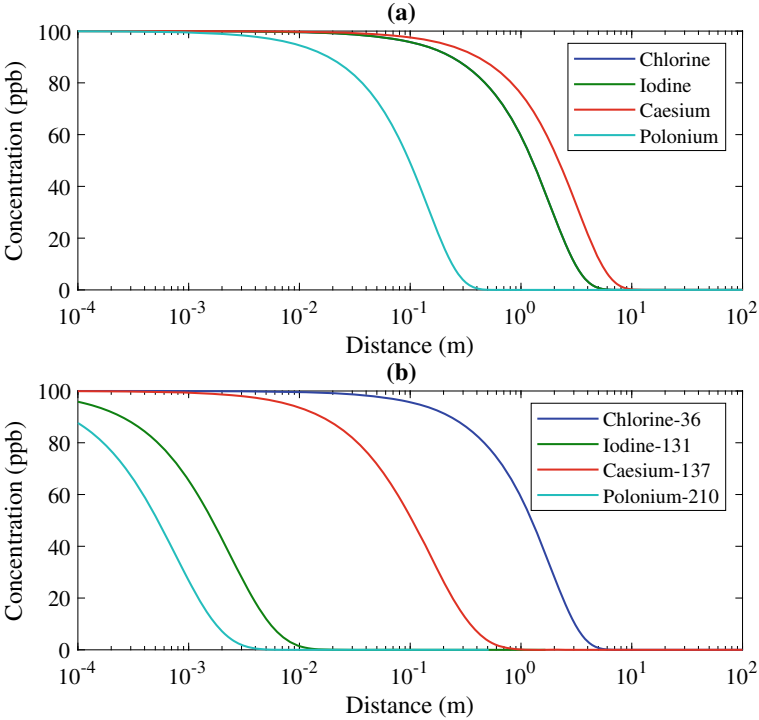


Fig. 9.3 Solute concentration profiles in bentonite clay after 10,000 years due to diffusion with adsorption from a fixed concentration boundary. **a** For stable isotopes (i.e., no decay). **b** For unstable isotopes (i.e., with decay)

Worked Solution 9.4 (see Problem 9.4)

(a) The dispersion coefficient, D_L , can be determined using Eq. (9.43) with the pore-water velocity, $u = 0.24 \text{ m day}^{-1}$, and the dispersivity, α_L , determined from Eq. (9.44) with the associated empirical parameters acquired from Table 9.4. In this context, the Peclet number, $Pe = \frac{x}{\alpha_L}$ (recall Eq. (6.71)). The results read as follows:

Lithology	$D_L \text{ (m}^2 \text{ day}^{-1}\text{)}$	$D_L \text{ (m}^2 \text{ s}^{-1}\text{)}$	Pe (-)
Sandstone	0.2411	2.79×10^{-6}	149
Carbonate	1.425	1.65×10^{-5}	25.3
Basalt	0.7651	8.86×10^{-6}	47.1
Granite	0.6490	7.51×10^{-6}	55.5

Converting the dispersion coefficients to m^2s^{-1} allows a comparison to be made with the effective diffusion coefficients given in Table 9.3. The dispersion coefficients

are several orders of magnitude larger the effective diffusion coefficients. Hydrodynamic dispersion is typically much more significant than molecular diffusion because hydrodynamic dispersion is driven by macro-scale features associated with geological heterogeneity, whereas molecular diffusion is driven by a much smaller molecular scale process. For this reason, it is common to assume that molecular diffusion is negligible in this context.

The Peclet number gives an indication of the relative importance of dispersion (recall Fig. 6.1). The higher the Peclet number the less important the dispersion is. Dispersion is more significant for carbonate aquifers and less significant for the sandstone aquifers. The reason for this is that flow pathways in carbonate aquifers tend to be dominated more by heterogeneous fracture networks. In contrast, flow pathways in sandstone are mostly due to more homogeneous pore-network pathways.

(b) Plots of salinity against time in the observation well can be determined using Eq. (8.22) in conjunction with the auxiliary equations, Eqs. (9.48) and (9.49). Furthermore, we can ignore the effects of adsorption, molecular diffusion and decay. Therefore $c = u$, $K = D_L$ and $\kappa = 0$ where $u = 0.24 \text{ m day}^{-1}$ and D_L is the dispersion coefficient, as found in part (a) above. The MATLAB code below utilizes the `OgataBanksDecay` function (Listing 8.2) to produce the desired results:

```
CI=450; %Initial concentration (ppm)
C0=550; %Boundary concentration (ppm)
u=0.24; %Pore-water velocity (m/day)
x=150; %Distance from source (m)
%Schulze-Makuch (2005) parameters
a1=[0.01 0.8 0.15 0.21]';
a2=[0.92 0.4 0.61 0.51]';
alphaL=a1.*x.^a2; %Dispersivity (m)
DL=alphaL*u; %Dispersion coefficient (m2/day)
%Specify times to solve for
t=linspace(0,1500,500);
%Determine concentration at observation point
C=OgataBanksDecay(x,t,C0,CI,DL,u,0);
figure(3);clf;box on %Plot results
plot(t,C,'linewidth',1)
legend('Sandstone','Carbonate','Basalt',...
'Granite','location','southeast')
xlabel('Time (days)')
ylabel('Salinity (ppm)')
```

The results are shown in Fig. 9.4. Such curves are often referred to as breakthrough curves (BTC), because they represent the time at which the solute concentration perturbations “breakthrough” the plane associated with the point of observation. It can be seen that the BTC is much sharper for the sandstone and less so for the carbonate. This reflects the idea that the variation in pathway lengths is much less in the sandstone as compared to in the carbonate. Shorter pathways lead to an early

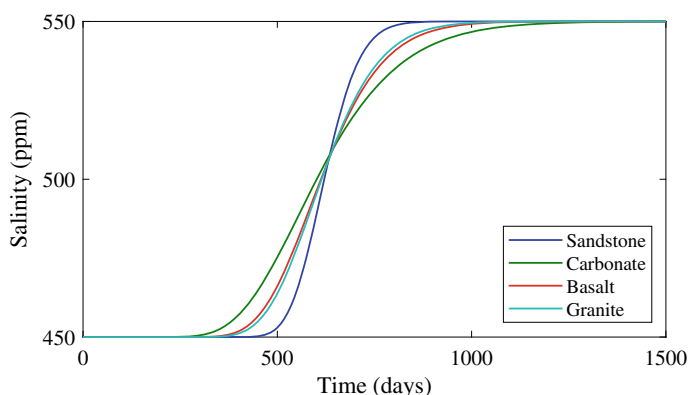


Fig. 9.4 Plot of observation well salinity against time due to advection and dispersion from a fixed concentration boundary assuming different dispersivities based on lithology, as indicated in the legend

time tailing effect. Longer pathways lead to a late time tailing effect. The basalt and granite aquifers represent something in between the carbonate and sandstone in terms of pathway heterogeneity.

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The Finite Difference Method

10

Abstract

This chapter introduces the finite difference method and develops finite difference solutions for the advection dispersion equation and a non-linear kinematic wave equation. Finite difference approximations are derived using Taylor series. Four different schemes are developed including ETCS (explicit time-stepping with central difference in space), ETBS (explicit time-stepping with backward difference in space), ITCS (implicit time-stepping with central difference in space) and ITBS (implicit time-stepping with backward difference in space). Each scheme is formulated in terms of a Jacobian matrix. Numerical stability constraints are defined in terms of Neumann, Courant and Peclet numbers. Taylor series truncation terms are used to derive expressions for quantifying numerical diffusion. A Newton iteration scheme is developed to solve non-linear partial differential equations. Practical applications are presented through a problem sheet with worked solutions and MATLAB code snippets.

Notation

A	Finite difference coefficient for Q_{i-1} .
B	Finite difference coefficient for Q_i .
c	Wave speed [LT^{-1}].
C	Finite difference coefficient for Q_{i+1} .
Cr	Courant number [–].
i	Index for solution points on the x -axis [–].
$\mathbf{J}$	Jacobian matrix [–].
K	Apparent diffusion coefficient [L^2T^{-1}].
K_{num}	Numerical diffusion coefficient [L^2T^{-1}].
L	Length [L].
n	Index for solution points on the t -axis [–].
Ne	Neumann number [–].

N_x	Number of solution points on the x -axis [–].
N_t	Number of solution points on the t -axis [–].
Pe	Peclet number [–].
Q	Flow rate [L^3T^{-1}].
Q_0	Constant boundary flow rate [L^3T^{-1}].
Q_I	Uniform initial flow rate [L^3T^{-1}].
Q_n	Array of flow rate solution values for the n -th time-step [L^3T^{-1}].
$R_{n+1,k}$	Residual vector containing errors associated with a solution from the k -th iteration [L^3T^{-1}].
t	Time [T].
u	Fluid velocity [LT^{-1}].
x	Horizontal distance in the x -direction [L].
Δt	Time-step [T].
Δx	Space-step [L].
ETBS	Explicit time-stepping with backward difference in space.
ETCS	Explicit time-stepping with central difference in space.
ITBS	Implicit time-stepping with backward difference in space.
ITCS	Implicit time-stepping with central difference in space.

10.1 Introduction

In many practical cases, it is not possible to derive analytical solutions to partial differential equations. Numerical solution procedures can be applied as an alternative, including the finite element method, finite-volume method and finite difference method [1]. The finite difference method represents the simplest of the three to understand and is often used to solve the shallow-water equation discussed in Chap. 6 (e.g. [2–4]). This chapter focuses on the development of finite difference solutions for the diffusion wave equation derived in Sect. 6.6. Following Chap. 9, analogous examples are presented (in the problem sheet at the end of this chapter) using heat conduction and chemical transport scenarios.

10.2 Boundary Value Problem

The boundary value problem discussed throughout this chapter utilizes the diffusion wave equation (recall Sect. 6.6)

$$\frac{\partial Q}{\partial t} = K \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} \quad (10.1)$$

subjected to the following initial and boundary conditions:

$$\begin{aligned} Q &= Q_I, \quad 0 < x < L, \quad t = 0 \\ Q &= Q_0, \quad x = 0, \quad t \geq 0 \\ Q &= Q_I, \quad x = L, \quad t \geq 0 \end{aligned} \quad (10.2)$$

where Q [L^3T^{-1}] is flow rate, t [T] is time, c [LT^{-1}] is wave speed, x [L] is distance, K [L^2T^{-1}] is a diffusion coefficient, Q_I [L^3T^{-1}] is a uniform initial flow rate, Q_0 [L^3T^{-1}] is a uniform boundary flow rate and L [L] is the spatial extent of the domain of concern.

10.3 Application of Taylor Series

Consider the following set of discrete points in time and space:

$$x_i = \Delta x \sum_{i=1}^{N_x} (i-1) \quad \text{and} \quad t_n = \Delta t \sum_{n=1}^{N_t} (n-1)$$

where N_x and N_t are the number of solution points on the x and t axes, respectively, and Δx [L] and Δt [L] are the space-step and time-step between each solution point, respectively. Note that $L = (N_x - 1)\Delta x$. A corresponding discrete set of values for $Q(x, t)$ can be found from

$$Q_{i,n} = Q(x_i, t_n)$$

The finite difference method exploits Taylor series expansions of dependent variables (e.g. $Q(x, t)$) to derive approximate expressions for partial derivatives in terms of discrete values (e.g. $Q_{i,n}$).

Consider a Taylor series for a function, $f(x)$, [5, p. 817]

$$f(x + \Delta x) = f(x) + \Delta x \frac{\partial f}{\partial x} + \frac{\Delta x^2}{2!} \frac{\partial^2 f}{\partial x^2} + \frac{\Delta x^3}{3!} \frac{\partial^3 f}{\partial x^3} + O(\Delta x^4)$$

Letting $f_i = f(x_i)$ and $f_{i+1} = f(x_i + \Delta x)$ it follows that

$$f_{i+1} = f_i + \Delta x \left. \frac{\partial f}{\partial x} \right|_i + \frac{\Delta x^2}{2!} \left. \frac{\partial^2 f}{\partial x^2} \right|_i + \frac{\Delta x^3}{3!} \left. \frac{\partial^3 f}{\partial x^3} \right|_i + O(\Delta x^4) \quad (10.3)$$

Similarly it can be said that

$$f_{i-1} = f_i - \Delta x \left. \frac{\partial f}{\partial x} \right|_i + \frac{\Delta x^2}{2!} \left. \frac{\partial^2 f}{\partial x^2} \right|_i - \frac{\Delta x^3}{3!} \left. \frac{\partial^3 f}{\partial x^3} \right|_i + O(\Delta x^4) \quad (10.4)$$

Challenge 10.1 Use Eqs. (10.3) and (10.4) to derive three different expressions for $\frac{\partial f}{\partial x}$ and one expression for $\frac{\partial^2 f}{\partial x^2}$, all to second-order accuracy.

Equation (10.3) can be rearranged to get [6, p. 91]

$$\left. \frac{\partial f}{\partial x} \right|_i = \frac{f_{i+1} - f_i}{\Delta x} - \frac{\Delta x}{2!} \left. \frac{\partial^2 f}{\partial x^2} \right|_i + O(\Delta x^2) \quad (10.5)$$

which is commonly referred to as a forward difference approximation because of its use of f_{i+1} .

Equation (10.4) can be rearranged to get [6, p. 91]

$$\left. \frac{\partial f}{\partial x} \right|_i = \frac{f_i - f_{i-1}}{\Delta x} + \frac{\Delta x}{2!} \left. \frac{\partial^2 f}{\partial x^2} \right|_i + O(\Delta x^2) \quad (10.6)$$

which is commonly referred to as a backward difference approximation because of its use of f_{i-1} .

Subtracting Eq. (10.4) from (10.3) and solving for $\left. \frac{\partial f}{\partial x} \right|_i$ leads to [6, p. 93]

$$\left. \frac{\partial f}{\partial x} \right|_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + O(\Delta x^2) \quad (10.7)$$

which is commonly referred to as a central difference approximation because of its use of both f_{i-1} and f_{i+1} .

Note that if we ignore the second-order derivatives, Eqs. (10.5) and (10.6) are only first order accurate whereas Eq. (10.7) remains second order accurate.

Adding Eqs. (10.3) and (10.4) together and solving for $\left. \frac{\partial^2 f}{\partial x^2} \right|_i$ leads to [6, p. 95]

$$\left. \frac{\partial^2 f}{\partial x^2} \right|_i = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} + O(\Delta x^2). \quad (10.8)$$

10.4 Four Different Schemes

10.4.1 Explicit Time-Stepping with Central Difference in Space (ETCS)

Challenge 10.2 Derive a finite difference approximation for Eq. (10.1) using a forward difference approximation for the time-derivative and a central difference approximation for the first-order space derivative.

From Eq. (10.5) we can say

$$\left. \frac{\partial Q}{\partial t} \right|_{i,n} = \frac{Q_{i,n+1} - Q_{i,n}}{\Delta t} - \frac{\Delta t}{2!} \left. \frac{\partial^2 Q}{\partial t^2} \right|_{i,n} + O(\Delta t^2) \quad (10.9)$$

From Eq. (10.7) we can say

$$\left. \frac{\partial Q}{\partial x} \right|_{i,n} = \frac{Q_{i+1,n} - Q_{i-1,n}}{2\Delta x} + O(\Delta x^2) \quad (10.10)$$

From Eq. (10.8) we can say

$$\left. \frac{\partial^2 Q}{\partial x^2} \right|_{i,n} = \frac{Q_{i+1,n} - 2Q_{i,n} + Q_{i-1,n}}{\Delta x^2} + O(\Delta x^2) \quad (10.11)$$

Substituting Eqs. (10.9), (10.11) and (10.10) into Eq. (10.1) leads to

$$\begin{aligned} \frac{Q_{i,n+1} - Q_{i,n}}{\Delta t} - \frac{\Delta t}{2!} \left. \frac{\partial^2 Q}{\partial t^2} \right|_{i,n} &= K \left(\frac{Q_{i+1,n} - 2Q_{i,n} + Q_{i-1,n}}{\Delta x^2} \right) \\ -c \left(\frac{Q_{i+1,n} - Q_{i-1,n}}{2\Delta x} \right) &+ O(\Delta x^2, \Delta t^2) \end{aligned} \quad (10.12)$$

It is common practice to ignore the second-order derivative in time and the second-order truncation error such that

$$\frac{Q_{i,n+1} - Q_{i,n}}{\Delta t} = K \left(\frac{Q_{i+1,n} - 2Q_{i,n} + Q_{i-1,n}}{\Delta x^2} \right) - c \left(\frac{Q_{i+1,n} - Q_{i-1,n}}{2\Delta x} \right) \quad (10.13)$$

which will be accurate to $O(\Delta x^2, \Delta t)$ as opposed to $O(\Delta x^2, \Delta t^2)$ because of the ignoring of the $\frac{\partial^2 Q}{\partial t^2}$ term.

Challenge 10.3 Solve Eq. (10.13) for $Q_{i,n+1}$ and collect the $Q_{i-1,n}$, $Q_{i,n}$ and $Q_{i+1,n}$ terms.

Equation (10.13) can be rearranged to get

$$Q_{i,n+1} = \left(\frac{K\Delta t}{\Delta x^2} + \frac{c\Delta t}{2\Delta x} \right) Q_{i-1,n} + \left(1 - \frac{2K\Delta t}{\Delta x^2} \right) Q_{i,n} + \left(\frac{K\Delta t}{\Delta x^2} - \frac{c\Delta t}{2\Delta x} \right) Q_{i+1,n} \quad (10.14)$$

The time-stepping scheme in Eq. (10.14) is commonly referred to as an Euler explicit time-stepping scheme. Because Eq. (10.14) also adopts a central difference approximation in space, this scheme is hereafter referred to as the explicit time-stepping with central difference in space (ETCS) scheme.

10.4.2 Explicit Time-Stepping with Backward Difference in Space (ETBS)

Challenge 10.4 Derive a finite difference approximation for Eq. (10.1) using a forward difference approximation for the time-derivative and a backward difference approximation for the first-order space derivative.

From Eq. (10.6) we can say

$$\left. \frac{\partial Q}{\partial x} \right|_{i,n} = \frac{Q_{i,n} - Q_{i-1,n}}{\Delta x} + \frac{\Delta x}{2!} \left. \frac{\partial^2 Q}{\partial x^2} \right|_{i,n} + O(\Delta x^2) \quad (10.15)$$

Substituting Eqs. (10.9), (10.11) and (10.15) into Eq. (10.1) leads to

$$\begin{aligned} \frac{Q_{i,n+1}-Q_{i,n}}{\Delta t} - \frac{\Delta t}{2!} \frac{\partial^2 Q}{\partial t^2} \Big|_{i,n} &= K \left(\frac{Q_{i+1,n}-2Q_{i,n}+Q_{i-1,n}}{\Delta x^2} \right) \\ -c \left(\frac{Q_{i,n}-Q_{i-1,n}}{\Delta x} \right) - \frac{c\Delta x}{2!} \frac{\partial^2 Q}{\partial x^2} \Big|_{i,n} &+ O(\Delta x^2, \Delta t^2) \end{aligned} \quad (10.16)$$

Ignoring the second-order derivative in time, the second-order derivative in space and the second-order truncation error leads to

$$\frac{Q_{i,n+1}-Q_{i,n}}{\Delta t} = K \left(\frac{Q_{i+1,n}-2Q_{i,n}+Q_{i-1,n}}{\Delta x^2} \right) - c \left(\frac{Q_{i,n}-Q_{i-1,n}}{\Delta x} \right) \quad (10.17)$$

which will be accurate to $O(\Delta x, \Delta t)$ as opposed to $O(\Delta x^2, \Delta t^2)$ because of the ignoring of both the $\frac{\partial^2 Q}{\partial t^2}$ and $\frac{\partial^2 Q}{\partial x^2}$ terms.

Challenge 10.5 Solve Eq. (10.17) for $Q_{i,n+1}$ and collect the $Q_{i-1,n}$, $Q_{i,n}$ and $Q_{i+1,n}$ terms.

Equation (10.17) can be rearranged to get

$$Q_{i,n+1} = \left(\frac{K\Delta t}{\Delta x^2} + \frac{c\Delta t}{\Delta x} \right) Q_{i-1,n} + \left(1 - \frac{2K\Delta t}{\Delta x^2} - \frac{c\Delta t}{\Delta x} \right) Q_{i,n} + \left(\frac{K\Delta t}{\Delta x^2} \right) Q_{i+1,n} \quad (10.18)$$

Equation (10.18) also uses an Euler explicit time-stepping scheme. However, because Eq. (10.18) adopts a backward difference approximation in space, this scheme is hereafter referred to as the explicit time-stepping with backward difference in space (ETBS) scheme.

10.4.3 Implicit Time-Stepping with Central Difference in Space (ITCS)

Challenge 10.6 Derive a finite difference approximation for Eq. (10.1) using a backward difference approximation for the time-derivative and a central difference approximation for the first-order space derivative.

From Eq. (10.6) we can say

$$\frac{\partial Q}{\partial t} \Big|_{i,n} = \frac{Q_{i,n}-Q_{i,n-1}}{\Delta t} + \frac{\Delta t}{2!} \frac{\partial^2 Q}{\partial t^2} \Big|_{i,n} + O(\Delta t^2) \quad (10.19)$$

Substituting Eqs. (10.19), (10.11) and (10.10) into Eq. (10.1) leads to

$$\begin{aligned} \frac{Q_{i,n}-Q_{i,n-1}}{\Delta t} + \frac{\Delta t}{2!} \frac{\partial^2 Q}{\partial t^2} \Big|_{i,n} &= K \left(\frac{Q_{i+1,n}-2Q_{i,n}+Q_{i-1,n}}{\Delta x^2} \right) \\ -c \left(\frac{Q_{i+1,n}-Q_{i-1,n}}{2\Delta x} \right) &+ O(\Delta x^2, \Delta t^2) = 0 \end{aligned} \quad (10.20)$$

Ignoring the second-order derivative in time and the second-order truncation error leads to

$$\frac{Q_{i,n} - Q_{i,n-1}}{\Delta t} = K \left(\frac{Q_{i+1,n} - 2Q_{i,n} + Q_{i-1,n}}{\Delta x^2} \right) - c \left(\frac{Q_{i+1,n} - Q_{i-1,n}}{2\Delta x} \right) \quad (10.21)$$

which will be accurate to $O(\Delta x^2, \Delta t)$.

Challenge 10.7 Solve Eq. (10.21) for $Q_{i,n-1}$ and collect the $Q_{i-1,n}$, $Q_{i,n}$ and $Q_{i+1,n}$ terms

Equation (10.21) can be rearranged to get

$$Q_{i,n-1} = \left(-\frac{K\Delta t}{\Delta x^2} - \frac{c\Delta t}{2\Delta x} \right) Q_{i-1,n} + \left(1 + \frac{2K\Delta t}{\Delta x^2} \right) Q_{i,n} + \left(-\frac{K\Delta t}{\Delta x^2} + \frac{c\Delta t}{2\Delta x} \right) Q_{i+1,n} \quad (10.22)$$

The time-stepping scheme in Eq. (10.22) is commonly referred to as an Euler implicit time-stepping scheme. Because Eq. (10.22) also adopts a central difference approximation in space, this scheme is hereafter referred to as the implicit time-stepping with central difference in space (ITCS) scheme.

10.4.4 Implicit Time-Stepping with Backward Difference in Space (ITBS)

Challenge 10.8 Derive a finite difference approximation for Eq. (10.1) using a backward difference approximation for the time-derivative and a backward difference approximation for the first-order space derivative.

Substituting Eqs. (10.19), (10.11) and (10.15) into Eq. (10.1) leads to

$$\begin{aligned} \frac{Q_{i,n} - Q_{i,n-1}}{\Delta t} + \frac{\Delta t}{2!} \frac{\partial^2 Q}{\partial t^2} \Big|_{i,n} &= K \left(\frac{Q_{i+1,n} - 2Q_{i,n} + Q_{i-1,n}}{\Delta x^2} \right) \\ -c \left(\frac{Q_{i,n} - Q_{i-1,n}}{\Delta x} \right) - \frac{c\Delta x}{2!} \frac{\partial^2 Q}{\partial x^2} \Big|_{i,n} &+ O(\Delta x^2, \Delta t^2) \end{aligned} \quad (10.23)$$

Ignoring the second-order derivative in time, the second-order derivative in space and the second-order truncation error leads to

$$\frac{Q_{i,n} - Q_{i,n-1}}{\Delta t} = K \left(\frac{Q_{i+1,n} - 2Q_{i,n} + Q_{i-1,n}}{\Delta x^2} \right) - c \left(\frac{Q_{i,n} - Q_{i-1,n}}{\Delta x} \right) \quad (10.24)$$

which will be accurate to $O(\Delta x, \Delta t)$.

Challenge 10.9 Solve Eq. (10.24) for $Q_{i,n-1}$ and collect the $Q_{i-1,n}$, $Q_{i,n}$ and $Q_{i+1,n}$ terms.

Equation (10.24) can be rearranged to get

$$Q_{i,n-1} = \left(-\frac{K\Delta t}{\Delta x^2} - \frac{c\Delta t}{\Delta x}\right) Q_{i-1,n} + \left(1 + \frac{2K\Delta t}{\Delta x^2} + \frac{c\Delta t}{\Delta x}\right) Q_{i,n} + \left(-\frac{K\Delta t}{\Delta x^2}\right) Q_{i+1,n} \quad (10.25)$$

Equation (10.25) also uses an Euler implicit time-stepping scheme. However, because Eq. (10.25) adopts a backward difference approximation in space, this scheme is hereafter referred to as the explicit time-stepping with backward difference in space (ITBS) scheme.

10.5 Explicit Versus Implicit Time-Stepping

Both of the explicit schemes, ETCS and ETBS (Eqs. (10.14) and (10.18)), can be written in the form

$$Q_{i,n+1} = A Q_{i-1,n} + B Q_{i,n} + C Q_{i+1,n} \quad (10.26)$$

where for the ETCS scheme

$$A = \frac{K\Delta t}{\Delta x^2} + \frac{c\Delta t}{2\Delta x}, \quad B = 1 - \frac{2K\Delta t}{\Delta x^2}, \quad C = \frac{K\Delta t}{\Delta x^2} - \frac{c\Delta t}{2\Delta x} \quad (10.27)$$

and for the ETBS scheme

$$A = \frac{K\Delta t}{\Delta x^2} + \frac{c\Delta t}{\Delta x}, \quad B = 1 - \frac{2K\Delta t}{\Delta x^2} - \frac{c\Delta t}{\Delta x}, \quad C = \frac{K\Delta t}{\Delta x^2} \quad (10.28)$$

Both of the implicit schemes, ITCS and ITBS (Eqs. (10.22) and (10.25)), can be written in the form

$$A Q_{i-1,n} + B Q_{i,n} + C Q_{i+1,n} = Q_{i,n-1} \quad (10.29)$$

where for the ITCS scheme

$$A = -\frac{K\Delta t}{\Delta x^2} - \frac{c\Delta t}{2\Delta x}, \quad B = 1 + \frac{2K\Delta t}{\Delta x^2}, \quad C = -\frac{K\Delta t}{\Delta x^2} + \frac{c\Delta t}{2\Delta x} \quad (10.30)$$

and for the ITBS scheme

$$A = -\frac{K\Delta t}{\Delta x^2} - \frac{c\Delta t}{\Delta x}, \quad B = 1 + \frac{2K\Delta t}{\Delta x^2} + \frac{c\Delta t}{\Delta x}, \quad C = -\frac{K\Delta t}{\Delta x^2} \quad (10.31)$$

To make Eqs. (10.26) and (10.29) easier to compare we can push the implicit scheme, Eq. (10.29), forward by a time-step to get

$$A Q_{i-1,n+1} + B Q_{i,n+1} + C Q_{i+1,n+1} = Q_{i,n} \quad (10.32)$$

In practice, Eqs. (10.26) and (10.32) are used to evaluate each $Q_{i,n+1}$ value with the assumption that values of $Q_{i-1,n}$, $Q_{i,n}$ and $Q_{i+1,n}$ are known a priori (see Fig. 10.1a). Eq. (10.26) appears more straightforward to evaluate because there is one equation and only one unknown value, $Q_{i,n+1}$. When using this method, it is

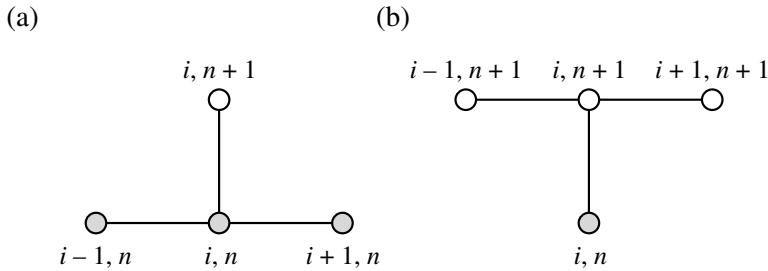


Fig. 10.1 Finite difference stencils for **a** an explicit time-stepping scheme and **b** an implicit time-stepping scheme. The shaded and white circles represent known and unknown values, respectively

said that $Q_{i,n+1}$ can be “explicitly” calculated from the $Q_{i-1,n}$, $Q_{i,n}$ and $Q_{i+1,n}$ values. Hence this method is referred to as an explicit time-stepping method.

In contrast, Eq. (10.32) appears more difficult to deal with because there apparently remains only one equation but three unknown values, $Q_{i-1,n+1}$, $Q_{i,n+1}$ and $Q_{i+1,n+1}$ (see Fig. 10.1b). When using this method, it is said that $Q_{i,n+1}$ is “implicitly” calculated from the $Q_{i-1,n+1}$, $Q_{i,n}$ and $Q_{i+1,n+1}$ values. Hence this method is referred to as an implicit time-stepping method.

Explicit methods are generally considered easier to implement as compared to implicit methods. However, explicit methods tend require much smaller time-steps to ensure numerical stability as compared to implicit methods. Hence, implicit methods are often preferred.

10.6 Numerical Stability

The approximate nature of the finite difference schemes described above gives rise to inevitable numerical error. In some cases, this error increases with each time-step leading chaotic and unrealistic results. When this occurs, the scheme is said to be numerically unstable. In other cases, the error is found to reduce with each time-step and the results provide realistic approximate solutions to the governing equations being solved. In this latter case, a scheme is said to be numerically stable. Most numerical schemes are conditionally stable. Conditions for stability can be found using Fourier stability analysis (e.g. [1, p. 103]).

10.6.1 Explicit Schemes

The conditions of stability for the explicit time-stepping schemes are that the coefficients A , B and C in Eq. (10.26) must all be greater than zero.

For the ETCS scheme, inspection of Eq. (10.27) reveals that numerical stability will be achieved providing [1, pp. 104 and 118]

$$\frac{2K\Delta t}{\Delta x^2} < 1 \quad \text{and} \quad \frac{c\Delta t}{2\Delta x} < \frac{K\Delta t}{\Delta x^2} \quad (10.33)$$

For the ETBS scheme, inspection of Eq. (10.28) reveals that numerical stability will be achieved providing [1, pp. 104 and 113]

$$\frac{2K\Delta t}{\Delta x^2} + \frac{c\Delta t}{\Delta x} < 1. \quad (10.34)$$

10.6.2 Implicit Schemes

The conditions of stability for the implicit time-stepping schemes are that the coefficient B in Eq. (10.32) must be greater than zero whilst the coefficients A and C must be less than zero.

For the ITCS scheme, inspection of Eq. (10.30) reveals that numerical stability will be achieved providing [1, p. 122]

$$\frac{c\Delta t}{2\Delta x} < \frac{K\Delta t}{\Delta x^2} \quad (10.35)$$

The ITBS scheme is unconditionally stable.

10.6.3 Neumann, Courant and Peclet Number

The three constraints provided in Eqs. (10.33) and (10.34) give rise to three important dimensionless groups, the Neumann number, Ne [–], the Courant number, Cr [–], and the Peclet number, Pe [–] [1, pp. 102, 111 and 118] :

$$Ne = \frac{K\Delta t}{\Delta x^2}, \quad Cr = \frac{c\Delta t}{\Delta x} \quad \text{and} \quad Pe = \frac{c\Delta x}{K} \quad (10.36)$$

Substituting the definitions for Cr and Pe into Eqs. (10.33) to (10.35) suggests that:

- ETCS requires $Ne < 0.5$ and $Pe < 2$.
- ETBS requires $2Ne + Cr < 1$.
- ITCS requires $Pe < 2$.

The velocity of diffusion waves within a finite difference solution is around $\frac{2K}{\Delta x}$. The Neumann number stability criterion, $Ne < 0.5$, suggests that, for explicit schemes, numerical instability occurs when the distance a diffusion wave travels during a time-step, $\frac{2K\Delta t}{\Delta x}$, is greater than the distance to the next solution point, Δx . A common method of dealing with this is to reduce the size of the time-steps, Δt . However, reductions in time-step size lead to increases in the number of computations required to simulate a specified time period.

Both of the implicit methods, ITCS and ITBS, are not restricted in this way, and will remain numerically stable regardless of the size of the time-step applied. This represents a significant advantage of implicit schemes over explicit schemes.

However, numerical stability does not ensure numerical accuracy. As we will see later in the chapter, large time-steps lead to excessive numerical diffusion.

The Peclet number stability criterion, $Pe < 2$, suggests that, for both the ETCS and ITCS schemes, numerical instability occurs when the advection velocity, c , exceeds the velocity of the diffusion waves. When $Pe > 2$, the changes in Q with x become very sharp and cannot be properly defined within the prescribed set of spatial solution points, $x_1, x_2, \dots, x_{N_x}$. A high Peclet number also affects the ETBS scheme by making the associated Courant number constraint harder to satisfy.

The Peclet number can be reduced by reducing the size of space steps. However, this will lead to increased computational requirements and, for explicit schemes, further reductions in the size of the time steps (due to the Neumann number and Courant number stability criteria). In contrast, the ITBS scheme is unaffected by Peclet number stability. However, as we will see later in the chapter, backward differencing in space leads to additional numerical diffusion.

10.7 Matrix Formulation

Let

$$\mathbf{Q}_n = \begin{bmatrix} Q_{1,n} \\ Q_{2,n} \\ Q_{3,n} \\ Q_{4,n} \\ \vdots \\ Q_{N_x-3,n} \\ Q_{N_x-2,n} \\ Q_{N_x-1,n} \\ Q_{N_x,n} \end{bmatrix}, \quad \mathbf{Q}_{n+1} = \begin{bmatrix} Q_{1,n+1} \\ Q_{2,n+1} \\ Q_{3,n+1} \\ Q_{4,n+1} \\ \vdots \\ Q_{N_x-3,n+1} \\ Q_{N_x-2,n+1} \\ Q_{N_x-1,n+1} \\ Q_{N_x,n+1} \end{bmatrix} \quad (10.37)$$

10.7.1 Explicit Time-Stepping Schemes

Challenge 10.10 Write Eq. (10.26), for the explicit time-stepping schemes, in matrix form, also taking into account the boundary conditions in Eq. (10.2).

Considering Eq. (10.37), the explicit time-stepping schemes described by Eq. (10.26) can be written as

$$\mathbf{Q}_{n+1} = \mathbf{J}\mathbf{Q}_n \quad (10.38)$$

where $\mathbf{J}$, is often referred to as a Jacobian matrix, and is found from

$$\mathbf{J} = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ A & B & C & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & A & B & C & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & A & B & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & B & C & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & A & B & C & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & A & B & C \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 1 \end{bmatrix} \quad (10.39)$$

with the top and bottom rows in Eq. (10.39) required to impose the two boundary conditions in Eq. (10.2) and A , B and C determined from either Eq. (10.27) or Eq. (10.28).

10.7.2 Implicit Time-Stepping Schemes

Challenge 10.11 Write Eq. (10.32), for the implicit time-stepping schemes, in matrix form, again taking into account the boundary conditions in Eq. (10.2).

Considering Eq. (10.37) again, the implicit time-stepping schemes described by Eq. (10.32) can be written as

$$\mathbf{J}\mathbf{Q}_{n+1} = \mathbf{Q}_n \quad (10.40)$$

where again $\mathbf{J}$ is described by Eq. (10.39) but with A , B and C determined from either Eq. (10.30) or Eq. (10.31).

Note that $\mathbf{Q}_{n+1}$ can be acquired directly from $\mathbf{Q}_n$ by multiplying both sides of Eq. (10.40) by the inverse of the Jacobian matrix, $\mathbf{J}^{-1}$, i.e.,

$$\mathbf{Q}_{n+1} = \mathbf{J}^{-1}\mathbf{Q}_n. \quad (10.41)$$

10.7.3 More about the Jacobian Matrix

Consider when $\mathbf{f} = \mathbf{J}\mathbf{x}$. The Jacobian matrix, $\mathbf{J}$, represents

$$\mathbf{J} = \left[\frac{\partial \mathbf{f}}{\partial x_1} \dots \frac{\partial \mathbf{f}}{\partial x_{N_x}} \right] = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \dots & \frac{\partial f_1}{\partial x_{N_x}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_{N_x}}{\partial x_1} & \dots & \frac{\partial f_{N_x}}{\partial x_{N_x}} \end{bmatrix} \quad (10.42)$$

For the explicit schemes (Eq. (10.38))

$$\mathbf{J} = \begin{bmatrix} \frac{\partial \mathbf{Q}_{n+1}}{\partial \mathbf{Q}_{1,n}} & \cdots & \frac{\partial \mathbf{Q}_{n+1}}{\partial \mathbf{Q}_{N_X,n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \mathbf{Q}_{N_X,n+1}}{\partial \mathbf{Q}_{1,n}} & \cdots & \frac{\partial \mathbf{Q}_{N_X,n+1}}{\partial \mathbf{Q}_{N_X,n}} \end{bmatrix} \quad (10.43)$$

Furthermore, comparing Eqs. (10.39) and (10.43) it can be understood that

$$A = \frac{\partial Q_{i,n+1}}{\partial Q_{i-1,n}}, \quad B = \frac{\partial Q_{i,n+1}}{\partial Q_{i,n}}, \quad C = \frac{\partial Q_{i,n+1}}{\partial Q_{i+1,n}}$$

For the implicit schemes (Eq. (10.40))

$$\mathbf{J} = \begin{bmatrix} \frac{\partial \mathbf{Q}_n}{\partial \mathbf{Q}_{1,n+1}} & \cdots & \frac{\partial \mathbf{Q}_n}{\partial \mathbf{Q}_{N_X,n+1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \mathbf{Q}_{N_X,n}}{\partial \mathbf{Q}_{1,n+1}} & \cdots & \frac{\partial \mathbf{Q}_{N_X,n}}{\partial \mathbf{Q}_{N_X,n+1}} \end{bmatrix} \quad (10.44)$$

Furthermore, comparing Eqs. (10.39) and (10.44) it can be understood that

$$A = \frac{\partial Q_{i,n}}{\partial Q_{i-1,n+1}}, \quad B = \frac{\partial Q_{i,n}}{\partial Q_{i,n+1}}, \quad C = \frac{\partial Q_{i,n}}{\partial Q_{i+1,n+1}}.$$

10.7.4 Implementation in MATLAB

The four different finite difference schemes described above can be implemented using the MATLAB function given in Listing 10.1.

Listing 10.1 A MATLAB function capable of evaluating four different finite difference schemes for the diffusion wave equation.

```
function [Q,x,t]=FDmodel(L,tend,Q0,QI,K,c,k,dx,dt,scheme)
%Finite difference solution for ADE
%Q - Flow rate (m3/s)
%x - Distance from inlet (m)
%t - Time (s)
%L - Length of spatial domain (m)
%tend - Duration of temporal domain (s)
%Q0 - Inlet flow rate (m3/s)
%QI - Uniform initial flow rate (m3/s)
%K - Apparent diffusion coefficient (m2/s)
%c - Wave speed (m/s)
%dx - Space-step (m)
%dt - Time-step (s)
%scheme - 'ETCS', 'ETBS', 'ITCS' or 'ITBS'
x=[0:dx:L]'; t=0:dt:tend; %Point locations
Nx=numel(x); Nt=numel(t); %Numer of points
Q=zeros(Nx,Nt); %Initialise solution matrix
%Apply initial and boundary conditions
Q(:,1)=QI; Q(1,:)=Q0; Q(Nx,:)=QI;
```



```

switch scheme %Jacobian matrix coefficients:
case 'ETCS'
A=K*dt/dx^2+c*dt/2/dx;
B=1-2*K*dt/dx^2;
C=K*dt/dx^2-c*dt/2/dx;
case 'ETBS'
A=K*dt/dx^2+c*dt/dx;
B=1-2*K*dt/dx^2-c*dt/dx;
C=K*dt/dx^2;
case 'ITCS'
A=-K*dt/dx^2-c*dt/2/dx;
B=1+2*K*dt/dx^2;
C=-K*dt/dx^2+c*dt/2/dx;
case 'ITBS'
A=-K*dt/dx^2-c*dt/dx;
B=1+2*K*dt/dx^2+c*dt/dx;
C=-K*dt/dx^2;
end
%Determine the Jacobian matrix
J=spdiags(ones(Nx,1)*[A B C],[-1 0 1],Nx,Nx);
%Apply boundary conditions
J(1,:)=0; J(1,1)=1; J(Nx,:)=0; J(Nx,Nx)=1;
for n=1:Nt-1 %Step through solution
switch scheme
case {'ETCS','ETBS'}
Q(:,n+1)=J*Q(:,n);
case {'ITCS','ITBS'}
Q(:,n+1)=J\Q(:,n);
end
end
end

```

MATLAB's `switch` command is used to determine the appropriate set of Jacobian matrix coefficients from either Eq. (10.27), (10.28), (10.30) or (10.31), depending on which scheme is selected (ETCS, ETBS, ITCS or ITBS).

MATLAB's `spdiags` command is used to form the sparse tri-diagonal matrix associated with the Jacobian matrix, Eq. (10.39). The benefit of using a sparse matrix is that diagonals containing only zeros do not contribute to the memory requirement. Consequently the memory requirement for the Jacobian matrix reduces from $N_x \times N_x$ to $N_x \times 3$.

The fixed Q boundary conditions, given in Eq. (10.2), are implemented within the Jacobian matrix by setting the associated coefficients to one on the central diagonal and zero on the neighbouring diagonals, either side, such that the value of Q remains unchanged at those nodes within the time-stepping schemes. The values of Q for the initial condition and boundary conditions are set following the initialisation of the solution matrix.

MATLAB's left-divide-operator (`\`) is used for both of the implicit schemes, ITCS and ITBS, to perform the inverse matrix calculation in Eq. (10.41).

10.8 Numerical Diffusion

It can be seen in Eqs. (10.16) and (10.23), that the backward difference space approximations in ETBS and ITBS lead to an additional diffusion term with a diffusion coefficient of $\frac{c\Delta x}{2!}$. This diffusion is commonly referred to as numerical diffusion [1, p. 113]. In fact, it can be shown that the $\frac{\partial^2 Q}{\partial t^2}$ leads to negative numerical diffusion for the explicit schemes and additional positive numerical diffusion for the implicit schemes.

Partially differentiating both sides of Eq. (10.1) with respect to t leads to

$$\begin{aligned}\frac{\partial^2 Q}{\partial t^2} &= K \frac{\partial}{\partial t} \left(\frac{\partial^2 Q}{\partial x^2} \right) - c \frac{\partial}{\partial t} \left(\frac{\partial Q}{\partial x} \right) \\ &= K \frac{\partial^2}{\partial x^2} \left(\frac{\partial Q}{\partial t} \right) - c \frac{\partial}{\partial x} \left(\frac{\partial Q}{\partial t} \right)\end{aligned}$$

Substituting Eq. (10.1) then leads to

$$\begin{aligned}\frac{\partial^2 Q}{\partial t^2} &= K \frac{\partial^2}{\partial x^2} \left(K \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} \right) - c \frac{\partial}{\partial x} \left(K \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} \right) \\ &= K^2 \frac{\partial^4 Q}{\partial x^4} - 2cK \frac{\partial^3 Q}{\partial x^3} + c^2 \frac{\partial^2 Q}{\partial x^2}\end{aligned}$$

and so

$$\frac{\partial^2 Q}{\partial t^2} = c^2 \frac{\partial^2 Q}{\partial x^2} + O\left(\frac{\partial^3 Q}{\partial x^3}\right). \quad (10.45)$$

10.8.1 Numerical Diffusion from the ETCS Scheme

Challenge 10.12 Substitute Eqs. (10.9), (10.11), (10.10) and (10.45) into Eq. (10.13) and determine the numerical diffusion coefficient, $K_{\text{num}} [\text{L}^2\text{T}^{-1}]$, associated with the ETCS scheme.

Substituting Eqs. (10.9), (10.11) and (10.10) into the ETCS scheme, Eq. (10.13) leads to

$$\frac{\partial Q}{\partial t} + \frac{\Delta t}{2!} \frac{\partial^2 Q}{\partial t^2} = K \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} + O(\Delta x^2, \Delta t^2)$$

Substituting Eq. (10.45) then leads to

$$\frac{\partial Q}{\partial t} = \left(K - \frac{c^2 \Delta t}{2} \right) \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} + O(\Delta x^2, \Delta t^2)$$

from which it can be seen that numerical diffusion coefficient, $K_{\text{num}} [\text{L}^2\text{T}^{-1}]$, incurred by the ETCS scheme is

$$K_{\text{num}} = -\frac{c^2 \Delta t}{2} \quad (10.46)$$

which is negative.

It follows that one should add $\frac{c^2 \Delta t}{2}$ to the actual diffusion coefficient to counteract the effect of numerical diffusion when applying the ETCS scheme.

10.8.2 Numerical Diffusion from the ETBS Scheme

Challenge 10.13 Substitute Eqs. (10.9), (10.11), (10.15) and (10.45) into Eq. (10.17) and determine the numerical diffusion coefficient, $K_{\text{num}} [\text{L}^2\text{T}^{-1}]$, associated with the ETBS scheme.

Substituting Eqs. (10.9), (10.11) and (10.15) into the ETBS scheme, Eq. (10.17) leads to

$$\frac{\partial Q}{\partial t} + \frac{\Delta t}{2!} \frac{\partial^2 Q}{\partial t^2} = K \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} + \frac{c \Delta x}{2!} \frac{\partial^2 Q}{\partial x^2} + O(\Delta x^2, \Delta t^2)$$

Substituting Eq. (10.45) then leads to

$$\frac{\partial Q}{\partial t} = \left(K - \frac{c^2 \Delta t}{2} + \frac{c \Delta x}{2} \right) \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} + O(\Delta x^2, \Delta t^2)$$

from which it can be seen that numerical diffusion coefficient, $K_{\text{num}} [\text{L}^2\text{T}^{-1}]$, incurred by the ETBS scheme is [7, p. 390]

$$K_{\text{num}} = \frac{c}{2} (\Delta x - c \Delta t) \quad (10.47)$$

which becomes negative when $\text{Cr} > 1$.

It follows that one should subtract $\frac{c}{2} (\Delta x - c \Delta t)$ from the actual diffusion coefficient to counteract the effect of numerical diffusion when applying the ETBS scheme.

10.8.3 Numerical Diffusion from the ITCS Scheme

Challenge 10.14 Substitute Eqs. (10.19), (10.11), (10.10) and (10.45) into Eq. (10.21) and determine the numerical diffusion coefficient, $K_{\text{num}} [\text{L}^2\text{T}^{-1}]$, associated with the ITCS scheme.

Substituting Eqs. (10.19), (10.11) and (10.10) into the ITCS scheme, Eq. (10.21) leads to

$$\frac{\partial Q}{\partial t} - \frac{\Delta t}{2!} \frac{\partial^2 Q}{\partial t^2} = K \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} + O(\Delta x^2, \Delta t^2)$$

Substituting Eq. (10.45) then leads to

$$\frac{\partial Q}{\partial t} = \left(K + \frac{c^2 \Delta t}{2} \right) \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} + O(\Delta x^2, \Delta t^2)$$

from which it can be seen that numerical diffusion coefficient, $K_{\text{num}} [L^2 T^{-1}]$, incurred by the ITCS scheme is

$$K_{\text{num}} = \frac{c^2 \Delta t}{2} \quad (10.48)$$

which is positive.

It follows that one should subtract $\frac{c^2 \Delta t}{2}$ from the actual diffusion coefficient to counteract the effect of numerical diffusion when applying the ITCS scheme.

10.8.4 Numerical Diffusion from the ITBS Scheme

Challenge 10.15 Substitute Eqs. (10.19), (10.11), (10.15) and (10.45) into Eq. (10.24) and determine the numerical diffusion coefficient, $K_{\text{num}} [L^2 T^{-1}]$, associated with the ITBS scheme.

Substituting Eqs. (10.19), (10.11) and (10.15) into the ITBS scheme, Eq. (10.24) leads to

$$\frac{\partial Q}{\partial t} - \frac{\Delta t}{2!} \frac{\partial^2 Q}{\partial t^2} = K \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} + \frac{c \Delta x}{2!} \frac{\partial^2 Q}{\partial x^2} + O(\Delta x^2, \Delta t^2)$$

Substituting Eq. (10.45) then leads to

$$\frac{\partial Q}{\partial t} = \left(K + \frac{c^2 \Delta t}{2} + \frac{c \Delta x}{2} \right) \frac{\partial^2 Q}{\partial x^2} - c \frac{\partial Q}{\partial x} + O(\Delta x^2, \Delta t^2)$$

from which it can be seen that numerical diffusion coefficient, $K_{\text{num}} [L^2 T^{-1}]$, incurred by the ITBS scheme is [7, p. 390]

$$K_{\text{num}} = \frac{c}{2} (\Delta x + c \Delta t) \quad (10.49)$$

which is negative.

It follows that one should subtract $\frac{c}{2} (\Delta x + c \Delta t)$ from the actual diffusion coefficient to counteract the effect of numerical diffusion when applying the ITBS scheme.

10.8.5 Correcting all the Schemes for Numerical Diffusion

Adding the appropriate amount to the diffusion coefficient to counteract the effect of numerical dispersion for both the ETCS and ETBS schemes (recall Eqs. (10.27) and (10.28)) leads to the following set of modified A , B and C coefficients:

$$\begin{aligned} A &= \frac{K \Delta t}{\Delta x^2} + \frac{c \Delta t}{2 \Delta x} + \frac{1}{2} \left(\frac{c \Delta t}{\Delta x} \right)^2 \\ B &= 1 - \frac{2K \Delta t}{\Delta x^2} - \left(\frac{c \Delta t}{\Delta x} \right)^2 \\ C &= \frac{K \Delta t}{\Delta x^2} - \frac{c \Delta t}{2 \Delta x} + \frac{1}{2} \left(\frac{c \Delta t}{\Delta x} \right)^2 \end{aligned} \quad (10.50)$$

Adding the appropriate amount to the diffusion coefficient to counteract the effect of numerical dispersion for both the ITCS and ITBS schemes (recall Eqs. (10.30) and (10.31)) leads to the following set of modified A , B and C coefficients:

$$\begin{aligned} A &= -\frac{K \Delta t}{\Delta x^2} - \frac{c \Delta t}{2 \Delta x} + \frac{1}{2} \left(\frac{c \Delta t}{\Delta x} \right)^2 \\ B &= 1 + \frac{2K \Delta t}{\Delta x^2} - \left(\frac{c \Delta t}{\Delta x} \right)^2 \\ C &= -\frac{K \Delta t}{\Delta x^2} + \frac{c \Delta t}{2 \Delta x} + \frac{1}{2} \left(\frac{c \Delta t}{\Delta x} \right)^2. \end{aligned} \quad (10.51)$$

10.9 Implicit Schemes for Non-linear PDEs

As we saw earlier, only the ITBS scheme is unconditionally stable. Previously we focused on Eq. (10.1) with constant values for c and K . However, it is often the case that c and K are both functions of the dependent variable, Q . In this case, the Jacobian matrix, $\mathbf{J}$, is a function of $\mathbf{Q}_{n+1}$ and Eq. (10.41) cannot be directly used to derive values for $\mathbf{Q}_{n+1}$ from $\mathbf{Q}_n$. An iterative solution is required instead.

Let $\mathbf{Q}_{n+1,k}$ contain the estimated values of $\mathbf{Q}_{n+1}$ after the k -th iteration. A reasonable starting point is to take $\mathbf{Q}_{n+1,1} = \mathbf{Q}_n$. From Eq. (10.40) we can say

$$\mathbf{J}_{n+1,k} \mathbf{Q}_{n+1,k} - \mathbf{Q}_n = \mathbf{R}_{n+1,k} \quad (10.52)$$

where $\mathbf{J}_{n+1,k} = \mathbf{J}(\mathbf{Q}_{n+1,k})$ is the Jacobian matrix, calculated from Eq. (10.39) with values of $\mathbf{Q}_{n+1,k}$ from the latest iteration, and $\mathbf{R}_{n+1,k} = \mathbf{R}(\mathbf{Q}_{n+1,k})$ is a residual vector containing the errors associated with the solution from the latest iteration.

As the iterative solution starts to converge, the difference $\Delta \mathbf{Q}_{n+1} = \mathbf{Q}_{n+1,k+1} - \mathbf{Q}_{n+1,k}$ should be small and the residual vector from the next iteration, $\mathbf{R}_{n+1,k+1}$, can be found from the following truncated Taylor series (recall Eq. (10.3))

$$\mathbf{R}_{n+1,k+1} = \mathbf{R}_{n+1,k} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}_{n+1,k}} \right] \Delta \mathbf{Q}_{n+1} + O(\Delta \mathbf{Q}_{n+1}^2) \quad (10.53)$$

From Eq. (10.52) we can see that

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}_{n+1,k}} \right] = \mathbf{J}_{n+1,k} \quad (10.54)$$

Substituting Eq. (10.54) into Eq. (10.53) leads to

$$\mathbf{R}_{n+1,k+1} = \mathbf{R}_{n+1,k} + \mathbf{J}_{n+1,k} \Delta \mathbf{Q}_{n+1} + O(\Delta \mathbf{Q}_{n+1}^2) \quad (10.55)$$

We want to choose values for $\Delta \mathbf{Q}_{n+1}$ such that $\mathbf{R}_{n+1,k+1}$ goes to zero. It follows that a good choice for $\Delta \mathbf{Q}_{n+1}$ is found from

$$\mathbf{J}_{n+1,k} \Delta \mathbf{Q}_{n+1} = -\mathbf{R}_{n+1,k} \quad (10.56)$$

Multiplying both sides of Eq. (10.56) by the inverse of the Jacobian matrix, $\mathbf{J}_{n+1,k}^{-1}$, and adding $\mathbf{Q}_{n+1,k}$ to both sides leads to [1, p. 93]

$$\mathbf{Q}_{n+1,k+1} = \mathbf{Q}_{n+1,k} - \mathbf{J}_{n+1,k}^{-1} \mathbf{R}_{n+1,k} \quad (10.57)$$

Substituting Eq. (10.52) then leads to

$$\mathbf{Q}_{n+1,k+1} = \mathbf{J}_{n+1,k}^{-1} \mathbf{Q}_n \quad (10.58)$$

Equation (10.57) is often referred to as a Newton iteration. A Newton iteration scheme can be considered to have converged when $|\Delta \mathbf{Q}_{n+1}|$ has reached an acceptably low level.

10.10 Problem Sheet

Problem 10.1 (see Worked Solution 10.1)

Use the `FDmodel` function, given in Listing 10.1, to simulate heat conduction from a fixed temperature boundary condition. Assume the thermal diffusion coefficient, $K = 10^{-6} \text{ m}^2\text{s}^{-1}$, the initial temperature, $T_I = -1^\circ\text{C}$ and that the boundary temperature, $T_0 = 1^\circ\text{C}$. Also assume that the temperature is fixed to T_I at a 0.6 m distance from the T_0 boundary condition and solve with a space-step, $\Delta x = 2 \text{ cm}$.

(a) Explore the effect of time-step size, using an explicit time-stepping scheme, by simulating the problem described above with (i) 91 temporal-solution-points (i.e., $N_t = 91$), (ii) 89 temporal-solution-points, (iii) 88 temporal-solution-points and (iv) 87 temporal-solution-points. Compare plots of temperature against distance after 300 minutes and calculate the associated Neumann numbers. Also compare your results to a relevant analytical solution.

(b) Explore the effect of time-step size, using an implicit time-stepping scheme, by simulating the problem described above with (i) 40 temporal-solution-points (i.e., $N_t = 91$), (ii) 5 temporal-solution-points, (iii) 3 temporal-solution-points and (iv) 2 temporal-solution-points. Compare plots of temperature against distance after 300 minutes and calculate the associated Neumann numbers.

Problem 10.2 (see Worked Solution 10.2)

Use the `FDmodel` function, given in Listing 10.1, to simulate the propagation of a flood wave in a river. Assume the hydraulic diffusion coefficient, $K = 500 \text{ m}^2\text{s}^{-1}$, the wave speed, $c = 1 \text{ m s}^{-1}$, negligible decay, an initial flow rate, $Q_I = 60 \text{ m}^3\text{s}^{-1}$ and an inlet boundary flow rate, $Q_0 = 750 \text{ m}^3\text{s}^{-1}$. Also assume that the flow rate is fixed to Q_I at a 500 km distance from the inlet boundary and solve using 1001 temporal-solution-points.

(a) Explore the effect of space-step size using ITCS, by simulating the problem described above with (i) 25 spatial-solution-points (i.e., $N_x = 25$), (ii) 50 spatial-solution-points, (iii) 100 spatial-solution-points and (iv) 250 spatial-solution-points. Compare plots of flow rate against distance after 80h and calculate the associated numerical Peclet numbers. Also compare your results to a relevant analytical solution.

(b) Repeat part (a) but using ITBS.

(c) Calculate the numerical diffusion associated with the ITBS solution with 250 spatial-solution-points and compare the results from part b) with those from the analytical solution with the theoretical diffusion added.

(d) Explore the effect of time-step size using ITCS, by simulating the problem described above using 250 spatial-solution-points (i.e., $N_x = 250$) and with (i) 10 temporal-solution-points (i.e., $N_t = 25$), (ii) 30 temporal-solution-points, (iii) 100 temporal-solution-points and (iv) 1000 temporal-solution-points. Compare plots of flow rate against distance after 80h and calculate the associated Neumann numbers. Also compare your results to a relevant analytical solution.

(e) Calculate the numerical diffusion associated with the ITCS solution with 250 spatial-solution-points and 100 temporal-solution-points and compare the results with those from the analytical solution with the theoretical diffusion added.

Problem 10.3 (see Worked Solution 10.3)

Develop a finite difference solution for the kinematic wave equation

$$\frac{\partial u}{\partial t} = -\frac{5u}{3} \frac{\partial u}{\partial x} \quad (10.59)$$

subjected to the initial condition

$$u(x, 0) = \begin{cases} 1.2 \text{ m s}^{-1}, & x \in (0, 50 \text{ km}) \\ 0, & x \notin (0, 50 \text{ km}) \end{cases}$$

and boundary condition

$$u(0, t) = 0 \quad (10.60)$$

Plot the resulting fluid velocity values against distance after 5, 10, 20 and 40 h and compare these with values obtained using the Method of Characteristics (MoC) solution given in Listing 7.2. It is recommended to re-write the kinematic wave equation in conservative form and use a backward difference in time and space with a time-step, $\Delta t = 3$ minutes and a space-step, $\Delta x = 200$ m.

10.11 Worked Solutions

Worked Solution 10.1 (see Problem 10.1)

(a) Below is a MATLAB script for performing the desired task using an explicit time-stepping scheme. Note that for the `FDmodel` function, $Q = T$, $Q_0 = T_0$ and $Q_I = T_I$. The schemes, ETCS and ETBS, yield the same answers in this context because the wave speed, $c = 0$. The Neumann number, Ne , is calculated using Eq. (10.36). The `OgataBanksDecay` function, given in Listing 8.2, can be used as an analytical solution for checking purposes. Note that $c = 0$ and $\kappa = 0$ because there is no advection and no decay.

```
function HeatConductionExamples
K=1e-6; %Diffusion coefficient (m2/s)
c=0; %Wave speed (m/s)
k=0; %Decay rate (1/s)
L=0.6; %Distance (m)
tend=300*60; %Time (s)
TI=-1; %Initial temperature (deg C)
T0=1; %Boundary temperature (deg C)
dx=0.02; %Space-step (m)
Nt=[91 89 88 87]; %Number of time points
figure(1);clf;hold on;box on %Form figure
for n=1:numel(Nt) %Step through each solution
dt=tend/(Nt(n)-1); %Time step
Ne=K*dt/dx^2; %Neumann number
%Evaluate explicit time-stepping solution
[Tfd,x,t]=FDmodel(L,tend,T0,TI,K,c,k,dx,dt,'ETCS');
%Plot results
plot(Tfd(:,end),x*100)
%Compile strings for legend
MyLegend{n}=['Ne = ' num2str(Ne,3)...
' (' num2str(Nt(n)) ' time-points)'];
end
%Evaluate analytical solution
Ta=OgataBanksDecay(x,tend,T0,TI,K,c,k);
```



```
%Add extra legend entry
MyLegend{n+1}='Analytical solution';
plot(Ta,x*100,'ko')
set(gca,'ydir','reverse')
legend(MyLegend,'location','southeast')
xlim([-1.5 1.5])
xlabel('Temperature (^oC)')
ylabel('Depth (cm)')
```

The results are shown in Fig. 10.2, with the Neumann numbers displayed in the legend. Simulations with $Ne > 0.5$ are unstable, as predicted by Eq. (10.33). As Ne increases, the simulations become progressively more unstable. Nevertheless, the simulation with $Ne = 0.5$ provides an excellent approximation of the analytical solution.

(b) The additional MATLAB code below can be appended to the `HeatConductionExamples` function listed above to produce a set of simulations using an implicit time-stepping scheme with the requested number of temporal-solution-points. The schemes, ITCS and ITBS, yield the same answers in this context because the wave speed, $c = 0$.

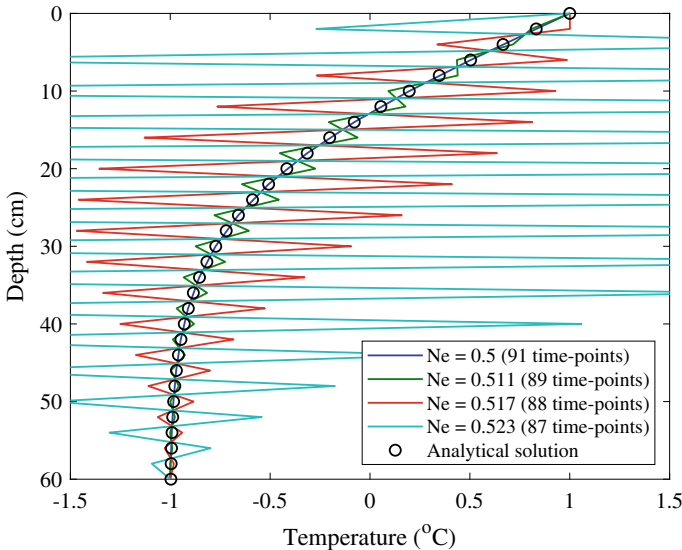


Fig. 10.2 Results from explicit finite difference solutions to a heat conduction problem showing the effect of the Neumann number, Nr

```

Nt=[40 5 3 2]; %Number of time points
figure(2);clf;hold on;box on %Form figure
for n=1:numel(Nt) %Step through each solution
dt=tend/(Nt(n)-1); %Time step
Ne=K*dt/dx^2; %Neumann number
%Evaluate implicit time-stepping solution
[Tfd,x,t]=FDmodel(L,tend,T0,TI,K,c,k,dx,dt,'ITCS');
%Plot results
plot(Tfd(:,end),x*100)
%Compile strings for legend
MyLegend{n}=['Ne = ' num2str(Ne,3)...
' (' num2str(Nt(n)) ' time-points)'];
end
%Plot analytical solution for comparison
plot(Ta,x*100,'ko')
set(gca,'ydir','reverse')
legend(MyLegend,'location','southeast')
xlim([-1 1])
xlabel('Temperature (^oC)')
ylabel('Depth (cm)')

```

The results are shown in Fig. 10.3, with the Neumann numbers displayed in the legend. Simulations remain stable regardless of the Neumann number when applying implicit time-stepping schemes (recall Sect. 10.6.3). Nevertheless, as Ne becomes

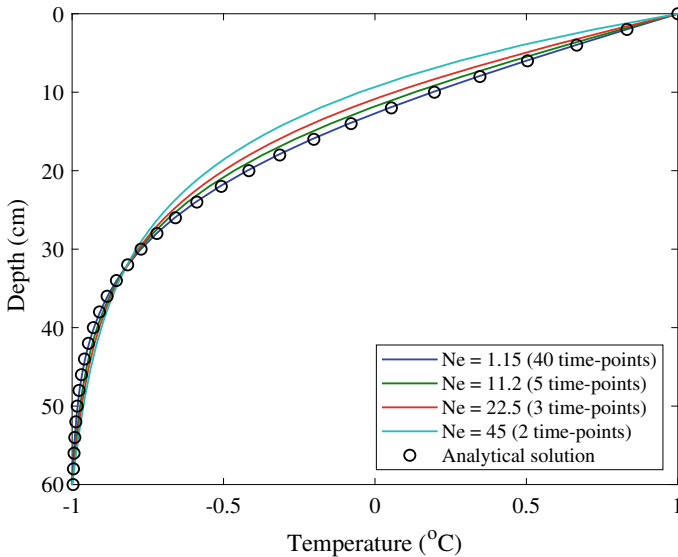


Fig. 10.3 Results from implicit finite difference solutions to a heat conduction problem showing the effect of the Neumann number, Ne

much greater than 0.5, the solutions become progressively less accurate, as indicated by the comparison with the analytical solution.

Worked Solution 10.2 (see Problem 10.2)

(a) Below is a MATLAB script for performing the desired task using ITCS. The numerical Peclet number, Pe , is calculated using Eq. (10.36). The function `OgataBanksDecay`, given in Listing 8.2, can be used as an analytical solution for checking purposes. Note that $\kappa = 0$ because there is no decay.

```
function DiffusionWaveExamples
K=500; %Diffusion coefficient (m2/s)
c=1; %Wave speed (m/s)
k=0; %Decay rate (1/s)
L=500e3; %Distance (m)
tend=80*60^2; %Time (s)
QI=60; %Initial flow rate (m3/s)
Q0=750; %Boundary flow rate (m3/s)
Nt=1001; %Number of time points
dt=tend/(Nt-1); %Time step
Nx=[25 50 100 250]; %Number of space points
figure(3);clf;hold on;box on %Form figure
for n=1:numel(Nx) %Step through each solution
dx=L/(Nx(n)-1); %Determine space-step
%Evaluate implicit time-stepping solution
[Qfd,x,t]=FDmodel(L,tend,Q0,QI,K,c,k,dx,dt,'ITCS');
%Plots results
plot(x/1000,Qfd(:,end),'.-')
Pe=c*dx/K; %Determine Peclet number
MyLegend{n}=['Pe = ' num2str(Pe,3)...
' (' num2str(Nx(n)) ' space-points)'];
end
%Evaluate analytical solution
Qa=OgataBanksDecay(x,tend,Q0,QI,K,c,k);
plot(x/1000,Qa) %Plot results
MyLegend{n+1}='Analytical solution';
legend(MyLegend,'location','southwest')
xlabel('Distance (km)')
ylabel('Flow rate (m^3 s^-1)')
```

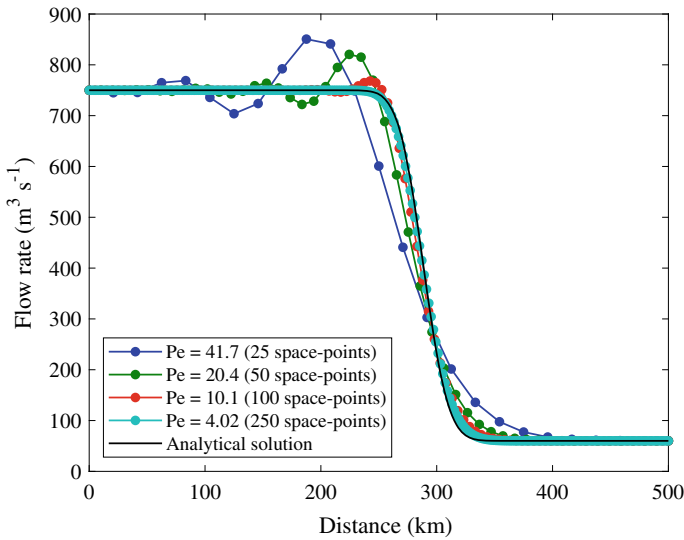


Fig. 10.4 Results from ITCS finite difference solutions to the diffusion wave problem showing the effect of the numerical Peclet number, Pe

The results are shown in Fig. 10.4, with the numerical Peclet numbers displayed in the legend. According to Eq. (10.35), simulations with $Pe > 2$ will exhibit numerical instability. As Pe increases, the simulations become progressively more unstable. Nevertheless, the simulation with $Pe = 4.01$ provides a very good approximation of the analytical solution. Note that a sufficient number of temporal-solution-points has been selected such that numerical diffusion due to implicit time-stepping is negligibly small.

(b) The additional MATLAB code below can be appended to the `DiffusionWaveExamples` function listed above to produce a set of simulations using ITBS with the requested number of spatial-solution-points.

```
figure(4);clf;hold on;box on
for n=1: numel(Nx) %Step through each solution
    dx=L/(Nx(n)-1); %Determine space-step
    %Evaluate implicit time-stepping solution
    [Qfd,x,t]=FDmodel(L,tend,Q0,QI,K,c,k,dx,dt,'ITBS');
    %Plots results
    plot(x/1000,Qfd(:,end),'.-')
end
%Plot analytical solution
plot(x/1000,Qa)
xlabel('Distance (km)')
ylabel('Flow rate (m^3 s^-1)')
```

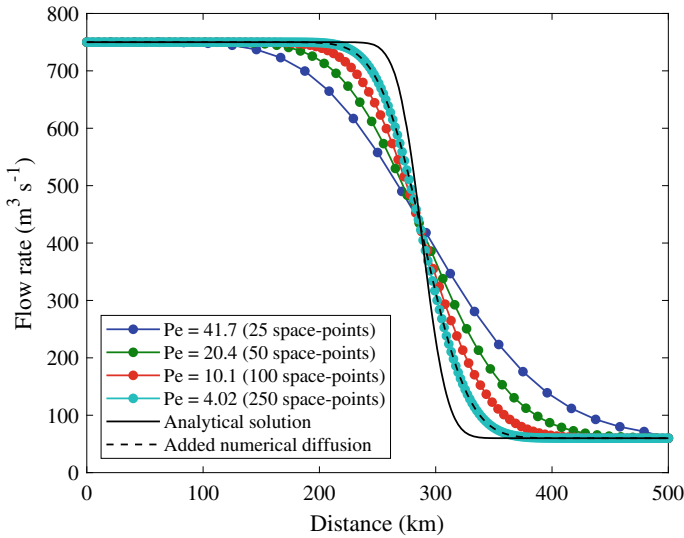


Fig. 10.5 Results from ITBS finite difference solutions to the diffusion wave problem showing the effect of the numerical Peclet number, Pe

The results are shown in Fig. 10.5, with the numerical Peclet numbers displayed in the legend. Simulations remain stable regardless of the numerical Peclet number when applying ITBS (recall Sect. 10.6.3). However, comparison with results from the analytical solution demonstrate that ITBS becomes progressively less accurate with increasing Pe due to numerical diffusion.

(c) The numerical diffusion can be quantified using Eq. (10.49). The additional MATLAB code below can be appended to `DiffusionWaveExamples` to evaluate the analytical solution, `OgataBanksDecay`, with the additional diffusion added to the existing diffusion coefficient.

```
%Analytical solution with numerical diffusion
Knum=c/2*(dx+c*dt); %Numerical diffusion
QaKnum=OgataBanksDecay(x,tend,Q0,QI,K+Knum,c,k);
plot(x/1000,QaKnum,'k--')
MyLegend{n+2}='Added numerical diffusion';
legend(MyLegend,'location','southwest')
```

The results are plotted as a dashed line in Fig. 10.5. The correspondence with the associated finite difference solution is excellent, corroborating the validity of the results derived in Sect. 10.8.

(d) The additional MATLAB code below can be appended to `DiffusionWaveExamples` to produce a set of simulations using ITCS with the requested number of spatial and temporal solution-points.

```
Nt=[10 30 100 1000]; %Number of time points
figure(5);clf;hold on;box on %Form figure
for n=1:numel(Nt) %Step through each solution
    dt=tend/(Nt(n)-1); %Time step
    Ne=K*dt/dx^2; %Neumann number
    %Evaluate implicit time-stepping solution
    [Qfd,x,t]=FDmodel(L,tend,Q0,QI,K,c,k,dx,dt,'ITCS');
    %Plot results
    plot(x/1000,Qfd(:,end),'.-')
    %Compile strings for legend
    MyLegend{n}=[ 'Ne = ' num2str(Ne,3)...
        ' ( ' num2str(Nt(n)) ' time-points)'];
end
%Plot analytical solution
plot(x/1000,Qa,'k')
xlabel('Distance (km)')
ylabel('Flow rate (m^3 s^-1)')
```

The results are shown in Fig. 10.6, with the Neumann numbers displayed in the legend. Simulations appear to remain stable regardless of the Neumann number when applying ITCS. This is because 250 spatial-solution-points are used, yielding a numerical Peclet number of 4.02 (see legend in Fig. 10.4), which is just sufficient to maintain Peclet number stability (recall Sect. 10.6.3). In contrast, ETCS would have led to highly unstable results for $Ne > 1$. However, comparison with results from the analytical solution demonstrate that ITCS becomes progressively less accurate with increasing Pe due to numerical diffusion associated with the implicit time-stepping, despite the use of central differencing for the advection term, even when $Ne = 0.361$.

(e) The numerical diffusion can be quantified for the 100 temporal-solution-points using Eq. (10.48). The additional MATLAB code below can be appended to `DiffusionWaveExamples` to evaluate the analytical solution, `OgataBanksDecay`, with the additional diffusion added to the existing diffusion coefficient.

```
%Analytical solution with numerical diffusion
dt=tend/(100-1); %Time step
Knum=c^2*dt/2; %Numerical diffusion
QaKnum=OgataBanksDecay(x,tend,Q0,QI,K+Knum,c,k);
plot(x/1000,QaKnum,'k--')
legend(MyLegend,'location','southwest')
```

The results are plotted as a dashed line in Fig. 10.6. The correspondence with the associated finite difference solution is excellent, again corroborating the validity of the results derived in Sect. 10.8.

Worked Solution 10.3 (see Problem 10.3)

Before deriving a finite difference solution for this problem it is worth to write the governing equation in conservative form (see Sect. 7.3). Comparing Eqs. (7.8) and (10.59) reveals that the flux function, $\phi = \frac{5u^2}{6}$, and therefore

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x} \left(\frac{5u^2}{6} \right)$$

Assuming a backward difference approximation for both derivatives leads to

$$\frac{u_{i,n} - u_{i,n-1}}{\Delta t} = -\frac{5}{6} \left(\frac{u_{i,n}^2 - u_{i-1,n}^2}{\Delta x} \right)$$

which can be rearranged to get

$$u_{i,n-1} = A_{i,n}u_{i-1,n} + B_{i,n}u_{i,n}$$

where

$$A_{i,n} = -\frac{5\Delta t u_{i-1,n}}{6\Delta x} \quad \text{and} \quad B_{i,n} = \frac{5\Delta t u_{i,n}}{6\Delta x} + 1$$

Similar to Eq. (10.41), it can be said that

$$\mathbf{u}_{n+1} = \mathbf{J}_{n+1}^{-1} \mathbf{u}_n$$

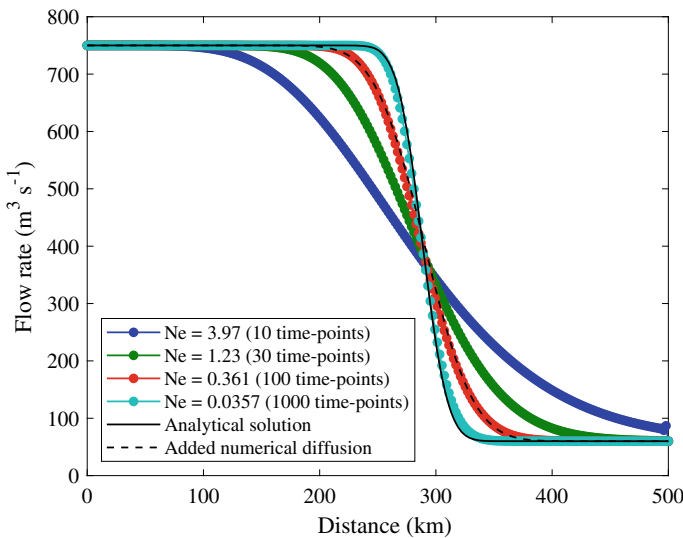


Fig. 10.6 Results from ITCS finite difference solutions to the diffusion wave problem showing the effect of the Neumann number, Ne

where in this case, the Jacobian matrix, $\mathbf{J}_n$, is found from

$$\mathbf{J}_n = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ A_{2,n} & B_{2,n} & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & A_{3,n} & B_{3,n} & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & A_{4,n} & B_{4,n} & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & B_{N_x-3,n} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & A_{N_x-2,n} & B_{N_x-2,n} & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & A_{N_x-1,n} & B_{N_x-1,n} & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & A_{N_x,n} & B_{N_x,n} \end{bmatrix}$$

Note that the boundary condition is incorporated through the one in the first row.

The non-linearity of the PDE being solved gives rise to the Jacobian matrix being dependent on the solution values that are sought. Therefore a Newton iteration scheme is required. Similar to Eq. (10.58), it can be said that

$$\mathbf{u}_{n+1,k+1} = \mathbf{J}_{n+1,k}^{-1} \mathbf{u}_n$$

where $\mathbf{u}_{n+1,k+1}$ represents the solution vector following the $(k+1)$ -th iteration, $\mathbf{J}_{n+1,k}$ is determined using the solution vector from the k -th iteration (i.e., $\mathbf{u}_{n+1,k}$) and $\mathbf{u}_n$ is the final solution vector from the previous time-step. The above scheme is implemented within the MATLAB code listed below:

```
L=200e3; dx=200; %Length and space-step (m)
tend=40*60^2; dt=3*60; %Duration and time-step (s)
x=[0:dx:L]'; t=0:dt:tend; %Point locations
Nx=numel(x); Nt=numel(t); %Numer of points
u=zeros(Nx,Nt); %Initialise solution matrix
%Apply initial and boundary conditions
u0=1.2; x0=50e3; %u0 (m/s) and x0 (m)
u(:,1)=u0*(x<x0); u(1,:)=0;
for n=1:Nt-1 %Step through solution
    uold=u(:,n); %Use previous time-step
    while max(abs(u(:,n+1)-uold))>1e-3
        %Jacobian matrix coefficients:
        A=-5/6*dt/dx*uold;
        B=5/6*dt/dx*uold+1;
        %Determine the Jacobian matrix
        J=spdiags([A B],[-1 0],Nx,Nx);
        %Apply boundary condition
        J(1,:)=0; J(1,1)=1;
        %Perform next iteration
        u(:,n+1)=J\u(:,n);
        uold=u(:,n+1); %Update uold
    end
end
%Obtain results for desired times
```

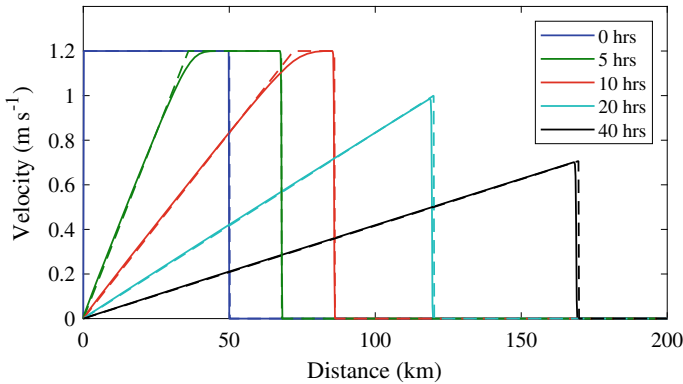



Fig. 10.7 Results from an ITBS Newton iteration scheme for the kinematic wave equation (solid lines) compared to results from a method of characteristics analytical solution (dashed lines)

```
tI=[0 5 10 20 40]*60^2;
u=interp1(t',u',tI');
uA=MoCsolBFun(x,tI,u0,x0); %Analytical solution
figure(6);clf;hold on;box on %Plot results
plot(x*1e-3,u)
set(gca,'ColorOrderIndex',1)
plot(x*1e-3,uA,'--')
legend('0 hrs','5 hrs','10 hrs','20 hrs','40 hrs')
xlabel('Distance (km)')
ylabel('Velocity (m s⁻¹)')
```

A for loop is used to progress through each time-step. The Newton iterations takes place within a while loop, nested within the for loop, which ceases once $|\mathbf{u}_{n+1,k+1} - \mathbf{u}_{n+1,k}| \leq 10^{-3}$. Solution values for the exact times of interest are obtained by linear interpolation using `interp1`. Comparison results from the MoC solution are obtained using the `MoCsolBFun` function, given in Listing 7.2.

The results are presented in Fig. 10.7. The MoC solution is an exact solution whereas the finite difference solution is an approximate solution. The finite difference solution compares favourably with the MoC solution. However, the finite difference solution is observed to be much smoother around discontinuities. This smoothness is due to numerical diffusion, which is strongly dependent on the size of time-step and space-step assumed.

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Part II

Hydrology and Water Resources

Abstract

This chapter introduces some basic aspects about hydrology and develops statistical theory commonly used for flood frequency analysis. The impact of climate and land surface on river flows is explored by comparing river flow observations from different catchments in the UK, Indonesia and Botswana. Various methods of measuring river flow and rainfall are described and explained. Various relevant statistical concepts are introduced, including return period, probability of non-exceedance, plotting positions, cumulative distribution functions and probability density functions. Mathematical equations are derived to relate normal and Gumbel distribution parameters to the mean and standard deviation of a given dataset. It is shown how to use annual maximum flow rates and annual minimum 7-day mean daily flow rates for flood frequency analysis and low flow frequency analysis, respectively. Practical applications are presented through a problem sheet with worked solutions.

Notation

A	Flowing cross-sectional area of the river channel [L^2].
B	Breadth of the river channel [L].
E	A single event [-].
$f(x)$	Probability density function.
$F(x)$	Cumulative distribution function [-].
i	Rank number [-].
h	Water depth [L].
j	Measurement number [-].
k	Number of successive years [-].
m	Hydraulic radius [L].
n	Manning coefficient [$L^{-1/3}T$].
N	Number of samples [-].

P	Probability [–].
Q	River flow rate [L^3T^{-1}].
Q_{50}	One in fifty years annual maximum river flow rate [L^3T^{-1}].
S_0	River channel slope [–].
T	Return period [T].
x	Some specified value.
X	A random variable.
z	Normalized argument [–].
α	Distribution parameter.
β	Distribution parameter.
γ	Euler-Mascheroni constant [–].
μ	Mean.
σ	Standard deviation.

11.1 Introduction

This chapter comprises two sections. The first is aimed at introducing students to key aspects of hydrology, including the hydrological cycle, the concept of a catchment water balance and how to acquire measurements of rainfall and river flow rate. The second section explains how to use frequency analysis to analyse hydrological data. The concept of a design event for a given return period is introduced and related to a cumulative distribution function (CDF). It is explained how to acquire an empirical CDF using a plotting position. Finally it is shown how to fit a theoretical CDF to a set of observations by moment matching. Practical examples, applying frequency analysis to solve engineering problems related to annual extremes in hydrological data, are provided in a problem sheet at the end of the chapter.

11.2 Fundamental Hydrology

11.2.1 The Hydrological Cycle

Some primary aspects of the hydrological cycle are illustrated in Fig. 11.1. Water precipitates within the atmosphere as either snow or rain. Open water bodies such as rivers, lakes and seas return water back to the atmosphere by evaporation. Snowfall forms snowpack and ice on the land surface. Some snow and ice evaporates directly back to the atmosphere; a process known as sublimation. Some snow and ice melts and runs off into gulleys, streams and rivers; a process known as runoff.

Some of the rainfall is intercepted by vegetative canopy (grass, shrubs, forest etc.) and evaporates directly back to the atmosphere. Some of the rainfall makes it to the land surface and infiltrates into the soil. Once infiltration capacity is reached,

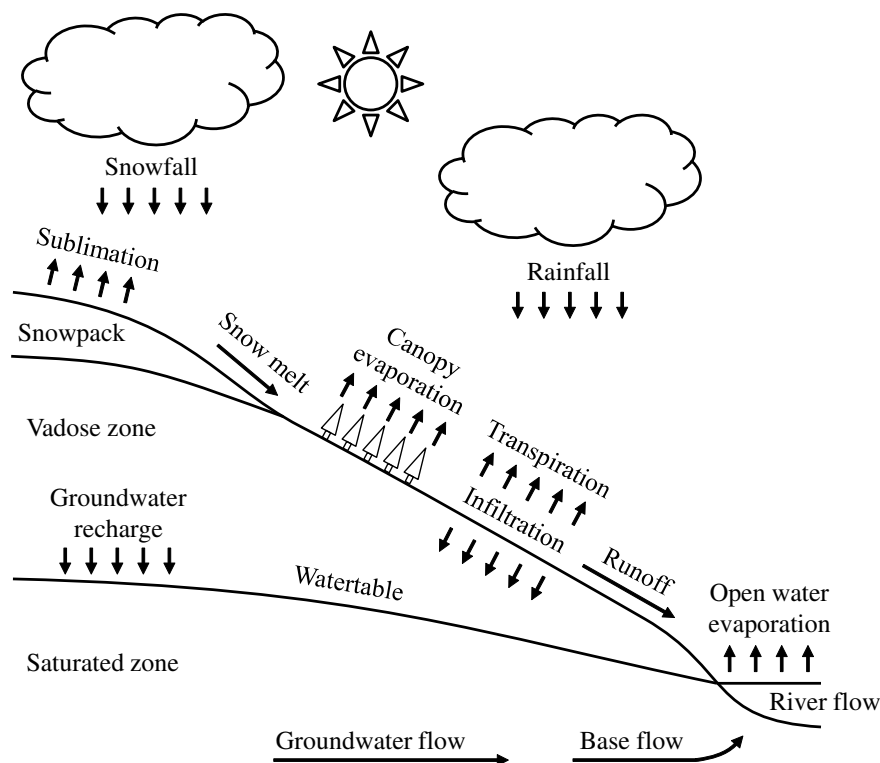


Fig. 11.1 Hydrological cycle

rainwater runs along the surface into gulleys, streams and rivers to form additional runoff.

Hydrologists partition the subsurface into the vadose zone and the saturated zone. The watertable represents the interface between these two zones. Within the saturated zone, the pore-space of rocks and soils is completely filled with liquid water. Within the vadose zone, the pore-space is partially filled with liquid water and air.

Some of the water that infiltrates into the vadose zone is abstracted by plant roots and transpired back to the atmosphere. The remainder mostly drains by gravity to the water table and recharges underlying aquifers. The movement of water in aquifers is referred to as groundwater flow. Groundwater can flow back out on to the land surface as springs. Some groundwater flows directly into rivers and streams, where its contribution to river flow is referred to as base flow.

11.2.2 Catchment Water Balance

Hydrologists partition land into river catchments, otherwise known as watersheds. River flow rates are measured at gauging stations. The main gauging station for the

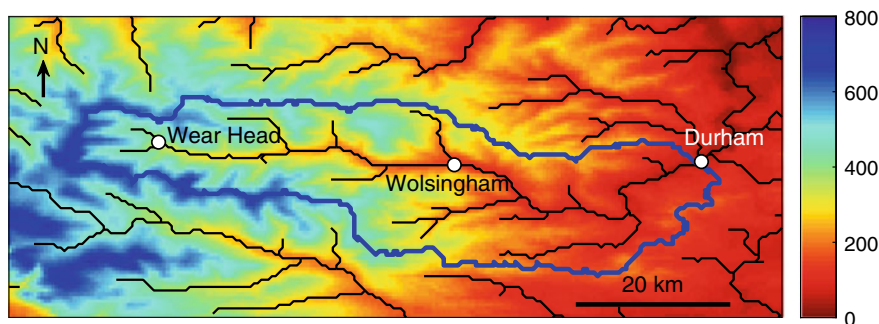


Fig. 11.2 Catchment area upstream of Sunderland Bridge (Durham) on the River Wear, as determined from land surface elevation (data acquired from [1]). The colour bar shows the scale for land surface elevation in m above sea level. The catchment boundary is shown in blue and river channels are shown in black

River Wear for Durham City is located at Sunderland Bridge. Figure 11.2 shows the catchment boundary upstream of Sunderland Bridge as a blue outline, which encloses a land area of 658 km^2 . Delineation of catchment boundaries are determined by studying the land surface elevation of the area. A river catchment is defined as the area of land upstream of an observation point on the river, whereby any rainfall landing on the land surface, within that area, will ultimately run-off and pass through the river observation point. Rainfall landing outside of the catchment area is assumed to drain to an alternative river.

Once a river catchment has been defined, a water balance can be developed whereby

$$\text{River flow} = \text{Precipitation} - \text{Evapotranspiration} - \text{Change in storage}$$

The “change in storage” term refers to the quantity of water held within the catchment whether it be in soil, aquifers, lakes or rivers. Evapotranspiration is a term used by hydrologists to lump to together both evaporation and transpiration.

11.2.2.1 Potential and Actual Evapotranspiration

Often we distinguish between potential and actual evapotranspiration. Potential evapotranspiration refers to how much evapotranspiration would occur in the presence of unlimited liquid water. Potential evapotranspiration is driven by meteorological variables such as solar radiation, temperature, humidity and wind-speed. Soils, lakes and rivers sometime dry out and available liquid water is limited. Consequently actual evapotranspiration rates are less than potential evapotranspiration rates.

11.2.2.2 Impact of Climate on River Flows

Figure 11.3 compares the hydrological response of three different rivers from around the world. Each has a similar sized catchment area. Nevertheless, all the variables have been transformed to a fortnightly (14 days) amount in mm so as to normalise out the effect of catchment size.

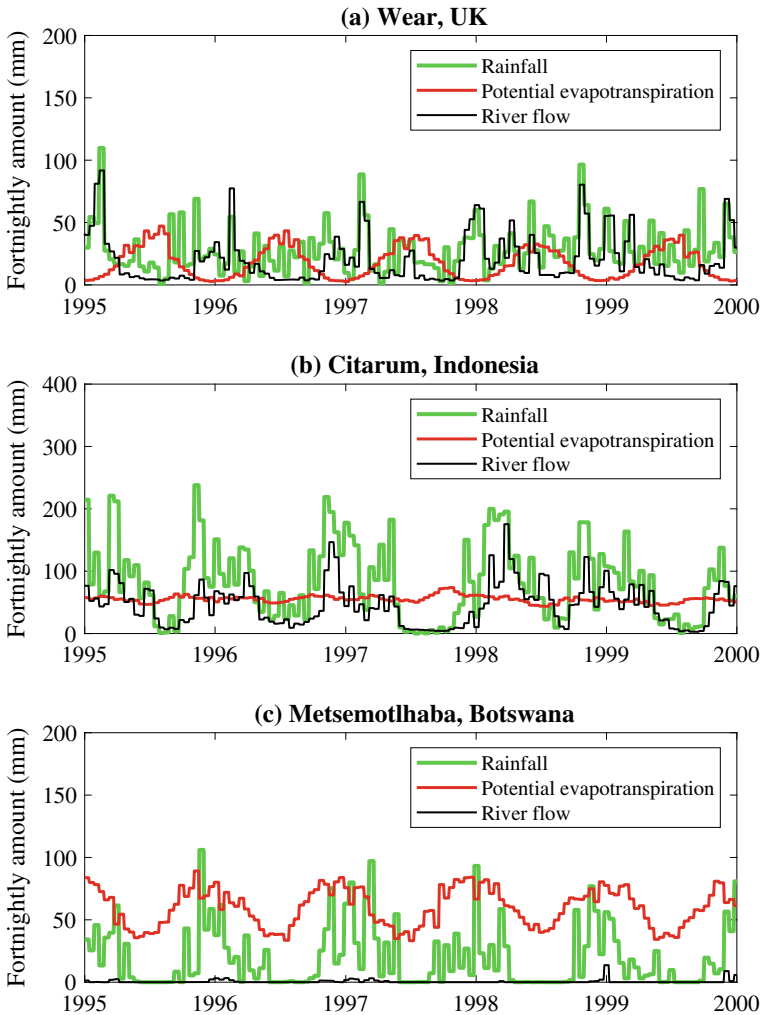


Fig. 11.3 How climate affects river flows around the world. Potential evapotranspiration was calculated from daily temperature data using the FAO56 method [4]. Rainfall and temperature data were acquired from [5]. Flow data for the rivers Wear, Citarum and Metsemotlhaba were provided by [6], Institute of Technology Bandung and the Department of Water and Sanitation, Botswana, respectively

Rainfall and evaporation are typically recorded as a daily depth in mm. A fortnightly amount is acquired by multiplying by 14. River flows are typically recorded in m^3s^{-1} . To transform river flows to a fortnightly amount in mm it is necessary to divide by the catchment area (in m^2) and then multiply by $14 \times 24 \times 60^2 \times 1000$. The reason for studying fortnightly quantities as opposed to daily is that this enables the rainfall and evaporation to be viewed at a similar time-scale to the primary variations commonly observed in river flows.

Figure 11.3a shows rainfall, potential evapotranspiration (PE) and river flow for the River Wear at Sunderland Bridge. The rainfall record appears chaotic with no obvious seasonal pattern although peak rates are slightly higher in the winter. The PE record shows strong seasonality with high values in the summer due to higher temperatures and more daylight hours. The river flow follows the rainfall pattern during the winter but then significantly reduces in the summer. The low summer flows are caused by higher PE as opposed to lower rainfall. More soil water is evaporated in the summer, which means that infiltration capacities remain high and there is less runoff.

Figure 11.3b shows rainfall, PE and river flow for the River Citarum in West Java, Indonesia. The rainfall record shows strong seasonality with highest values in the summer (from a Southern Hemisphere perspective), very typical of monsoonal rainfall associated with Southeast Asia [2]. In contrast, the PE record is close to uniform over time, due to the tropical climate of the region; this means that temperature and daylight hours are close to constant throughout the year.

The river flow in Citarum apparently shows a similar pattern as compared to the River Wear, with high flows in January and low flows in August. However, in Citarum, high and low flows are purely caused by high and low rainfall rates in the winter and summer, respectively. Also of note is that the rainfall and river flow are around double that in the Wear. Hence, not surprisingly, flooding causes significant economic damage in this region.

Figure 11.3c shows rainfall, PE and river flow for the River Metsemotlhaba in Botswana. The transient pattern of rainfall looks slightly similar to that at Citarum. However, annual rainfall in Botswana is less than a quarter of that in West Java. Botswana is semi-arid and land-locked. Seasonal rainfall is mostly driven by migration of the intertropical convergence zone.

Botswana is subtropical and hence seasonality is apparent in the PE record. Winter and summer are interchanged, as compared to the UK, due to Botswana being located in the Southern Hemisphere. Of note is that wintertime PE in Botswana is at a similar rate to summertime PE in the UK. Furthermore, summertime PE in Botswana is double that in the UK. Another important point is that rainfall rates are substantially less than PE rates, hence most the rain evaporates and river flows are very low. For most of the year, the River Metsemotlhaba does not flow and appears as a dry sand filled channel [3]. The word, metsemotlhaba, means sand river. Water shortage is a primary obstacle for economic development in this region.

11.2.2.3 Impact of Land Surface on River Flows

River flows are also strongly controlled by land surface characteristics. Figure 11.4 shows daily rainfall and river flow records for two very different river systems in the UK.

The river Urr flows over granite rocks in Southwest Scotland. Granite rocks are close to being impermeable. Therefore, there is very little groundwater flow in this region. As a consequence, most of the water in this catchment flows along the land surface. The river responds very quickly to individual rainfall events. During the summer, the soil layer dries out and river flows are frequently reduced to near zero.

In contrast, the river Kennet flows over fractured chalk rocks in Southern England. Fracture chalk is highly permeable and forms the main water supply aquifer for this region. There is very little surface runoff because most of the rain infiltrates into the underlying Chalk aquifer. However, groundwater flow drains into low-lying river valleys. Most of the water in the River Kennet is supplied by drainage from the surrounding Chalk aquifer. As a consequence, it can be seen that the river does not respond strongly to individual rainfall events. Furthermore, the river does not dry out during the summer, due to the fact that it is continuously sustained by a base flow from aquifers.

The rivers Urr and Kennet are examples of surface water dominated and groundwater dominated rivers, respectively. From a societal perspective, the response of a groundwater dominated river is preferred. The fact that the river does not respond quickly to individual rainfall events makes it less prone to surprise flood events.

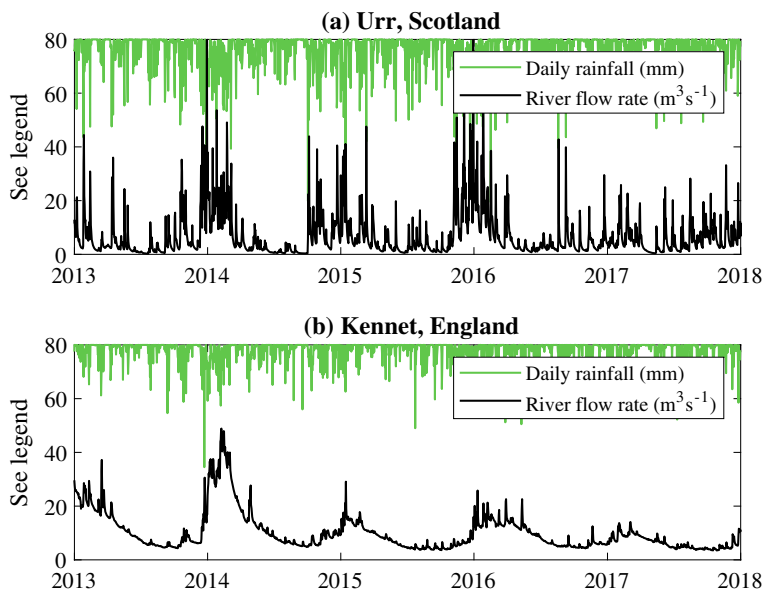


Fig. 11.4 Rainfall and river flow rates in **a** a surface water dominated catchment and **b** a groundwater dominated catchment (data acquired from [6])

The fact that the river maintains a relatively high flow throughout the summer dry-period makes it easier to manage as a water resource. Unfortunately, the paving and building over of natural landscapes, associated with urbanisation, has a tendency of transforming river systems towards being surface water dominated.

11.2.3 Rainfall Measurement

11.2.3.1 Precipitation Processes

Air temperature decreases with elevation and cooler temperatures lead to condensation of vapour. This is because the vapour holding capacity of air reduces with reducing temperature.

Rainfall in the UK is heavily controlled by warm humid air, from the Atlantic Ocean, being forced over the central highlands where it precipitates as snow and rain. This type of precipitation is referred to as orographic precipitation. Air that travels over the central highlands becomes water depleted leading to a rain shadow in the East (see Fig. 11.5). More extreme examples of an orographic rain shadow effect include the Atacama Desert and the Tibetan Plateau.

Other types of precipitation include convectonal precipitation and frontal precipitation [7]. These are less dependent on topography.

Convectonal precipitation occurs when moist air from the sea is driven over warm land. As the air temperature increases, the air rises due to reduced density and forms a convection cell. As the warm moist air rises it reduces in temperature and vapour precipitates. This process is particularly common in tropical regions.

Frontal precipitation occurs when a warm moist air body meets a colder air body. The interface is referred to as a front. At a weather front, warm moist air is cooled leading to precipitation. There are many different types of weather fronts. See [7] for more detail.

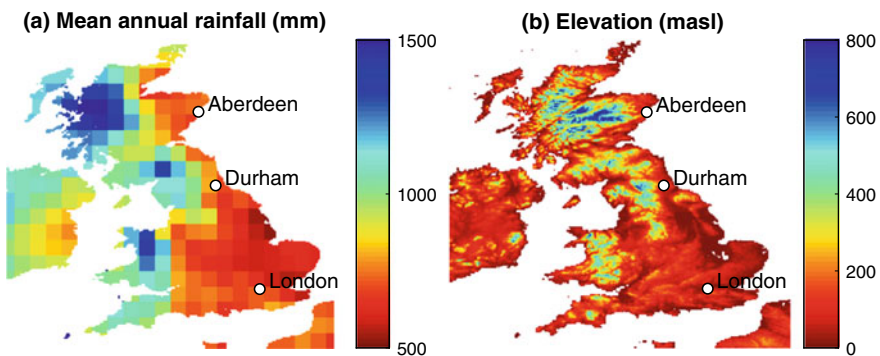


Fig. 11.5 **a** Mean annual rainfall across the UK for 2000 to 2020 (data acquired from [5]). **b** Land surface elevation in m above sea level (masl) (data acquired from [1])

11.2.3.2 Direct Rainfall Measurement

The classical method of measuring rainfall is to use a non-recording gauge, which looks like a small bucket. Typically the gauge is visited on a daily basis, the depth of water within the gauge is recorded, and the gauge is emptied to measure the rainfall for the following day. The measurement is in the form of a daily rainfall depth.

A common example of a recording rain gauge is the so-called tipping bucket rain gauge. This consists of two small buckets on a pivot, which are attached to a magnet. Each bucket typically measures 0.2 mm of rainfall. Once a bucket is full, it swings on the pivot, the magnet passes over a reed switch, the bucket empties and the previously empty bucket is emplaced, ready to collect the next 0.2 mm of rainfall. In this way the two buckets tip backwards and forwards as it rains. A logger records when each tip occurs using the electrical signal from the reed switch. Such a device can be used to continuously measure sub-daily rainfall rates.

Other measuring devices include weighing gauges (these can measure snow as it happens), optical gauges and disdrometers (these latter two can measure drop size distribution) [8].

11.2.3.3 Indirect Precipitation Measurement

Radar is often used for indirect precipitation measurement. Radar works by sending out electromagnetic pulses and measuring how long they take to return from a target. In this case the target is rain, hail and snow. Empirical relationships between reflectivity and precipitation rate have been developed by calibration to data from networks of direct precipitation measurements.

The UK and Ireland weather radar network currently comprises 18 weather radars, of which 15 are operated and maintained by the Met. Office [9].

The Tropical Rainfall Measuring Mission (TRMM) provided radar observations of the Earth from a satellite enabling measurement of precipitation. TRMM also provided conventional passive remote sensing observations including microwave, infrared and visible radiation. TRMM was active from 1997 to 2015.

By developing correlations between rainfall and passive observations, TRMM enabled the development of a historic global daily rainfall dataset going back to 1983. In 2014 the Global Precipitation Measurement (GPM) system was established, which provides global hourly precipitation data dating back to 2003 [10].

11.2.4 River Flow Measurement

For spot measurements of river flow rate, a hand-held flowmeter can be used. Flowmeters use either mechanical impellers or electromagnetic sensors to measure fluid velocity. A sequence of spot measurements of fluid velocity and river depth are obtained along a cross-section of the river. These are then integrated using trapezoidal integration to obtain a measurement of flow rate. An important problem with this method is that it is often very dangerous to take the probe into the river and measure the velocity.

Acoustic Doppler current profiler (ADCP) methods, exploit the doppler effect of sound waves scattered back from flowing water particles to resolve a three-dimensional velocity field within the near vicinity of an ADCP probe. An ADCP probe can be transported on a radio-controlled boat. The boat moves backwards and forwards along a river cross-section to collect sufficient data to calculate the flow rate. ADCP represents a safer and more accurate method of obtaining spot measurements of flow rate. Other new gauging systems include processing images of the water surface recorded by hovering drones. Like ADCPs, these are not fixed to one location. Unlike ADCPs, you can take them out in severe floods.

However, most river flow data is acquired using a stilling well and a weir. The stilling well is a well dug out close to a river with a pipe connecting the well to the river. The well is used to continuously monitor the elevation of the water surface in the river. The water level of a river is commonly referred to as the stage. The purpose of the weir is to enable the determination of a theoretical relationship between river flow rate and stage, known as a stage-discharge relationship. River flow data can then be calculated from the stage data.

The current trend is away from weirs and towards fixed time-of-flight gauges, because these are less of a problem for migrating fish. Time-of-flight gauges fire ultrasonic pulses diagonally across a river, back and forth between two emitter/receivers. A normal setup has several pairs of emitter/receivers at different depths. Flow is inferred from the time difference between upstream and downstream firing.

11.3 Frequency Analysis

Hydrological engineering often involves designing infrastructure to deal with a “design event” occurring. A “design event” is commonly considered to be some form of worst case scenario likely to happen within a specified duration of time, referred to as a return period. For example, a flood wall might be designed to deal with a 1 in 50 year flood event; 50 years is the return period. A wastewater discharge to a river might be designed to deal with a 1 in 10 year low-flow event (in this case it is important to have enough river flow to ensure sufficient dilution takes place). Hydrologists use frequency analysis to determine the magnitude of design events for specified return periods.

The notion of a return period is stochastic as opposed to deterministic. Let Q_{50} be a 1 in 50 year annual maximum flow rate for a given river. If the flow rate exceeds Q_{50} today it does not necessarily mean that the flow rate will not exceed Q_{50} for another 50 years. Rather, it implies we would expect the annual maximum flow rate to exceed Q_{50} around 10 times within a 500 year period. Furthermore, within that 500 year period, there is a remote possibility that the annual maximum flow rate could exceed Q_{50} for 10 consecutive years.

Below we will develop the necessary statistical theory to determine design events from a given set of hydrological observations. First we will look at the relationship between return period, probability and the cumulative distribution function (CDF).

The concept of a plotting position is introduced to determine an empirical CDF from a given set of observations. It is then shown how to extrapolate an empirical CDF using statistical distribution functions and moment matching. Examples are then presented in the context of flood frequency analysis and low-flow frequency analysis.

11.3.1 Return Period and Probability

The probability of a single event, E , is defined as the relative number of occurrences after a long series of trials. If E occurs k times during N trials, the probability of E , $P(E) = \frac{k}{N}$, providing N is sufficiently large.

Let X be a random variable (flow rate, rainfall etc.). The term, $P(X > x)$, denotes the probability that X will be greater than a specified value, x , referred to as the probability of exceedance.

Suppose that each trial takes place after a fixed interval of time. The return period of an event, T [T], can be found from

$$T = \frac{1}{P(X > x)}$$

where the units of T will be the same as the interval duration of each trial.

Suppose each trial represents a daily measured flow rate, then the units of the return period, T , will be days. Alternatively, if each trial represents an annual maximum flow rate, then the units of the return period, T , will be years.

The term $P(X \leq x)$ denotes the probability that X will not be greater than a specified value, x , referred to as the probability of non-exceedance. Probability of exceedance is related to probability of non-exceedance by

$$P(X > x) = 1 - P(X \leq x)$$

Challenge 11.1 Consider a design flow, x , with a return period of T years. Determine an expression for the probability that x will be exceeded at least once within k successive years. Your expression should be purely in terms of T and k .

For a given return period, T , in years, the probability that x will be exceeded at least once in a given year is

$$P(X > x) = \frac{1}{T}$$

The probability that x will not be exceeded in a given year is

$$P(X \leq x) = 1 - P(X > x) = 1 - \frac{1}{T}$$

The probability that x will not be exceeded in k successive years is

$$[P(X \leq x)]^k = \left(1 - \frac{1}{T}\right)^k$$

The probability that x will be exceeded at least once within k successive years is

$$1 - [P(X \leq x)]^k = 1 - \left(1 - \frac{1}{T}\right)^k$$

A significant problem with the above approach is an assumption of stationarity, which means that the underlying statistical distributions are assumed to be constant with time. Incorporation of climate change and/or land-use change require a non-stationary approach. Nevertheless, stationary approaches continue to be used in practice.

11.3.2 Cumulative Distribution Functions

The cumulative distribution function (CDF), $F(x) \equiv P(X \leq x)$, represents a mathematical way of describing a random process.

Suppose that the CDF for flow rates in a given river is $F(x)$. The probability that a design flow rate, x , will be exceeded at least once within k successive years is

$$1 - [P(X \leq x)]^k = 1 - F(x)^k$$

The CDF can be found from

$$F(x) = \int_{-\infty}^x f(x)dx \quad (11.1)$$

where $f(x)$ is the underlying probability density function (PDF).

A PDF can be thought of as a continuous form of a histogram. However, an important property of the PDF is that

$$\int_{-\infty}^{\infty} f(x)dx = 1. \quad (11.2)$$

11.3.3 Empirical CDF

It is possible to construct an empirical CDF from a discrete set of measurements. Consider N number of measurements, x_j ($j = 1, 2, \dots, N$). Let x_i ($i = 1, 2, \dots, N$) be the same set of measurements but ranked from largest to smallest; i is referred to as the rank number. The probability of exceedance for x_i can be found from empirical functions of i and N , referred to as plotting positions.

Two popular heuristic plotting positions in hydrology are the Gringorten formula [7, p. 314]

$$P(X > x_i) = \frac{i - 0.44}{N + 0.12} \quad (11.3)$$

and the Weibull formula [7, p. 316]

$$P(X > x_i) = \frac{i}{N + 1} \quad (11.4)$$

Table 11.1 Example showing an application of the Gringorten and Weibull plotting positions

Measurements		Ranked data		Gringorten	Weibull
j	x_j	i	x_i	$P(X > x_i)$	$P(X > x_i)$
1	35	1	35	0.11	0.17
2	27	2	30	0.30	0.33
3	30	3	27	0.50	0.50
4	10	4	25	0.70	0.67
5	25	5	10	0.89	0.83

The empirical CDF can be obtained from

$$F(x_i) = 1 - P(X > x_i)$$

A simple example is presented in Table 11.1 where probability estimates from the Gringorten and Weibull plotting positions are compared. Of note is that the Gringorten plotting position provides extreme probabilities closer to zero and one. Both plotting positions will provide identical results as the number of measurements approaches infinity.

11.3.4 Extrapolation by Moment Matching

The problem with empirical CDFs is that they limit our analysis to the range of our observations. For example, if our data record is of 30 years duration, it is not possible to use the empirical CDF to estimate a 1 in 100 year event.

An alternative approach is to fit a continuous theoretical distribution function to the data, which can then be extrapolated to estimate values with higher return periods.

Moment matching is a convenient method of fitting a distribution to a set of observations. In particular we will exploit the first absolute moment and the second central moment of the probability density function, $f(x)$, which represent the mean, μ , and variance, σ^2 , respectively, defined as follows [11, p. 1035]:

$$\mu = \int_{-\infty}^{\infty} xf(x)dx \quad (11.5)$$

$$\sigma^2 = \int_{-\infty}^{\infty} (x - \mu)^2 f(x)dx \quad (11.6)$$

A given probability density function can be fitted to empirical data by choosing function parameter values such that the mean and variance match that of the empirical data, found from [11, pp. 1013–1014]

$$\mu = \frac{1}{N} \sum_{j=1}^N x_j$$

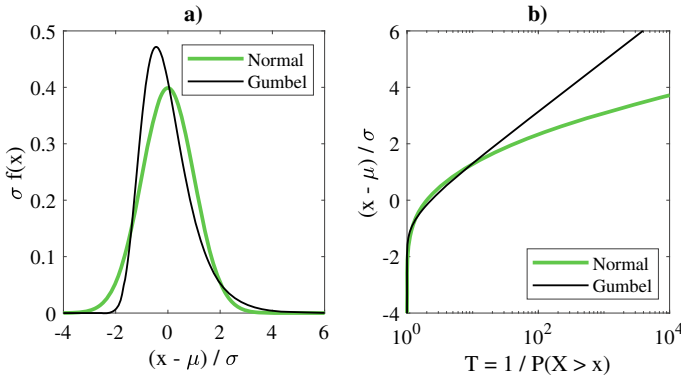


Fig. 11.6 A comparison of the normal and Gumbel distribution functions

$$\sigma^2 = \frac{1}{N-1} \sum_{j=1}^N (x_j - \mu)^2$$

The normal distribution function is arguably the most commonly applied PDF for studying statistics of scientific observations. However, extreme value distributions are preferred for hydrological frequency analysis because they bias towards extreme values, leading to a more conservative design. As an example, we will study the Gumbel distribution.

A comparison of the normal PDF and Gumbel PDF is presented in Fig. 11.6a. To aid comparison, the two distributions have been moment matched, i.e., they have been forced to provide the same mean and variance. An important characteristic of the normal distribution is its symmetry about the mean. In contrast, the Gumbel distribution is skewed towards higher values, by virtue of it being an extreme value distribution.

The consequence of this skewness, in the context of hydrological frequency analysis, can be understood by studying the corresponding plot of $(x - \mu)/\sigma$ against return period, T , shown in Fig. 11.6b. For a given mean and variance, the Gumbel distribution predicts higher values of x (as compared with the normal distribution) for return periods greater than 10 units (units are not specified here and are dependent on the interval of trials).

Below we will develop the necessary equations to moment match both the normal distribution and the Gumbel distribution to a given set of empirical observations.

In practice, L-moments are used as an alternative to moments [12]. However, the underlying concept is very similar and moment matching (as opposed to L-moment matching) is more amenable to developing a preliminary understanding in this area.

11.3.5 The Normal Distribution

The CDF associated with the normal distribution takes the form

$$F(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - \alpha}{\beta\sqrt{2}} \right) \right] \quad (11.7)$$

where α and β are empirical parameters and erf denotes the error function, defined as [11, p. A67]

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-x^2} dx \quad (11.8)$$

An important quality of $\operatorname{erf}(x)$ is that $\operatorname{erf}(\infty) = 1$.

Challenge 11.2 Use Eq. (11.1) to determine the underlying PDF associated with Eq. (11.7).

From Eq. (11.1) it is understood that the underlying PDF, $f(x)$, is obtained by differentiating Eq. (11.7) with respect to x .

Making the substitution

$$z = \frac{x - \alpha}{\beta\sqrt{2}}$$

it can be seen that [11, p. 1045]

$$\begin{aligned} f(x) &\equiv \frac{\partial F}{\partial x} = \frac{1}{2} \frac{\partial z}{\partial x} \frac{\partial(\operatorname{erf}(z))}{\partial z} \\ &= \frac{1}{\beta\sqrt{2\pi}} \exp \left[- \left(\frac{x - \alpha}{\beta\sqrt{2}} \right)^2 \right] \end{aligned} \quad (11.9)$$

Challenge 11.3 Use Eq. (11.5) to determine an expression for the mean, μ , in terms of α .

Substituting Eq. (11.9) into Eq. (11.5) leads to

$$\mu = \int_{-\infty}^{\infty} \frac{x}{\beta\sqrt{2\pi}} \exp \left[- \left(\frac{x - \alpha}{\beta\sqrt{2}} \right)^2 \right] dx$$

Letting

$$z = \frac{x - \alpha}{\beta\sqrt{2}}$$

it can then be seen that

$$\begin{aligned}
 \mu &= \int_{-\infty}^{\infty} \frac{x}{\sqrt{\pi}} e^{-z^2} dz = \int_{-\infty}^{\infty} \frac{\alpha + \beta z \sqrt{2}}{\sqrt{\pi}} e^{-z^2} dz \\
 &= \int_{-\infty}^0 \frac{\alpha + \beta z \sqrt{2}}{\sqrt{\pi}} e^{-z^2} dz + \int_0^{\infty} \frac{\alpha + \beta z \sqrt{2}}{\sqrt{\pi}} e^{-z^2} dz \\
 &= \int_0^{\infty} \frac{\alpha - \beta z \sqrt{2}}{\sqrt{\pi}} e^{-z^2} dz + \int_0^{\infty} \frac{\alpha + \beta z \sqrt{2}}{\sqrt{\pi}} e^{-z^2} dz \\
 &= \alpha \int_0^{\infty} \frac{2}{\sqrt{\pi}} e^{-z^2} dz = \alpha \operatorname{erf}(\infty) = \alpha
 \end{aligned}$$

Challenge 11.4 Use Eq. (11.6) to determine an expression for the variance, σ^2 , in terms of β . Hint: take advantage of Eq. (11.2).

An expression for the variance, σ^2 , in terms of β , is found as follows:

Substituting Eq. (11.9) into Eq. (11.6) leads to

$$\sigma^2 = \int_{-\infty}^{\infty} \frac{(x - \mu)^2}{\beta \sqrt{2\pi}} \exp \left[- \left(\frac{x - \alpha}{\beta \sqrt{2}} \right)^2 \right] dx$$

But recall that $\mu = \alpha$ in this case so

$$\sigma^2 = \int_{-\infty}^{\infty} \frac{(x - \alpha)^2}{\beta \sqrt{2\pi}} \exp \left[- \left(\frac{x - \alpha}{\beta \sqrt{2}} \right)^2 \right] dx \quad (11.10)$$

Equation (11.2) tells us that

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp \left[- \left(\frac{x - \alpha}{\beta \sqrt{2}} \right)^2 \right] dx = \beta \quad (11.11)$$

Interestingly it can be seen that an equation of similar form to Eq. (11.10) is obtained by differentiating both sides of Eq. (11.11) with respect to β :

$$\int_{-\infty}^{\infty} \frac{2}{\beta^3} \left(\frac{x - \alpha}{\sqrt{2}} \right)^2 \frac{1}{\sqrt{2\pi}} \exp \left[- \left(\frac{x - \alpha}{\beta \sqrt{2}} \right)^2 \right] dx = 1 \quad (11.12)$$

Comparing Eqs. (11.10) and (11.12) it is then clear that

$$\sigma^2 = \beta^2$$

So for the normal distribution (Eq. (11.7)), α and β can be defined in terms of μ and σ as follows:

$$\alpha = \mu \quad \text{and} \quad \beta = \sigma. \quad (11.13)$$

11.3.6 The Gumbel Distribution

The CDF associated with the Gumbel distribution takes the form [7, p. 317]

$$F(x) = \exp \left\{ -\exp \left[-\left(\frac{x - \alpha}{\beta} \right) \right] \right\} \quad (11.14)$$

where α and β are empirical parameters.

Challenge 11.5 Use Eq. (11.1) to determine the underlying PDF associated with Eq. (11.14).

The underlying PDF, $f(x)$, is obtained by differentiating Eq. (11.14) with respect to x .

Making the substitution

$$z = \exp \left[-\left(\frac{x - \alpha}{\beta} \right) \right]$$

it can be seen that

$$\begin{aligned} f(x) &\equiv \frac{\partial F}{\partial x} = -\frac{\partial z}{\partial x} e^{-z} \\ &= \frac{1}{\beta} \exp \left[-\left(\frac{x - \alpha}{\beta} \right) \right] e^{-z} \\ &= \frac{ze^{-z}}{\beta} \end{aligned} \quad (11.15)$$

Challenge 11.6 Use Eq. (11.5) to determine an expression for the mean, μ , in terms of α and β . You will need to exploit the identity [13, p. 581],

$$\int_0^{\infty} \ln z e^{-z} dz = -\gamma$$

where $\gamma = 0.5772$ is the Euler-Mascheroni constant.

Substituting Eq. (11.15) into Eq. (11.5) leads to

$$\mu = \int_{-\infty}^{\infty} \frac{xze^{-z}}{\beta} dx$$

where

$$z = \exp \left[-\left(\frac{x - \alpha}{\beta} \right) \right]$$

Noting that

$$\frac{\partial z}{\partial x} = -\frac{z}{\beta}$$

and

$$x = \alpha - \beta \ln z$$

it follows that

$$\begin{aligned}\mu &= - \int_{\infty}^0 (\alpha - \beta \ln z) e^{-z} dz \\ &= \int_0^{\infty} (\alpha - \beta \ln z) e^{-z} dz \\ &= \alpha \int_0^{\infty} e^{-z} dz - \beta \int_0^{\infty} \ln z e^{-z} dz\end{aligned}$$

It turns out that [13, p. 581]

$$\int_0^{\infty} \ln z e^{-z} dz = -\gamma$$

where $\gamma = 0.5772$ is the Euler-Mascheroni constant.

It therefore follows that

$$\mu = \alpha + \gamma\beta$$

Challenge 11.7 Use Eq. (11.6) to determine an expression for the variance, σ^2 , in terms of α and β . You will need to exploit the identity [13, p. 581]

$$\int_0^{\infty} (\ln z)^2 e^{-z} dz = \gamma^2 + \frac{\pi^2}{6}$$

An expression for the variance, σ^2 , in terms of α and β , is found as follows:

Substituting Eq. (11.15) into Eq. (11.6) gives that

$$\sigma^2 = \int_{-\infty}^{\infty} \frac{(x - \mu)^2 z e^{-z}}{\beta} dx$$

Changing the integration variable to z and substituting the definition of μ for the Gumbel distribution gives that

$$\begin{aligned}\sigma^2 &= \beta^2 \int_0^{\infty} (\gamma + \ln z)^2 e^{-z} dz \\ &= \beta^2 \int_0^{\infty} [\gamma^2 + 2\gamma \ln z + (\ln z)^2] e^{-z} dz \\ &= -\beta^2 \gamma^2 + \beta^2 \int_0^{\infty} (\ln z)^2 e^{-z} dz\end{aligned}$$

It turns out that [13, p. 581]

$$\int_0^{\infty} (\ln z)^2 e^{-z} dz = \gamma^2 + \frac{\pi^2}{6}$$

and therefore

$$\begin{aligned}\sigma^2 &= -\beta^2\gamma^2 + \beta^2\left(\gamma^2 + \frac{\pi^2}{6}\right) \\ &= \beta^2\frac{\pi^2}{6}\end{aligned}$$

So for the Gumbel distribution (Eq. (11.14)), α and β can be defined in terms of μ and σ as follows [7, p. 317]:

$$\alpha = \mu - \gamma\beta \quad \text{and} \quad \beta = \frac{\sigma\sqrt{6}}{\pi}. \quad (11.16)$$

11.3.7 Analysis of Annual Flow Statistics

11.3.7.1 Flood Frequency Analysis

Flood frequency analysis typically involves annual maximum daily flow rates, commonly referred to as flood data.

Annual maximum daily flows are obtained by choosing the maximum observed daily value in a given hydrological year. The UK hydrological year runs from July to June so as to encompass a complete wet-season of river flows. In this way, the annual maximum daily flow of 2020 will be the maximum daily flow for the period from July 1st 2019 to June 30th 2020.

An empirical CDF, $F(x_i)$ can be obtained by ranking the annual maxima from high to low values and plotting them against $1 - P(X > x_i)$ where $P(X > x_i)$ is found using a plotting position. The return period for a given x_i value is obtained from

$$T_i = \frac{1}{1 - F(x_i)}$$

In this context, x_i is an observed annual maximum flow rate and T_i is the return period (in years) of that value being exceeded.

Alternatively, the mean and variance of the annual maxima can be used to derive parameters for a theoretical CDF (normal, Gumbel etc.), $F(x)$. The return period for a given x value is then obtained from

$$T = \frac{1}{1 - F(x)}$$

In this context, x is an annual maximum flow rate and T is the return period (in years) of that value being exceeded.

11.3.7.2 Low Flow Frequency Analysis

An instantaneous flow rate is used for flood frequency analysis because flood inundation will cause economic damage regardless of its duration. However, low flows can often be tolerated over a short period of time without too much difficulty. Therefore,

low flow frequency analysis typically involves acquisition of annual minimum 7-day mean daily flow rates, as opposed to instantaneous rates.

Annual minimum 7-day mean daily flows are obtained by applying a 7-day moving average to the observed daily data and choosing the minimum 7-day mean in a given solar year. The UK solar year runs from January to December and encompasses a complete dry-season of river flows. In this way, the annual minimum 7-day mean daily flow of 2020 will be the minimum 7-day mean for the period from January 1st 2020 to December 31st 2020.

An empirical CDF, $F(x_i)$ can be obtained by ranking the annual minima from high to low values and plotting them against $1 - P(X > x_i)$ where $P(X > x_i)$ is found using a plotting position. The return period for a given x_i value, in this case, is obtained from

$$T_i = \frac{1}{F(x_i)}$$

In this context, x_i is an observed annual minimum 7-day mean daily flow rate and T_i is the return period (in years) of that value not being exceeded.

Alternatively, the mean and variance of the annual minima can be used to derive parameters for a theoretical CDF, $F(x)$. The return period for a given x value is then obtained from

$$T = \frac{1}{F(x)}$$

In this context, x is an annual minimum 7-day mean daily flow rate and T is the return period (in years) of that value not being exceeded.

11.3.7.3 Flow Statistics at Sunderland Bridge

Figure 11.7a shows 25 years of flow rate data from the Sunderland Bridge gauging station on the River Wear near Durham City. The green line shows the observed daily flow data. The black line shows the 7-day moving average of the daily flow data. The black circular markers show the annual maximum daily flow rates. The white-filled circular markers show the annual minimum 7-day mean daily flow rates.

Figure 11.7b, c compare results using the normal distribution, Gumbel distribution and the Gringorten plotting position for the annual maximum daily flow rates. Both theoretical CDFs closely follow the empirical CDF obtained using the Gringorten plotting position. However, the plots against return period show how the Gumbel distribution biases more towards the high values, as compared to the normal distribution. Consequently, extrapolating the data using the Gumbel distribution leads to a more conservative flood estimate (i.e., higher in this context) for long return periods.

Figure 11.7d, e compare results using the normal distribution and the Gringorten plotting position for the annual minimum 5-day mean daily flow rates. The Gumbel distribution is not used here because we want to focus on small values. The normal CDF closely follows the empirical CDF obtained using the Gringorten plotting position. The normal distribution function also provides a convincing extrapolation of the data in terms of return period.

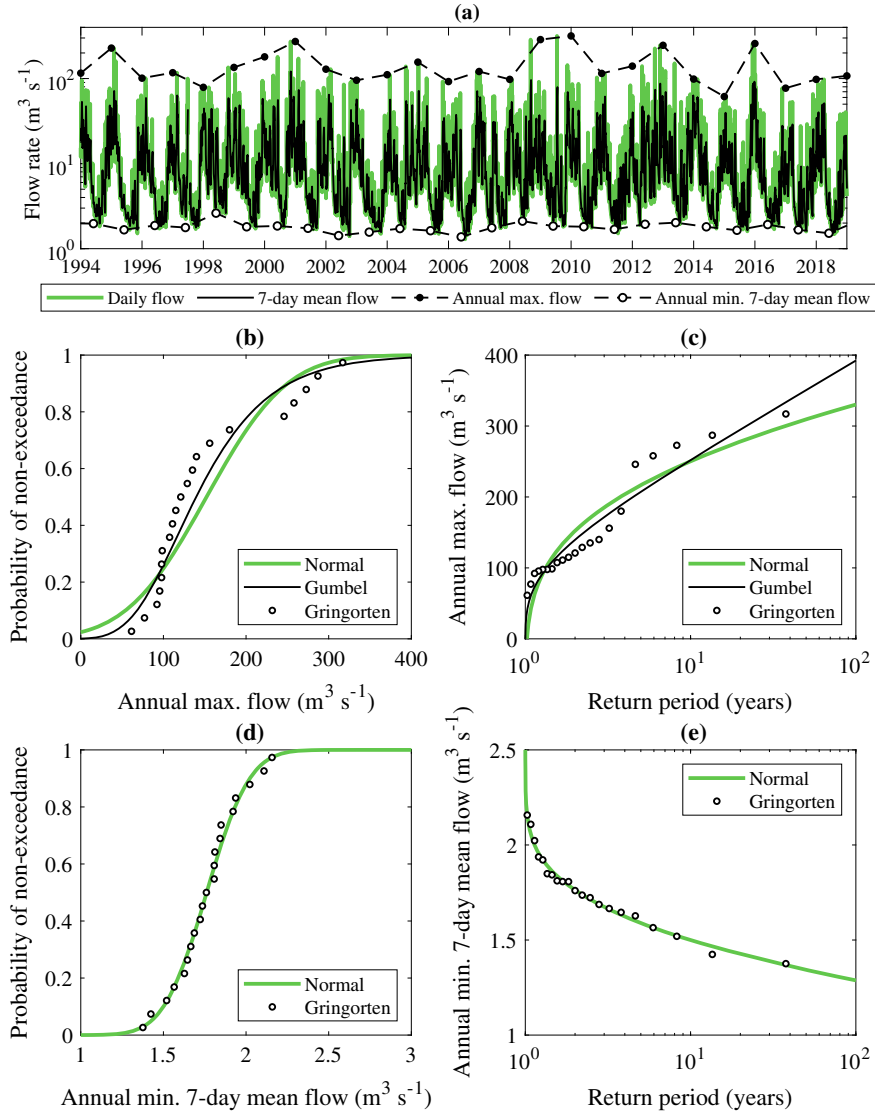


Fig. 11.7 Frequency analysis of flow data from the Sunderland Bridge gauging station on the River Wear (river flow data acquired from [6])

11.4 Problem Sheet

Problem 11.1 (see Worked Solution 11.1)

A contractor plans to build a cofferdam in a river subject to annual flooding. Hydrological records over 30 years indicate a maximum annual maximum flow of $7800 \text{ m}^3\text{s}^{-1}$ and a minimum annual maximum flow of $2000 \text{ m}^3\text{s}^{-1}$. The observed annual maxima plot as a straight line on semi-logarithmic paper where return period is plotted logarithmically. The cofferdam will be in the river during four consecutive flood seasons and it is decided to build it sufficiently high to protect against a 1 in 20 year event. Use the Gringorten plotting position and evaluate (without plotting) the 20-year event and determine the probability of its occurrence during the cofferdam's life.

Problem 11.2 (see Worked Solution 11.2)

A rainwater harvesting scheme is designed for a useful life of 20 years. It can tolerate an annual rainfall of up to 1800 mm. The mean and standard deviation for annual rainfall in the area is 1260 mm and 180 mm, respectively. Use a Gumbel distribution to determine the probability of an annual rainfall of 1800 mm occurring once in the next 20 years.

Problem 11.3 (see Worked Solution 11.3)

Table 11.2 contains ten years of annual maximum daily river flow and annual minimum 7-day mean daily river flow data from the Sunderland Bridge gauging station.

- (a) Write a MATLAB script to (i) compute the empirical CDF for the annual maximum flows using the Gringorten plotting position, (ii) compute a moment matched Gumbel CDF, (iii) compare your results by plotting annual maximum flow against return period using the two distribution functions.
- (b) Write a MATLAB script to (i) compute the empirical CDF for the annual minimum 7-day mean flows using the Gringorten plotting position, (ii) compute a moment matched normal CDF, (iii) compare your results by plotting annual minimum 7-day mean flow against return period using the two distribution functions.
- (c) Use the Gumbel distribution to determine the 1 in 50 year annual maximum flow.
- (d) Use the normal distribution to determine the 1 in 50 year annual minimum 7-day mean flow.

Table 11.2 Annual maximum daily river flow and annual minimum 7-day mean daily river flow data from the Sunderland Bridge gauging station (determined from [6])

Year	Max. flow (m^3s^{-1})	Min. flow (m^3s^{-1})
2010	317	1.81
2011	115	1.68
2012	140	1.94
2013	246	2.02
2014	98.6	1.81
2015	61.4	1.65
2016	258	1.92
2017	77.1	1.67
2018	97.8	1.52
2019	108	2.16

(e) Determine the 1 in 50 year low and high water depths in the river. Assume that the river channel is rectangular, has a breadth of 38 m, a slope of 0.01 and a Manning's coefficient of $0.035 \text{ m}^{-\frac{1}{3}}\text{s}$.

Under normal flow conditions, the Manning equation (see Sect. 2.5.2) gives that $A^2 m^{\frac{4}{3}} S_0 = n^2 Q^2$ where $A [\text{L}^2]$ is the flowing cross-sectional area of the river channel, $m [\text{L}]$ is the hydraulic radius, $S_0 [-]$ is the slope of the river bed, $n [\text{L}^{-\frac{1}{3}}\text{T}]$ is the Manning coefficient and $Q [\text{L}^3\text{T}^{-1}]$ is river flow rate.

11.5 Worked Solutions

Worked Solution 11.1 (see Problem 11.1)

Given there is a 30 year record, the number of annual maxima in the series will be $N = 30$. If the annual maxima, x_j , are ranked from highest to lowest, $x_1 = 7800 \text{ m}^3\text{s}^{-1}$ and $x_N = 2000 \text{ m}^3\text{s}^{-1}$. Given the Gringorten plotting position (Eq. (11.3)), the corresponding probability of exceedance are:

$$P(x > x_1) = \frac{1 - 0.44}{30 + 0.12} = 0.01859$$

$$P(x > x_N) = \frac{30 - 0.44}{30 + 0.12} = 0.9814$$

The corresponding return periods are $T_1 = 53.79$ years and $T_N = 1.019$ years.

If the annual maxima plot as a straight line on semi-logarithmic paper it follows

that

$$x = m \ln T + c$$

where m and c are the slope and intercept of the straight line.

It further follows that:

$$m = \frac{x_1 - x_N}{\ln(T_1/T_N)} = \frac{7800 - 2000}{\ln(53.79/1.019)} = 1462 \text{ m}^3 \text{ s}^{-1}$$

$$c = x_1 - m \ln T_1 = 7800 - 1462 \times \ln 53.79 = 1974 \text{ m}^3 \text{ s}^{-1}$$

The 20-year event is therefore

$$1462 \times \ln 20 + 1974 = 6354 = 6350 \text{ m}^3 \text{ s}^{-1}$$

The probability of the 20-year event occurring once in the life-time of the cofferdam is $1 - (1 - 1/20)^4 = 0.186$

Worked Solution 11.2 (see Problem 11.2)

First use Eq. (11.16) to determine the α and β parameters for the Gumbel distribution:

$$\beta = \frac{180\sqrt{6}}{\pi} = 140.3 \text{ mm}$$

$$\alpha = 1260 - 0.5772 \times 140.3 = 1179 \text{ mm}$$

The probability of annual rainfall not exceeding 1800 mm in a given year is

$$P(X \leq 1800) = \exp \left\{ -\exp \left[-\left(\frac{1800 - 1179}{140.3} \right) \right] \right\} = 0.9881$$

Therefore the probability of the annual rainfall exceeding 1800 mm once within the next 20 years is (from Eq. (11.14))

$$1 - [P(X \leq 1800)]^{20} = 1 - 0.9881^{20} = 0.213$$

Worked Solution 11.3 (see Problem 11.3)

(a) The following MATLAB script computes the analysis and plots the results:

```
%Rank the annual maximum flows
xMAX=[317,115,140,246,98.6,61.4,258,77.1,97.8,108];
xMAX=sort(xMAX,'descend');
%Determine the P(X>xi) using Gringorten
N=numel(xMAX);
Pi=( [1:N]' -0.44)/(N+0.12);
%Determine return period
```

```

Ti=1./Pi;
%Determine Gumbel distribution parameters
beta=std(xMAX)*sqrt(6)/pi;
alpha=mean(xMAX)-double(eulergamma)*beta;
%Compute theoretical CDF
x=linspace(0,400)';
F=exp(-exp(-(x-alpha)/beta));
%Determine return period
T=1./(1-F);
figure(1);clf %Plot results
plot(T,x,Ti,xMAX,'o')
set(gca,'xscale','log')
xlabel('Return period (years)')
ylabel('Annual max. flow (m^3 s^-1)')
legend('Gumbel','Gringorten')

```

The plot should look similar to Fig. 11.7c.

(b) The following MATLAB script computes the analysis and plots the results:

```

%Rank the annual minimum flows
xMIN=[1.81,1.68,1.94,2.02,1.81,1.65,1.92,1.67,1.52,2.16];
xMIN=sort(xMIN,'descend')';
%Determine the P(X>xi) using Gringorten
N=numel(xMIN);
Pi=( [1:N]' -0.44)/(N+0.12);
%Determine return period
Ti=1./(1-Pi);
%Determine normal distribution parameters
alpha=mean(xMIN);
beta=std(xMIN);
%Compute theoretical CDF
x=linspace(1,2.5)';
F=(1+erf((x-alpha)/beta/sqrt(2)))/2;
%Determine return period
T=1./F;
figure(2);clf %Plot results
plot(T,x,Ti,xMIN,'o')
set(gca,'xscale','log')
xlabel('Return period (years)')
ylabel('Annual min. flow (m^3 s^-1)')
legend('Normal','Gringorten')

```

The plot should look similar to Fig. 11.7e.

(c) Assuming $T = \frac{1}{P(X>x)}$, the Gumbel CDF (Eq. (11.14)) can be rearranged to get

$$x = \alpha - \beta \ln \left[-\ln \left(1 - \frac{1}{T} \right) \right]$$

From 11.3a above we have that $\alpha = 112.1 \text{ m}^3\text{s}^{-1}$ and $\beta = 68.94 \text{ m}^3\text{s}^{-1}$. For a return period of 50 years it can therefore be determined that $x = 381.1 \text{ m}^3\text{s}^{-1}$.

(d) Assuming $T = \frac{1}{P(X>x)}$, the normal CDF (Eq. (11.7)) can be rearranged to get

$$x = \alpha + 2^{1/2} \beta \operatorname{erf}^{-1} \left(\frac{2}{T} - 1 \right)$$

where erf^{-1} denotes the inverse of the error function.

From 11.3b above we have that $\alpha = 1.818 \text{ m}^3\text{s}^{-1}$ and $\beta = 0.1947 \text{ m}^3\text{s}^{-1}$. For a return period of 50 years it can therefore be determined that $x = 1.418 \text{ m}^3\text{s}^{-1}$.

(e) Let B [L] be the breadth of the river channel and h [L] be the water depth. For a rectangular channel, the flowing cross-sectional area, $A = Bh$ and the wetted perimeter is $B + 2h$. It follows that the hydraulic radius, $m = \frac{Bh}{B+2h}$. Substituting these expressions into the Manning equation gives that

$$\left(\frac{Bh}{B+2h} \right)^{4/3} S_0 = \left(\frac{nQ}{Bh} \right)^2$$

which can be rearranged to get

$$h^{5/3} - \frac{nQ}{S_0^{1/2} B^{5/3}} (B+2h)^{2/3} = 0$$

The above equation can be solved iteratively for h . A good initial guess, h_0 , can be obtained by assuming $B \gg h$ such that

$$h_0 = \left(\frac{nQ}{S_0^{1/2} B} \right)^{3/5}$$

A MATLAB script for the iterative solution is provided below:

```
B=38; %Channel breadth (m)
S0=0.01; %Channel slope (m)
n=0.035; %Manning's coefficient
Q=[1.418 381.1]; %Flow rates (m^3/s)
for k=1: numel(Q)
    %Step through each flow rate to be studied
    %Initial guess for water depth (m)
    h0=(n*Q(k)/sqrt(S0)/B)^(3/5);
    %Iterative solution for water depth (m)
    U=n*Q(k)/sqrt(S0)/B^(5/3);
    h=fzero(@(h) h^(5/3)-U*(B+2*h)^(2/3),h0)
end
```

On evaluation, it is found that the 1 in 50 year low and high water depth is 0.0742 m and 2.22 m, respectively.

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Abstract

This chapter develops some basic mathematical theory concerning fluid flow in porous media. Relevant concepts covered include aquifers, aquicludes, aquitards, porosity, void ratio, hydraulic conductivity and permeability. The Kozeny-Carman equation for permeability is derived by comparing Darcy's law with the Darcy-Weisbach equation. The Ergun equation, which represents a semi-theoretical form of the Forchheimer equation, is derived by combining theoretical equations for laminar flow and turbulent flow head losses. The Kozeny-Carman equation is combined with an empirical equation for the Forchheimer parameter to uncover a Reynolds number criterion for non-Darcian flow. Practical applications are presented through a problem sheet with worked solutions.

Notation

a	Fracture aperture [L].
A	Cross-sectional area [L^2].
A_p	Cross-sectional area of a pipe [L^2].
A_v	Surface area of void-space [L^2].
b	Forchheimer parameter [L^{-1}].
B	Breadth [L].
c_0	Geometrical factor [–].
E	Total head [L].
f	Darcy-Weisbach friction factor [–].
Fo	Forchheimer number [–].
g	Gravitational acceleration [LT^{-2}].
h	Hydraulic head [L].
H	Formation thickness [L].
k	Permeability [L^2].
K	Hydraulic conductivity [LT^{-1}].

L	Length [L].
L_p	Length of pipe [L].
m	Volume to surface area ratio of the voids (i.e., hydraulic radius) [L].
m_g	Volume to surface area ratio of solid grains [L].
N	Number of pipes [-].
p	Pressure [$\text{ML}^{-1}\text{T}^{-2}$].
q	Darcy flux [LT^{-1}].
Q	Flow rate [L^3T^{-1}].
r_g	Radius of grain [L].
Re	Reynolds number [-].
s	Distance in the direction of flow [L].
s_p	Distance along a tortuous pathway [L].
S	Fracture spacing [L].
t	Time [T].
T	Transmissivity [L^2T^{-1}].
v	Pore-water velocity [LT^{-1}].
V_S	Volume of solid material [L^3].
V_T	Total volume of sample [L^3].
V_V	Volume of voids [L^3].
z	Elevation [L].
ε	Void ratio [-].
μ	Dynamic viscosity [$\text{ML}^{-1}\text{T}^{-1}$].
ρ	Fluid density [ML^{-3}].
τ	Tortuosity [-].
ϕ	Porosity [-].
ψ	Pressure head [L].

12.1 Introduction

This chapter introduces the topic of groundwater flow. First we look at what properties make a geological formation an aquifer. The terms porosity and void ratio are introduced, which are important because these describe how much water can be stored within an aquifer formation. We then introduce the empirical equation, Darcy's law, which enables the determination of groundwater flow rates from measurements of hydraulic head. The difference between water level measurements from open boreholes and piezometers are discussed. A theoretical comparison between Darcy's law and the Darcy-Weisbach equation for flow in pipes is used to derive a theoretical relationship between permeability and geometrical properties of a pore-space. The concept of non-Darcian flow is also studied using the Forchheimer equation and the Ergun equation.

12.2 Aquifers, Aquicludes and Aquitards

An aquifer is a term frequently given to geological formations that are potentially useful for water production. Most geological formations are porous to some level. The porosity of a formation represents the volume fraction comprised of void-space. Voids are present for a multitude of reasons including deformation induced fractures, packing efficiency of grains in sedimentary rocks, and vesicles in volcanic rocks. Much of this void-space is filled with water.

However, whether a formation should be defined as an aquifer depends more on its ability to transmit water as opposed to storing water. For example, large quantities of water are held within clay formations. However, it is very difficult to remove water from clay. Therefore, clay formations are not identified as aquifers. Geological formations typically identified as aquifers include gravels, sand, sandstone, limestones and some fractured crystalline rocks.

In this context it is useful to consider the following three definitions (adapted from [1, p. 47]):

- **Aquifer:** A saturated permeable geological formation that can transmit significant quantities of water under ordinary hydraulic gradients.
- **Aquiclude:** A saturated geological formation that is incapable of transmitting significant quantities of water under ordinary hydraulic gradients.
- **Aquitard:** A saturated permeable geological formation that can transmit significant quantities of water under ordinary hydraulic gradients but is not sufficiently permeable to yield economic quantities of water.

12.3 Porosity and Void Ratio

Many fluids are stored in rocks and soils including water, air, oil and gas. They reside in small pores within the porous material of concern. An important property often used to describe a material's ability to store fluid is porosity, ϕ [–], defined by

$$\phi = \frac{V_V}{V_T} \quad (12.1)$$

where V_V [L^3] is the volume of voids and V_T [L^3] is the total volume of the porous material of concern.

A related property is the void ratio, ε [–], found from

$$\varepsilon = \frac{V_V}{V_S} \quad (12.2)$$

where V_S [L^3] is the volume of solid material contained within a porous material. Note that $V_T = V_V + V_S$.

Challenge 12.1 Derive expressions relating ϕ to ε and ε to ϕ .

Porosity and void ratio can be related to each other as follows:

$$\phi = \frac{V_V}{V_T} = \frac{V_V}{V_V + V_S} = \left(1 + \frac{V_S}{V_V}\right)^{-1} = \left(1 + \frac{1}{\varepsilon}\right)^{-1} = \frac{\varepsilon}{1 + \varepsilon}$$

$$\varepsilon = \frac{V_V}{V_S} = \frac{V_V}{V_T - V_V} = \left(\frac{V_T}{V_V} - 1\right)^{-1} = \left(\frac{1}{\phi} - 1\right)^{-1} = \frac{\phi}{1 - \phi}$$

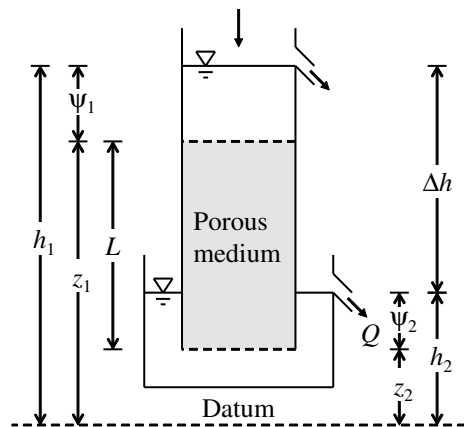
12.4 Darcy's Law

For a geological formation to qualify as an aquifer it needs to be able to transmit significant quantities of fluid under ordinary hydraulic gradients. The ability of a given formation to transmit water is quantitatively defined by its hydraulic conductivity, K [LT^{-1}], which represents the main controlling parameter contained within Darcy's law for flow in porous media.

Henry Darcy was a 19th century civil engineer from Dijon in France. He worked on many infrastructure projects related to water supply. He developed the Darcy-Weisbach equation for describing flow in pipes and Darcy's law to describe water flow in sand filters.

A schematic diagram of Darcy's sand filter experiment is presented in Fig. 12.1. The objective of the apparatus is to provide sufficient water at the top such that both overflow pipes continuously flow and the water levels in the upper and lower overflow tanks remain constant at the overflow points. The upper overflow rate will likely be transient and dependent on the inflow rate. However, the lower overflow rate should be constant because it is driven by a constant hydraulic gradient.

Fig. 12.1 Schematic diagram of Darcy's experiment



Darcy measured the lower overflow rate, Q [L^3T^{-1}], for different overflow water level differences, Δh [L], and determined empirically that

$$Q \propto \frac{A\Delta h}{L}$$

where A [L^2] and L [L] are the cross-sectional area and length of the filter, respectively.

In fact Δh represents the hydraulic head loss across the filter:

$$\Delta h = h_1 - h_2$$

where h_1 [L] and h_2 [L] are the hydraulic head at the top and bottom of the sand filter, respectively.

Recall that

$$h = \psi + z \quad (12.3)$$

where ψ [L] is the pressure head and z [L] is the elevation head above a reference level referred to as the datum. Also recall that

$$\psi = \frac{p}{\rho g} \quad (12.4)$$

where p [$ML^{-1}T^{-2}$] is the fluid pressure, ρ [L^3T^{-1}] is the fluid density and g [LT^{-2}] is gravitational acceleration.

The empirical coefficient of proportionality represents what was previously referred to as the hydraulic conductivity, K [LT^{-1}]. Consequently, Darcy's law is typically stated as

$$q \equiv \frac{Q}{A} = -K \frac{\partial h}{\partial s} \quad (12.5)$$

where $\frac{\partial h}{\partial s}$ [–] is the hydraulic gradient, s [L] is distance along the flow direction and q [LT^{-1}] is the flow per unit area of porous media, often referred to as the Darcy flux.

Hydraulic conductivity is a material property dependent on the geometry of the pore-space as well as the density and viscosity of the transported fluid. Representative values of porosity and hydraulic conductivity for a range of different geological formations are given in Table 12.1. Note that many geological media have relatively high porosities whilst not necessarily having high hydraulic conductivity as well.

12.5 Boreholes and Piezometers

A common method for assessing the performance of an aquifer is to record and observe measurements of hydraulic head in open boreholes and piezometers. The differences between open boreholes and piezometers are illustrated in Fig. 12.2.

Open boreholes contain a large open response zone, commonly referred to as a well-screen, where the borehole is in hydraulic contact with the aquifer. The water level measurement in an open borehole represents a vertically averaged hydraulic

Table 12.1 Porosity, ϕ , and hydraulic conductivity, K , for a range of different geological media [2, pp. 38 and 93]

	ϕ (%)	K (m day ⁻¹)
Gravel, coarse	28	150
Gravel, medium	32	270
Gravel, fine	34	450
Sand, coarse	39	45
Sand, medium	39	12
Sand, fine	43	2.5
Silt	46	0.08
Clay	42	0.0002
Sandstone, fine grained	33	0.2
Sandstone, medium grained	37	3.1
Limestone	30	0.94
Dune sand	45	20
Loess	49	0.08
Peat	92	5.7
Schist	38	0.2
Till, predominantly silt	34	0.49
Till, predominantly sand	31	30
Tuff	41	0.2

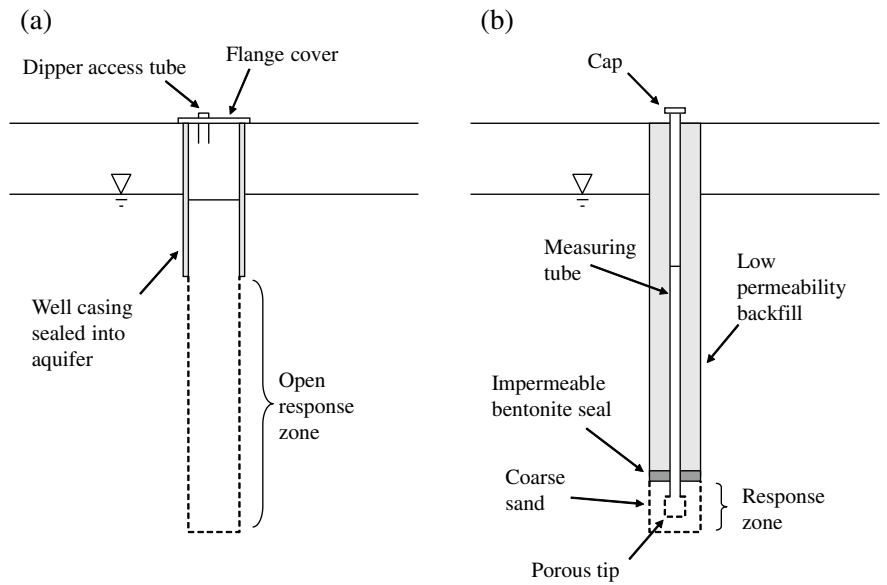


Fig. 12.2 Schematic diagrams showing **a** an open borehole and **b** a piezometer

head, over the interval of the well-screen. The advantage of such a measurement is that it provides average information about the entire aquifer thickness with just one borehole.

In contrast, a piezometer is designed to obtain a measurement of hydraulic head over a very narrow vertical region. The advantage here is that multiple piezometers at different depths can provide information about vertical hydraulic gradients.

12.6 Insights from the Darcy-Weisbach Equation

The Darcy-Weisbach equation for steady-state fluid flow in a non-cylindrical pipe gives that (recall Eq. (2.21))

$$\frac{\partial E}{\partial s} = -\frac{fv^2}{2gm} \quad (12.6)$$

where s [L] is distance along the flow direction, f [L] is the friction factor, v [LT⁻¹] is the cross-sectional mean fluid velocity within the pipe, m [L] is the hydraulic radius of the pipe and E [L] is the total head found from

$$E = h + \frac{v^2}{2g} \quad (12.7)$$

Under laminar flow conditions (recall Eq. (2.33))

$$f = \frac{8c_0}{\text{Re}} \quad (12.8)$$

where c_0 [–] is a geometrical factor and Re [–] is the Reynolds number, found from

$$\text{Re} = \frac{4\rho mv}{\mu} \quad (12.9)$$

where ρ [ML⁻³] is the fluid density and μ [ML⁻¹T⁻¹] is the dynamic viscosity of the fluid.

It can be shown that $c_0 = 2$ for flow through a cylindrical pipe and $c_0 = 3$ for flow between two parallel plates (see Sect. 2.4.4). For realistic pore-geometries, c_0 is unknown but likely to be greater than 3.

The hydraulic radius, m , is defined as the ratio of the flowing area to wetted perimeter for the pipe. In the context of porous media, m , can be estimated from

$$m = \frac{V_V}{A_V} \quad (12.10)$$

where V_V [L³] and A_V [L²] are the volume and surface area of the void-space within a porous system, respectively.

In what follows we will derive a theoretical equation to describe hydraulic conductivity in terms of the porosity, ϕ [–], void ratio, ε [–] and grain size, m_g [L], of a porous material using the Darcy-Weisbach equation. Because the Darcy-Weisbach equation is written in terms of fluid velocity, v [LT⁻¹], and Darcy's law is written in

terms of Darcy flux, q [LT^{-1}], the first step involves developing an expression that relates q to v . The next step involves deriving an expression that relates the hydraulic radius, m [L], with grain size and void ratio. Because Darcy's law assumes that q is a linear function of head gradient, it is clear that the Darcy-Weisbach equation can only be related to Darcy's law under laminar flow conditions. By assuming laminar flow conditions we will finally relate both equations together to derive a theoretical relationship for hydraulic conductivity.

12.6.1 Darcy Flux and Pore-Water Velocity

Consider a prismatic solid block with cross-sectional area, A [L^2], and length, L [L] (Fig. 12.3). The solid block is penetrated by N [–] number of identical, prismatic, non-cylindrical pipes, each of cross-sectional area, A_p [L^2], and length, L_p [L]. Fluid flows through the pipes at a steady and uniform velocity, v [LT^{-1}]. Each pipe is tortuous and therefore not parallel to the longitudinal axis of the prismatic block. However, each pipe starts from a common face normal to this longitudinal axis and ends on the opposite normal face. Therefore, the bulk flow of fluid through the entire porous block is parallel to its longitudinal axis.

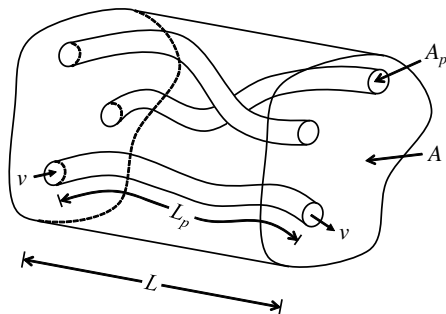
The tortuosity, τ [–], of the system is a property that describes how twisted and tortuous the pipes are. A simple model is to assume

$$\tau = \frac{L_p}{L} \quad (12.11)$$

Note that the system becomes more tortuous with increasing L_p .

Challenge 12.2 Determine an expression for the porosity of the block, ϕ [–], and then determine an expression for the Darcy flux, q [LT^{-1}] in terms of v , τ and ϕ .

Fig. 12.3 Schematic diagram of porous block with tortuous pathways



Recall that the porosity of the block, ϕ , can be found from $\phi = \frac{V_V}{V_T}$ where V_T [L^3] is the total volume of the block and V_V [L^3] is the total volume of voids within the block.

In this context $V_T = AL$ and $V_V = NA_p L_p$ so

$$\phi = \frac{NA_p L_p}{AL} = \frac{\tau NA_p}{A}$$

The total flow rate through the pipes, Q [$L^3 T^{-1}$], is found from

$$Q = NA_p v$$

Substituting in the expression for porosity leads to

$$Q = \frac{A\phi v}{\tau}$$

where v , in this context, is referred to as the pore-water velocity.

It follows that the Darcy flux is found from

$$q \equiv \frac{Q}{A} = \frac{\phi v}{\tau} \quad (12.12)$$

12.6.2 Hydraulic Radius, Grain Geometry and Void Ratio

The presence of the pipes within the porous block described above is due to the block comprising an agglomeration of solid grains characterised by a volume to surface area ratio, m_g [L] (referred to earlier as the grain size). For spherical grains of radius, r_g [L], it can be shown that $m_g = \frac{r_g}{3}$. The hydraulic radii of the pipes, m [L], represent the volume to surface area ratio of the pore-space within the block.

Challenge 12.3 Determine an expression for m in terms of m_g and void-ratio, ε .

The hydraulic radius, m , is defined by Eq. (12.10). The surface area of the void-space will be the same as the surface area of the solid grains. Therefore, the volume to surface area ratio of the grains can be found from

$$m_g = \frac{V_S}{A_V} \quad (12.13)$$

where V_S [L^3] is the volume of solids in the porous block.

Dividing Eq. (12.10) by Eq. (12.13) leads to

$$\frac{m}{m_g} = \frac{V_V}{V_S}$$

Substituting Eq. (12.2) then gives us

$$m = \varepsilon m_g \quad (12.14)$$

12.6.3 A Theoretical Hydraulic Conductivity Relationship

Challenge 12.4 Use the above expressions to derive an equation for the hydraulic head gradient, $\frac{\partial h}{\partial s_p}$, in terms of the Darcy flux, q , and τ , f , ϕ , m_g , ε and g where s_p [L] is the distance along one of the tortuous pipes within the porous block.

From Eq. (12.6) we have

$$\frac{\partial E}{\partial s_p} = -\frac{fv^2}{2gm}$$

Recall that the pipes in the porous block are prismatic, which means their cross-sectional area does not vary with s_p . It follows that for steady-state flow of an incompressible fluid, v is constant with s_p . Given Eq. (12.7), it follows that $\frac{\partial E}{\partial s_p} = \frac{\partial h}{\partial s_p}$ and therefore

$$\frac{\partial h}{\partial s_p} = -\frac{fv^2}{2gm} \quad (12.15)$$

Substituting Eqs. (12.12) and (12.14) into Eq. (12.15) leads to

$$\frac{\partial h}{\partial s_p} = -\frac{f\tau^2 q^2}{2g\phi^2 \varepsilon m_g} \quad (12.16)$$

Challenge 12.5 The independent variable in Eq. (12.16), represents the distance along a tortuous pipe within the porous block, s_p [L]. Use the tortuosity parameter, τ [–], to modify Eq. (12.16) such that the independent variable is instead the distance along the porous block, s [L], associated with Darcy's law (Eq. (12.5)).

Let s [L] be the distance along the porous block associated with Darcy's law (Eq. (12.5)). If we assume that $s_p = f(s)$ it can be further stated that

$$\frac{\partial s}{\partial s_p} \frac{\partial h}{\partial s} = -\frac{f\tau^2 q^2}{2g\phi^2 \varepsilon m_g}$$

In fact for our case,

$$\frac{\partial s}{\partial s_p} \approx \frac{L}{L_p} = \frac{1}{\tau}$$

so [3]

$$\frac{\partial h}{\partial s} = -\frac{f\tau^3 q^2}{2g\phi^2 \varepsilon m_g} \quad (12.17)$$

which is known as the Burke-Plummer equation [4, p.191].

Challenge 12.6 Eliminate the friction factor in Eq. (12.17) by assuming laminar flow conditions.

Under laminar flow conditions, Eq. (12.8) applies and

$$f = \frac{2c_0\mu}{\rho mv} \quad (12.18)$$

Substituting Eqs. (12.12) and (12.14) into Eq. (12.18) leads to

$$f = \frac{2c_0\mu\phi}{\rho\epsilon m_g \tau q} \quad (12.19)$$

and substituting Eq. (12.19) into Eq. (12.17) leads to [5]

$$\frac{\partial h}{\partial s} = -\frac{c_0\mu\tau^2 q}{\rho g \phi \epsilon^2 m_g^2} \quad (12.20)$$

which is known as the Blake-Kozeny equation [4, p.191].

Challenge 12.7 Compare Eqs. (12.5) and (12.20) and derive a theoretical relationship for the hydraulic conductivity.

A theoretical relationship for the hydraulic conductivity parameter, K , in Darcy's law can be obtained by comparing Darcy's law with the Blake-Kozeny equation.

Solving Eq. (12.20) for q leads to

$$q = -\frac{\rho g \phi \epsilon^2 m_g^2}{c_0 \mu \tau^2} \frac{\partial h}{\partial s} \quad (12.21)$$

Equating Eqs. (12.5) and (12.21) gives us

$$K = \frac{\rho g \phi}{c_0 \mu} \left(\frac{\epsilon m_g}{\tau} \right)^2 \quad (12.22)$$

12.7 Permeability

Equation (12.22) shows that hydraulic conductivity is controlled by two types of properties: (1) geometrical properties associated with the pore-space; (2) physical properties of the fluid being considered.

Often these types of properties are separated out as follows:

$$K = \frac{\rho g k}{\mu} \quad (12.23)$$

where k [L^2] is known as the permeability. The advantage of determining the permeability of a material is that it can be used to describe the transport of different types of fluids with varying viscosity and density.

Darcy's law written in terms of permeability takes the form

$$q = -\frac{\rho g k}{\mu} \frac{\partial h}{\partial s} \quad (12.24)$$

According to Eq. (12.22)

$$k = \frac{\phi}{c_0} \left(\frac{\varepsilon m_g}{\tau} \right)^2 \quad (12.25)$$

which is often referred to as the Kozeny-Carman equation.

The higher the permeability the more permeable a porous medium is. Large grain size increases permeability. High porosity or void ratio increases permeability. High tortuosity reduces permeability.

12.8 Non-Darcian Flow

12.8.1 The Forchheimer Equation

The derivation of Eq. (12.25) requires an assumption of laminar flow conditions. This in turn assumes that pore-water velocities are sufficiently small to ensure that the Reynolds number is less than 2000 (see Sect. 2.4.3). In most ambient groundwater scenarios, pore-water velocities are small and such an assumption holds well. However, close to groundwater production wells, velocities are enhanced due to active pumping of water. In such cases, Darcy's law is found to be inadequate and the following empirical formula is preferred [6]:

$$\frac{\partial h}{\partial s} = -\frac{\mu q}{\rho g k} - \frac{b|q|q}{g} \quad (12.26)$$

where b [L^{-1}] is referred to as the Forchheimer coefficient. Equation (12.26) is commonly referred to as the Forchheimer equation.

An estimate of the Forchheimer parameter can be obtained using the following additional empirical correlation due to [7]:

$$k^{\frac{1}{2}} b = 0.005 \phi^{-5.5} \quad (12.27)$$

12.8.2 The Ergun Equation

Under purely laminar flow conditions, hydraulic head loss in porous media can be determined using the Blake-Kozeny equation (Eq. (12.20)). Under purely turbulent flow conditions, hydraulic head loss in porous media can be determined using the Burke-Plummer equation (Eq. (12.17)) with a constant friction factor.

Ergun [8] argued that a Forchheimer-type equation can be obtained by assuming that laminar flow-like and turbulent flow-like head losses occur simultaneously and added the right-hand-sides of the Blake-Kozeny and Burke-Plummer equations together to get

$$\frac{\partial h}{\partial s} = -\frac{c_0 \mu \tau^2 q}{\rho g \phi \varepsilon^2 m_g^2} - \frac{f \tau^3 q^2}{2g \phi^2 \varepsilon m_g} \quad (12.28)$$

which is often referred to as the Ergun equation [4, p.191].

Substituting Eq. (12.25) into Eq. (12.28) leads to

$$\frac{\partial h}{\partial s} = -\frac{\mu q}{\rho g k} - \frac{f \tau^2 q^2}{2g (c_0 \phi^3 k)^{\frac{1}{2}}} \quad (12.29)$$

Equating Eqs. (12.26) and (12.29) then suggests that

$$k^{\frac{1}{2}} b = \frac{f \tau^2}{2c_0^{\frac{1}{2}} \phi^{\frac{3}{2}}} \quad (12.30)$$

which has a similar form to the empirical equation of [7], given in Eq. (12.27).

12.8.3 Reynolds Number Criterion for Non-Darcian Flow

Equation (12.26) can be rearranged to get

$$\frac{\partial h}{\partial s} = -(1 + \text{Fo}) \frac{\mu q}{\rho g k} \quad (12.31)$$

where Fo [–] is referred to as the Forchheimer number and defined by [9]

$$\text{Fo} = \frac{\rho k b |q|}{\mu} \quad (12.32)$$

Non-Darcian effects are likely to be significant when $\text{Fo} > 1$.

Challenge 12.8 Derive a semi-empirical equation for the Reynolds number, Re , in terms of the Forchheimer number, Fo , geometrical factor, c_0 , tortuosity, τ , and porosity, ϕ .

Substituting Eq. (12.9) into Eq. (12.32) and solving for Re leads to

$$\text{Re} = \frac{4m|v|}{kb|q|} \text{Fo} \quad (12.33)$$

Substituting Eq. (12.12) into Eq. (12.33) leads to

$$\text{Re} = \frac{4m\tau}{kb\phi} \text{Fo} \quad (12.34)$$

Substituting Eq. (12.27) into Eq. (12.34) leads to

$$\text{Re} = \frac{800m\tau}{k^{\frac{1}{2}}\phi^{-4.5}}\text{Fo} \quad (12.35)$$

Substituting Eq. (12.25) into Eq. (12.35) leads to

$$\text{Re} = \frac{800c_0^{\frac{1}{2}}m\tau^2}{\varepsilon m_g\phi^{-4}}\text{Fo} \quad (12.36)$$

Substituting Eq. (12.14) into Eq. (12.36) leads to

$$\text{Re} = 800c_0^{\frac{1}{2}}\tau^2\phi^4\text{Fo} \quad (12.37)$$

The geometrical factor, c_0 , is unlikely to be greater than 3, the tortuosity, τ , is unlikely to be greater than 4 and the porosity, ϕ , is unlikely to be greater than 0.3. It follows that $800c_0^{\frac{1}{2}}\tau^2\phi^4$ is unlikely to be greater than 180. It follows that non-Darcian effects can generally be expected to become significant when $\text{Re} > 180$ (see [10] for further discussion).

12.9 Problem Sheet

Problem 12.1 (see Worked Solution 12.1)

A sample of a cylindrical drill core of sandstone, 3.17 cm in diameter and 6.10 cm long, is to be analysed to determine its porosity. The sample is dried in a vacuum oven for several hours at 105°C and then weighed. The mass is 94.2 g. The sample is then vacuum saturated by first placing it in a dry vacuum tank and subjecting it to a vacuum of 800 Pa for about 30 minutes. With the vacuum pump remaining in operation, water with a density of 1.0 g cm^{-3} is allowed to enter the tank until the sample is completely submerged. The tank is then returned to atmospheric pressure. The sample is removed, the excess water is carefully wiped away and the sample mass is measured and found to be 103 g. Determine the porosity of the sandstone.

Problem 12.2 (see Worked Solution 12.2)

The following field notes were taken at a nest of piezometers installed in close proximity to each other:

Piezometer	A	B	C
Elevation at surface (mAOD)	350	330	345
Depth of piezometer (m)	100	70	75
Depth to water level (m)	70	49	63

- (a) Calculate the hydraulic head at A, B and C in mAOD.
- (b) Calculate the elevation head at A, B and C in mAOD.
- (c) Calculate the pressure head at A, B and C in m.
- (d) Calculate the vertical hydraulic gradient and determine the direction of flow.
- (e) If the hydraulic conductivity of the profile is 0.02 m day^{-1} , calculate the flow rate per unit area.

Note that mAOD stands for metres above ordnance datum.

Problem 12.3 (see Worked Solution 12.3)

Consider a vertically orientated cylindrical sand filter of 75 cm length and 10 cm diameter. Water is forced up the filter at a rate of $0.1 \text{ cm}^3\text{s}^{-1}$. During this time the pressure at the top and bottom of the cylinder is observed to be 0.982 kPa and 11.3 kPa, respectively. Assume steady-state conditions and use Darcy's law to calculate the hydraulic conductivity of the packed sand.

Problem 12.4 (see Worked Solution 12.4)

A cuboid fractured granite aquifer is of length, breadth and thickness, L [L], B [L] and H [L], respectively. The fractures are identical, horizontal, smooth and planar and are equally spaced by a distance, S [L]. The aperture of the fractures is a distance, a [L]. The unfractured portion of the granite is impermeable. Use the Kozeny-Carman formula to derive an expression for the permeability of the fractured rock mass in terms of S and a .

12.10 Worked Solutions

Worked Solution 12.1 (see Problem 12.1)

From Eq. (12.1), the porosity, $\phi = V_V / V_T$, where V_V is the volume of voids and V_T is the total volume.

The total volume of rock $= \pi(3.17/2)^2 \times 6.10 = 48.14 \text{ cm}^3$.

Given that the core is saturated with water, the volume of voids equals the volume of water in the core.

The mass of water = $103 - 94.2 = 8.8$ g.

The volume of water = $\frac{\text{mass of water}}{\text{density of water}} = \frac{8.8}{1.0} = 8.8 \text{ cm}^3$.

So the porosity, $\phi = 8.8/48.14 = 0.1828 = 0.183$.

Worked Solution 12.2 (see Problem 12.2)

(a) The hydraulic head represents the elevation of the water level in the piezometers relative to the datum. It follows that Hydraulic head = Elevation at surface – Depth to water level.

(b) The elevation head represents the elevation at which the piezometer is measuring hydraulic head relative to the datum. It follows that Elevation head = Elevation at surface – Depth of piezometer.

(c) From Eq. (12.3), Pressure head = Hydraulic head – Elevation head. It follows that the hydraulic head, elevation head and pressure head at locations A, B and C are as follows:

Piezometer	A	B	C
Elevation at surface (m)	350	330	345
Depth of piezometer (m)	100	70	75
Depth to water level (m)	70	49	63
(a) Hydraulic head (mAOD)	280	281	282
(b) Elevation head (mAOD)	250	260	270
(c) Pressure head (m)	30	21	12

(d) The hydraulic gradient is found from

$$\frac{\partial h}{\partial z} = \frac{281 - 280}{260 - 250} = \frac{282 - 281}{270 - 260} = \frac{1}{10}$$

which is positive, therefore the flow must be downwards.

(e) From Darcy's law (Eq. (12.5))

$$q = -K \frac{\partial h}{\partial z} = -0.02 \times \frac{1}{10} = -0.002 \text{ m day}^{-1}$$

Worked Solution 12.3 (see Problem 12.3)

Recall from Darcy's law

$$Q = -AK \frac{\partial h}{\partial z}$$

Note that A and K are constants. Furthermore, under steady-state conditions, Q will also be constant. Integrating both sides of the equation with respect to z therefore leads to

$$Qz = -AKh + C$$

where C is an integration constant.

Let h_1 and h_2 be the hydraulic heads at the top and bottom of the filter, respectively. Similarly let z_1 and z_2 be the elevation heads at the top and bottom of the filter. Setting $h = h_1$ when $z = z_1$ reveals that $C = Qz_1 + AKh_1$. Now setting $h = h_2$ when $z = z_2$ gives us

$$Q(z_1 - z_2) = -AK(h_1 - h_2)$$

So the hydraulic conductivity can be found from

$$K = \frac{Q(z_1 - z_2)}{A(h_2 - h_1)}$$

From Eqs. (12.3) and (12.4) we have that

$$h = \frac{p}{\rho g} + z$$

and so

$$K = \frac{Q(z_1 - z_2)}{A} \left(\frac{p_2 - p_1}{\rho g} + z_2 - z_1 \right)^{-1}$$

Note that the length of the filter, $L = z_1 - z_2$ so

$$K = \frac{QL}{A} \left(\frac{p_2 - p_1}{\rho g} - L \right)^{-1}$$

From the information in the question we have that $L = 0.75$ m, $A = \pi \times 0.1^2/4 = 0.007854$ m², $Q = 10^{-7}$ m³s⁻¹, $p_1 = 982$ Pa and $p_2 = 11,300$ Pa. Noting that $\rho = 1000$ kg m⁻³ and $g = 9.81$ m s⁻²,

$$K = \frac{10^{-7} \times 0.75}{0.007854} \left(\frac{11300 - 982}{1000 \times 9.81} - 0.75 \right)^{-1} = 3.164 \times 10^{-5} \text{ m s}^{-1}$$

So the hydraulic conductivity is $31.6 \mu\text{m s}^{-1}$.

Worked Solution 12.4 (see Problem 12.4)

Consider again the Kozeny-Carman equation (Eq. (12.25))

$$k = \frac{\phi}{c_0} \left(\frac{\varepsilon m_g}{\tau} \right)^2$$

From Eqs. (12.1), (12.2) and (12.13):

$$\phi = \frac{V_V}{V_T}, \quad \varepsilon = \frac{V_V}{V_S}, \quad m_g = \frac{V_S}{A_V}$$

where V_T is the total volume of rock, V_V is the volume of voids, V_S is the volume of solid rock and A_V is the surface area of the void-space.

Let N [-] be the number of fractures in the rock-mass such that:

$$V_T = BHL, \quad V_V = BNaL, \quad V_S = B(H - Na)L, \quad A_V = 2NBL$$

Note that $N = H/S$ so:

$$V_V = \frac{BHaL}{S}, \quad V_S = BH \left(1 - \frac{a}{S}\right) L, \quad A_V = \frac{2HBL}{S}$$

It therefore follows that

$$\phi = \frac{a}{S}, \quad \varepsilon = \frac{a}{S} \left(1 - \frac{a}{S}\right)^{-1}, \quad m_g = \frac{S}{2} \left(1 - \frac{a}{S}\right)$$

which, when substituted into the Kozeny-Carman, equation lead to

$$k = \frac{a^3}{4c_0 S \tau^2}$$

Because the fractures are horizontal, smooth and planar, $\tau = 1$. Furthermore, flow in the fractures is analogous to flow between two parallel plates, for which $c_0 = 3$ (see Sect. 2.4.4). It therefore follows that [11]

$$k = \frac{a^3}{12S}$$

which is widely referred to as the cubic law.

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Confined and Unconfined Aquifers

13

Abstract

This chapter looks at confined and unconfined aquifers. An explanation is provided concerning the difference between water table wells, artesian wells and flowing wells. A comparison is presented concerning groundwater distribution for unconfined aquifers in temperate and arid environments. Steady-state analytical solutions are derived for ground water flow in a confined aquifer, an unconfined aquifer and an unconfined aquifer with recharge. Practical applications are presented through a problem sheet with worked solutions.

Notation

A	Cross-sectional area [L^2].
B	Breadth [L].
h	Hydraulic head [L].
h_0	Boundary hydraulic head [L].
h_1	Boundary hydraulic head [L].
H	Formation thickness [L].
K	Hydraulic conductivity [LT^{-1}].
L	Length [L].
q	Darcy flux [LT^{-1}].
Q	Flow rate [L^3T^{-1}].
t	Time [T].
T	Transmissivity [L^2T^{-1}].
x	Distance along the x -axis [L].
W	Aquifer recharge rate [LT^{-1}].
ρ	Fluid density [ML^{-3}].

13.1 Introduction

This chapter focuses on two important aquifer types, namely confined and unconfined aquifers. First we consider how boreholes are likely to respond in such aquifers. We compare the behaviour of an unconfined aquifer in a temperate environment with that in an arid environment. We then go on to apply Darcy's law to derive analytical solutions for steady-state flow in a confined aquifer, an unconfined aquifer without recharge and finally an unconfined aquifer with recharge.

13.2 Two Types of Aquifer

Two important aquifer types to distinguish between are confined and unconfined aquifers (see Fig. 13.1). Confined aquifers are aquifer formations bounded above and below by aquitards and/or aquicludes. An unconfined aquifer is an aquifer which is unbounded such that the water table forms its upper boundary.

In an unconfined aquifer, the water level in a well will be located at the top of the aquifer, which is the water table. Such a well is referred to as a watertable well.

In a confined aquifer, the water level in a well will rise above the top of the aquifer. When this occurs, the well is said to be artesian. The reason this happens is that the presence of the confining layer above allows water in the aquifer to become overpressured (whereby fluid pressure is greater than hydrostatic pressure). The elevation of the water level in an artesian well should not be referred to as a water table. Instead, this level should be referred to as the piezometric surface.

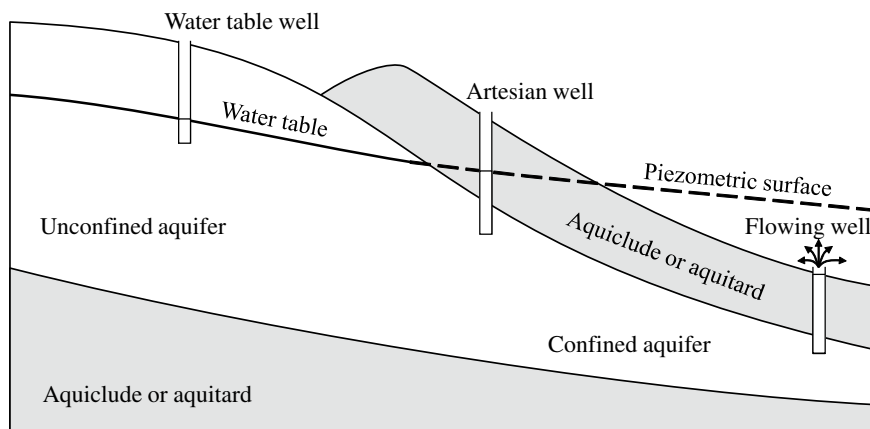


Fig. 13.1 Schematic diagram showing the difference between an unconfined and confined aquifer (inspired by [1])

In some cases the piezometric surface exists above the ground surface. Such a scenario leads to a so-called artesian flowing well, whereby water discharges from the well without pumping and is purely driven by the overpressure of the aquifer. A comparison of these three types of wells is illustrated in Fig. 13.1.

13.3 Temperate and Arid Environments

Whereas confined aquifers derive their water from regional groundwater flows, unconfined aquifers are open to the atmosphere and are subject to recharge by distributed rainfall infiltration at the land surface. Consequently groundwater distributions within unconfined aquifers are very much controlled by regional climatic conditions.

In temperate environments rainfall is both frequent and spatially distributed. Consequently, recharge to unconfined aquifers is continuous and relatively uniform. In such cases, groundwater flows to topographic lows associated with river valleys (see Fig. 13.2). The frictional resistance to water flow within the aquifer gives rise to water table mounding underneath topographic highs. A consequence of this is that groundwater flow tends to be in a downward direction below topographic highs and in an upward direction below topographic lows. This means that groundwater fed rivers often receive water as both an upwelling from below and as drainage of springs from above.

A directional change in groundwater flow occurs at the peak of groundwater mounds. Such a point is referred to as a groundwater divide. Groundwater divides occur where the watertable elevation exhibits a zero-gradient.

In arid environments, rainfall is episodic and tends to occur in small focused regions rather than in a uniformly distributed manor. Furthermore, the ground surface tends to be coated in a dry low permeability crust such that infiltration is significantly

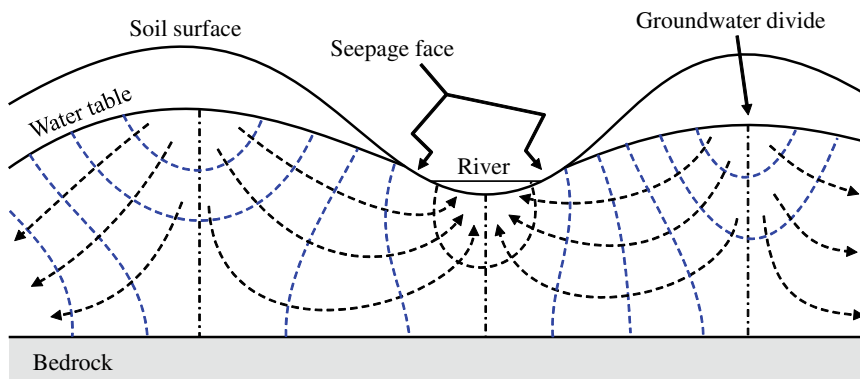


Fig. 13.2 Flow distribution in an unconfined aquifer in a temperate environment (inspired by [2])

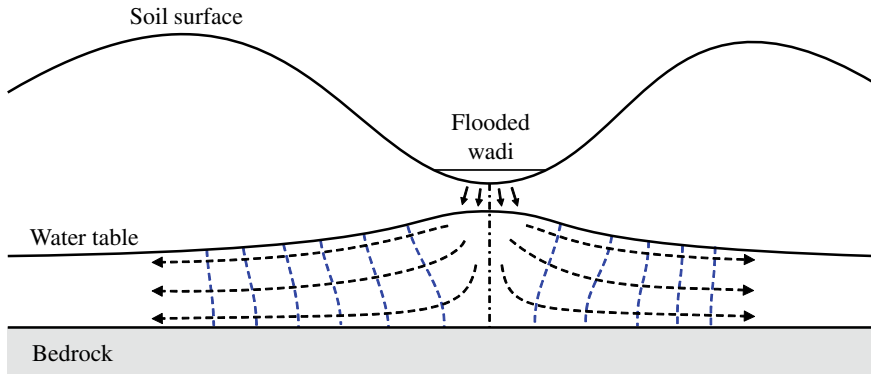


Fig. 13.3 Flow distribution in an unconfined aquifer in an arid environment (inspired by [2])

reduced. Consequently rainfall leads to surface runoff, which focuses in gulleys and channels to the main local river channel. Once the water reaches the river channel it infiltrates into the river bed deposits and recharges the underlying aquifer. Because groundwater recharge mainly occurs underneath the river channel there tends to be a groundwater mound directly underneath the river (see Fig. 13.3). In contrast to in temperate environments, groundwater in arid environments tends to flow away from river channels.

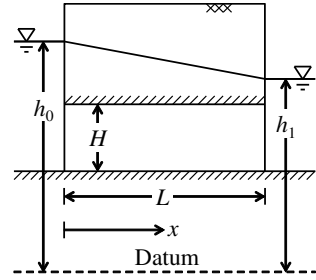
13.4 Applications of Darcy's Law

13.4.1 Confined Aquifers

Consider a steady-state horizontally orientated homogeneous confined aquifer of uniform vertical thickness, H [L], lateral thickness (i.e., thickness into the page), B [L], and hydraulic conductivity, K [LT^{-1}]. On the left-hand-side, the aquifer is bounded by an ocean where the elevation of the water level is h_0 [L] above an arbitrary datum. On the right-hand-side, the aquifer is bounded by a laterally extensive lake where the elevation of the water is h_1 [L] above an arbitrary datum. The distance along the aquifer from the ocean to the lake is L [L]. A schematic diagram of the system is shown in Fig. 13.4.

Challenge 13.1 Use Darcy's law to determine expressions for the volumetric flow rate through the aquifer and the hydraulic head distribution within the aquifer.

Fig. 13.4 Steady-state flow in a confined aquifer



Recall that Darcy's law (Eq. (12.5)) states that

$$Q = -AK \frac{dh}{dx}$$

where Q [L^3T^{-1}] is the flow rate, A [L^2] is the cross-sectional area, K [LT^{-1}] is hydraulic conductivity, h [L] is hydraulic head and x [L] is distance.

In this case, the cross-sectional area, $A = BH$ such that

$$Q = -BHK \frac{dh}{dx}$$

Integrating both sides of the above equation with respect to x leads to

$$\int Q dx = - \int BHK \frac{dh}{dx} dx$$

Because Q , B , H and K are constant, these can be moved outside of the integrals. Furthermore, the right-hand-side integral variable can be changed from x to h by the chain-rule. Therefore it can be said that

$$Q \int dx = -BHK \int dh$$

and

$$Qx = -BHKh + C$$

where C is an integration constant.

To eliminate the integration constant we need to impose one of the boundary conditions. If we choose the ocean to be at $x = 0$, then we can say that at $x = 0$, $h = h_0$ and

$$0 = -BHKh_0 + C$$

which gives that $C = BHKh_0$ and

$$Qx = BHK(h_0 - h) \quad (13.1)$$

To impose the lake boundary, we can say that $h = h_1$ at $x = L$ and therefore [3, p.146]

$$Q = \frac{BHK}{L}(h_0 - h_1) \quad (13.2)$$

Substituting Eq. (13.2) into Eq. (13.1) then leads to

$$\frac{BHKx}{L}(h_0 - h_1) = BHK(h_0 - h)$$

which after some further rearranging yields an equation describing the hydraulic head distribution within the aquifer:

$$h = h_0 - (h_0 - h_1)\frac{x}{L} \quad (13.3)$$

Often, hydrogeologists like to reduce the number of unknown parameters by replacing the product, HK , with a term known as transmissivity, $T = HK$ [L^2T^{-1}], such that Eq. (13.2) reduces further to

$$Q = \frac{BT}{L}(h_0 - h_1) \quad (13.4)$$

13.4.2 Unconfined Aquifers

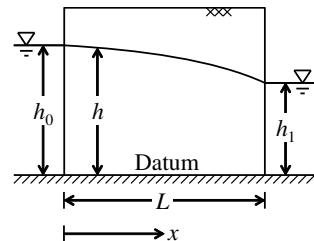
Consider a steady-state horizontally orientated homogeneous unconfined aquifer of lateral thickness (i.e., thickness into the page), B [L], and hydraulic conductivity, K [LT^{-1}]. On the left-hand-side, the aquifer is bounded by an ocean where the elevation of the water level is h_0 [L] above the base of the unconfined aquifer. On the right-hand-side, the aquifer is bounded by a laterally extensive lake where the elevation of the water is h_1 [L] above the base of the unconfined aquifer. The distance along the aquifer from the ocean to the lake is L [L]. A schematic diagram of the system is shown in Fig. 13.5.

Challenge 13.2 Use Darcy's law to determine expressions for the volumetric flow rate through the aquifer and hydraulic head distribution within the aquifer.

This problem is more complicated than the previous scenario because the aquifer thickness is not constant. Instead, the aquifer thickness is a linear function of the hydraulic head. Nevertheless, our starting point is Darcy's law:

$$Q = -AK \frac{dh}{dx}$$

Fig. 13.5 Steady-state flow in an unconfined aquifer



In this case, the cross-sectional area is found from $A = Bh$ such that

$$Q = -BhK \frac{dh}{dx}$$

Integrating both sides of the above equation with respect to x leads to

$$Q \int dx = -BK \int h dh$$

such that

$$Qx = -BK \frac{h^2}{2} + C$$

where C is an integration constant.

Choosing again the ocean to be at $x = 0$, we can say that at $x = 0$, $h = h_0$ such that $C = BK h_0^2/2$ and

$$Qx = \frac{BK}{2}(h_0^2 - h^2) \quad (13.5)$$

Imposing the lake boundary condition, $h = h_1$ at $x = L$, then yields [3, p.148]

$$Q = \frac{BK}{2L}(h_0^2 - h_1^2) \quad (13.6)$$

Substituting Eq. (13.6) into Eq. (13.5) then leads to

$$\frac{BKx}{2L}(h_0^2 - h^2) = \frac{BK}{2}(h_0^2 - h^2)$$

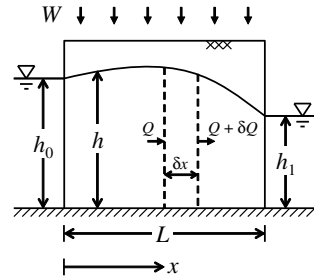
which after some further rearranging leads to an expression for the hydraulic head distribution:

$$h^2 = h_0^2 - (h_0^2 - h_1^2) \frac{x}{L} \quad (13.7)$$

13.4.3 The Dupuit-Forchheimer Assumption

An important assumption being made in Sects. 13.4.1 and 13.4.2 is that vertical flow is negligible. For the confined aquifer scenario, this assumption is consistent with our conceptual model. In contrast, for the unconfined aquifer scenario this is not exactly the case because there will be vertical flow due to the variation in aquifer thickness. However, ignoring vertical flow often leads to acceptably accurate results in this context. The assumption of negligible vertical flow in unconfined aquifers is often referred to as the Dupuit-Forchheimer assumption. Jules Dupuit and Philip Forchheimer were 19th century civil engineers interested in deriving analytical solutions for unconfined aquifer problems similar to that described above.

Fig. 13.6 Steady-state flow in an unconfined aquifer with recharge



13.4.4 Unconfined Aquifers with Recharge

Consider a steady-state horizontally orientated homogeneous unconfined aquifer of lateral thickness (i.e., thickness into the page), B [L], and hydraulic conductivity, K [LT^{-1}]. On the left-hand-side, the aquifer is bounded by an ocean where the elevation of the water level is h_0 [L] above the base of the unconfined aquifer. On the right-hand-side, the aquifer is bounded by a laterally extensive lake where the elevation of the water is h_1 [L] above the base of the unconfined aquifer. The distance along the aquifer from the ocean to the lake is L [L]. The unconfined aquifer also receives a uniform and constant recharge of water from rainfall at a rate, W [LT^{-1}] (this is a volumetric rate per unit plan area of aquifer). A schematic diagram of the system is shown in Fig. 13.6.

Challenge 13.3 Use Darcy's law to determine expressions for the volumetric flow rate through the aquifer and hydraulic head distribution within the aquifer.

This problem is more complicated than the previous scenario because the recharge gives rise to a non-uniform volumetric flow rate, Q .

To explore this further we need to consider mass conservation of water across a control-volume (CV) extracted from the aquifer. The CV is δx [L] long with a breadth and height of B and h , respectively, where h is the height of the water table above the base of the aquifer. Because the system is steady-state, the principle of mass conservation implies that the mass of water entering the CV equals the mass of water leaving the CV.

If we consider a designated time period, δt [T], we can say that the mass of water entering the CV equals $\rho Q \delta t + \rho W B \delta x \delta t$ where ρ [ML^{-3}] is the density of the water. The mass of water leaving the CV during that time equals $\rho(Q + \delta Q) \delta t$. Equating the two quantities together leads to

$$\rho Q \delta t + \rho W B \delta x \delta t = \rho(Q + \delta Q) \delta t$$

which simplifies to get

$$\frac{\delta Q}{\delta x} = BW$$

Note that

$$\lim_{\delta x \rightarrow 0} \frac{\delta Q}{\delta x} = \frac{dQ}{dx}$$

so for an infinitesimally thin CV (i.e., when $\delta x \rightarrow 0$)

$$\frac{dQ}{dx} = BW$$

Integrating both sides of the above equation leads to

$$\int \frac{dQ}{dx} dx = \int BW dx$$

Because B and W are constants these can be moved outside of the integral. Furthermore, the left-hand-side integral variable can be changed from x to Q by the chain-rule. Therefore it can be said that

$$\int dQ = BW \int dx$$

and

$$Q = BWx + C_1 \quad (13.8)$$

where C_1 is an integration constant.

Again applying the Dupuit-Forchheimer assumption, we can use Darcy's law as follows

$$Q = -AK \frac{dh}{dx}$$

where A [L^2] is cross-sectional area, K [LT^{-1}] is hydraulic conductivity and x [L] is distance.

The cross-sectional area is found from $A = Bh$ such that

$$Q = -BhK \frac{dh}{dx}$$

Substituting Eq. (13.8) then gives us

$$BWx + C_1 = -BhK \frac{dh}{dx}$$

Integrating both sides of the above equation with respect to x , bringing out the constants and changing the integration variables using the chain-rule where appropriate then allows us to say

$$BW \int x dx + C_1 \int dx = -BK \int h dh$$

from which we can obtain

$$BW \frac{x^2}{2} + C_1 x = -BK \frac{h^2}{2} + C_2$$

where C_2 is another integration constant.

Imposing the ocean boundary condition, $h = h_0$ at $x = 0$, yields

$$C_2 = BK \frac{h_0^2}{2}$$

and

$$BW \frac{x^2}{2} + C_1 x = BK \frac{(h_0^2 - h^2)}{2} \quad (13.9)$$

Imposing the lake boundary condition, $h = h_1$ at $x = L$, yields

$$BW \frac{L^2}{2} + C_1 L = BK \frac{(h_0^2 - h_1^2)}{2}$$

which can be rearranged to get

$$C_1 = BK \frac{(h_0^2 - h_1^2)}{2L} - BW \frac{L}{2}$$

Substituting the expression for C_1 into Eq. (13.8) leads to the following expression for the volumetric flow rate [3, p.150]

$$Q = B \left[K \frac{(h_0^2 - h_1^2)}{2L} + W \left(x - \frac{L}{2} \right) \right] \quad (13.10)$$

and substituting the expression for C_1 into Eq. (13.9) gives us

$$BW \frac{x^2}{2} + BK \frac{(h_0^2 - h_1^2)x}{2L} - BW \frac{Lx}{2} = BK \frac{(h_0^2 - h^2)}{2}$$

which can be simplified and solved for h to reveal that [3, p.150]

$$h^2 = h_0^2 - (h_0^2 - h_1^2) \frac{x}{L} + \frac{Wx}{K} (L - x) \quad (13.11)$$

13.5 Problem Sheet

Problem 13.1 (see Worked Solution 13.1)

A large lake drains water from the sea via a 10 km long confined sandstone aquifer. The level of the lake is 113 m below sea-level. The thickness of the aquifer is 100 m and its hydraulic conductivity is 2.2 m day^{-1} . Determine the flow rate per unit length of lake edge into the lake.

Problem 13.2 (see Worked Solution 13.2)

Determine the flow rate per unit length of lake edge into the lake for the same situation as in Problem 13.1 above but assuming the aquifer to be unconfined (such that a constant aquifer thickness no longer applies) but with no recharge, with an impermeable base at 213 m below sea-level.

Problem 13.3 (see Worked Solution 13.3)

Calculate the flow rate per unit length of lake edge into the lake for the same case given in Problem 13.2 but now assuming an aquifer recharge rate of 1 mm day^{-1} .

Problem 13.4 (see Worked Solution 13.4)

For the case depicted in Problem 13.3, there is a groundwater divide. Water on the left-hand-side drains to the sea and water on the right-hand-side drains to the lake. Calculate the distance of the divide line from the sea.

Problem 13.5 (see Worked Solution 13.5)

For the same situation again, determine the minimum recharge required to ensure water does not travel from the sea to the lake.

13.6 Worked Solutions

Worked Solution 13.1 (see Problem 13.1)

Consider the equation for steady-state flow in a confined aquifer (Eq. (13.2))

$$Q = \frac{BHK}{L}(h_0 - h_1)$$

In this case L is the distance between the sea and the lake, the $(h_0 - h_1)$ is the difference between the sea water level and lake water level, H is the thickness of the aquifer and K is the hydraulic conductivity. It follows that $L = 10,000 \text{ m}$, $(h_0 - h_1) = 113 \text{ m}$, $H = 100 \text{ m}$ and $K = 2.2 \text{ m day}^{-1}$. The flow rate per unit length of lake edge into the lake is found from

$$\frac{Q}{B} = \frac{HK(h_0 - h_1)}{L} = \frac{100 \times 2.2 \times 113}{10,000} = 2.486$$

So the flow rate per unit length of lake edge is $2.49 \text{ m}^2 \text{ day}^{-1}$.

Worked Solution 13.2 (see Problem 13.2)

Now consider the equation for steady-state flow in an unconfined aquifer (Eq. (13.6))

$$Q = \frac{BK}{2L}(h_0^2 - h_1^2)$$

For an unconfined aquifer we need to make the datum at the base of the aquifer due to the fact that h represents both the hydraulic head and the thickness of the aquifer.

Given that an impermeable base exists 213 m below sea-level, $h_0 = 213$ m.

Given that $(h_0 - h_1) = 113$ m, $h_1 = 213 - 113 = 100$ m.

It follows that

$$\frac{Q}{B} = \frac{K(h_0^2 - h_1^2)}{2L} = \frac{2.2 \times (213^2 - 100^2)}{2 \times 10,000} = 3.891$$

So the flow rate per unit length of lake edge is $3.90 \text{ m}^2 \text{ day}^{-1}$.

Worked Solution 13.3 (see Problem 13.3)

Now consider the equation for steady-state flow in an unconfined aquifer with recharge (Eq. (13.10))

$$Q = B \left[K \frac{(h_0^2 - h_1^2)}{2L} + W \left(x - \frac{L}{2} \right) \right]$$

All the parameters are the same as in Problem 13.2 except that also $W = 0.001 \text{ m day}^{-1}$. Because we have chosen (in this case) that the lake is located where $h = h_1$, it follows that $x = 10,000$ m and

$$\frac{Q}{B} = 3.891 + 0.001 \left(10,000 - \frac{10,000}{2} \right) = 8.891$$

So the flow rate per unit length of lake edge is $8.89 \text{ m}^2 \text{ day}^{-1}$.

Worked Solution 13.4 (see Problem 13.4)

The groundwater divide occurs where $Q = 0$. The location of the groundwater divide is the x value that satisfies Eq. (13.10) when $Q = 0$:

$$0 = B \left[K \frac{(h_0^2 - h_1^2)}{2L} + W \left(x - \frac{L}{2} \right) \right]$$

Solving for x then leads to

$$x = \frac{L}{2} - \frac{K}{W} \frac{(h_0^2 - h_1^2)}{2L} = \frac{10,000}{2} - \frac{2.2}{0.001} \frac{(213^2 - 100^2)}{2 \times 10,000} = 1109$$

So the groundwater divide exists 1100 m from the sea.

Worked Solution 13.5 (see Problem 13.5)

The minimum recharge rate, $W_{\min}$, corresponds to that which leads to the groundwater divide moving back to the sea, at $x = 0$. From the equation above it therefore follows that

$$0 = \frac{L}{2} - \frac{K}{W_{\min}} \frac{(h_0^2 - h_1^2)}{2L}$$

which on rearranging yields

$$\begin{aligned} W_{\min} &= \frac{2K}{L} \frac{(h_0^2 - h_1^2)}{2L} \\ &= \frac{2 \times 2.2}{10,000} \frac{(213^2 - 100^2)}{2 \times 10,000} \\ &= 7.781 \times 10^{-4} \text{ m day}^{-1} \end{aligned}$$

So the minimum recharge rate is 0.778 mm day⁻¹.

Interestingly, even though the groundwater divide was originally 1.1 km from the sea, a reduction of recharge rate by 22% leads to saline intrusion of an otherwise freshwater lake.

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Steady-State Radial Flow to Wells

14

Abstract

This chapter is concerned with the derivation and application of analytical solutions for describing steady-state groundwater flow around production and injection wells. We derive the Thiem equation for steady-state flow to a production well in a homogeneous and isotropic confined aquifer of infinite lateral extent. The principle of superposition is invoked to account for the co-existence of multiple production and injection wells. The method of images is explained, whereby fixed head and impermeable boundaries are represented by superimposing image wells. It is demonstrated how to use a step-drawdown test to simultaneously determine the formation loss and well loss coefficients of a given aquifer. The Forchheimer equation is used to derive an analytical solution for steady-state, non-Darcian flow to a production well or injection well. Practical applications are presented through a problem sheet with worked solutions.

Notation

a	Distance of a well from an aquifer boundary [L].
A	Cross-sectional area [L ²].
A_J	Formation loss coefficient [L ⁻² T].
b	Forchheimer parameter [L ⁻¹].
B_J	Well-loss coefficient [L ⁻⁵ T ²].
c	Intercept of a straight line.
g	Gravitational acceleration [LT ⁻²].
h	Hydraulic head [L].
h_e	Unperturbed hydraulic head [L].
h_w	Hydraulic head at a production well [L].
H	Formation thickness [L].
k	Permeability [L ²].
K	Hydraulic conductivity [LT ⁻¹].

q	Darcy flux [LT^{-1}].
Q	Flow rate [L^3T^{-1}].
Q_w	Production rate [L^3T^{-1}].
Q_{wn}	Production rate from the n th well [L^3T^{-1}].
r	Radial distance from well [L].
r_e	Radius of influence [L].
r_i	Radial distance from an image well [L].
r_n	Radial distance from the n th well [L].
r_p	Radial distance from a production well [L].
r_w	Radius of well [L].
t	Time [T].
T	Transmissivity [L^2T^{-1}].
x_0	Location of an observation point on the x -axis [L].
x_n	Location of the n th well on the x -axis [L].
y_0	Location of an observation point on the y -axis [L].
y_n	Location of the n th well on the y -axis [L].
η	Piezometric drawdown [L].
η_i	Drawdown due to an image well [L].
η_n	Drawdown due to the n th well [L].
η_p	Drawdown due to a production well [L].
η_w	Drawdown at a production well [L].
μ	Dynamic viscosity of water [$\text{ML}^{-1}\text{T}^{-1}$].
ρ	Fluid density [ML^{-3}].

14.1 Introduction

The main way that societies interact with aquifers is through water production wells. When a well is pumped to produce groundwater from an aquifer, the water level in the well is drawn down and a cone of depression in hydraulic head evolves around the well.

If an aquifer is homogeneous and isotropic (i.e., its properties do not vary in space and direction) the cone of depression will be perfectly circular in cross-section. Furthermore, the hydraulic head around the well will be radially symmetric about the axis of the well. In this chapter, the assumption of radial symmetry is imposed and an analytical solution, known as the Thiem equation, is derived to describe steady-state flow to a production well.

The Thiem equation assumes the production well of concern is situated within a confined aquifer of infinite horizontal extent. However, it will be shown that fixed hydraulic head boundaries and impermeable boundaries can be incorporated by utilizing the so-called method of images, which comes about from the principle of superposition.

Following on from this, the implications of step-drawdown tests are discussed, which show that the relationship between production rate and drawdown of hydraulic

head is non-linear. This implies that Darcy's law is inadequate for describing groundwater processes around fast flowing pumped wells. A non-linear correction to Darcy's law, known as the Forchheimer equation, is reintroduced. The Thiem equation is then re-derived, using the Forchheimer equation, to incorporate so-called non-Darcian well losses.

14.2 The Thiem Equation

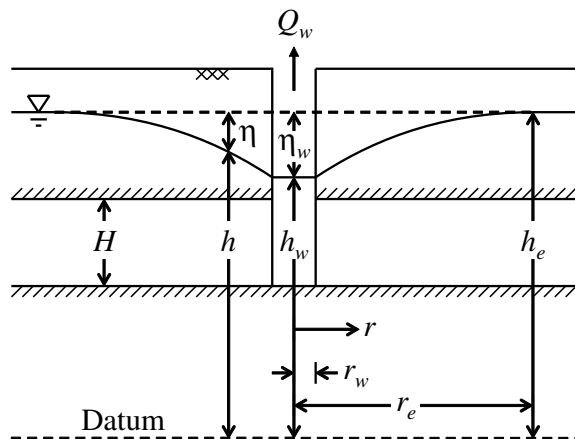
Water is produced at a steady-state rate, Q_w [L^3T^{-1}], from a fully penetrating production well within a homogeneous and isotropic confined aquifer of infinite lateral extent (see Fig. 14.1). The aquifer has a uniform thickness of H [L] and a hydraulic conductivity of K [LT^{-1}]. The production well has a radius of influence, r_e [L], beyond which the aquifer is unaffected by the pumped well and the hydraulic head is fixed to its unperturbed value, denoted h_e [L]. The drawdown in hydraulic head (referred to hereafter as the piezometric drawdown), η [L], due to the pumping well is defined as $\eta = h_e - h$.

Challenge 14.1 Use Darcy's law to determine an expression for the piezometric drawdown as a function of radial distance from the production well.

From Darcy's law (Eq. (12.5)) we have that

$$Q = -AK \frac{dh}{dr}$$

Fig. 14.1 Schematic diagram of radial flow to a production well in a confined aquifer



where Q [L^3T^{-1}] is the volumetric flow rate, A [L^2] is cross-sectional area, K [LT^{-1}] is hydraulic conductivity, h [L] is hydraulic head and r [L] is distance from the production well.

The cross-sectional area in this case is

$$A = 2\pi Hr$$

such that

$$Q = -2\pi HKr \frac{dh}{dr}$$

Before integrating the above equation it is important to separate out the two different variables: h and r . Bringing the r -factors on the left-hand-side and the h -factors on the right-hand-side leads to

$$\frac{Q}{r} = -2\pi HK \frac{dh}{dr}$$

Integrating both sides of the above equation with respect to r , bringing out the constant values from the integrals and changing the integral variable using the chain-rule where appropriate leads to

$$Q \int \frac{1}{r} dr = -2\pi HK \int dh$$

from which it can be seen that

$$Q \ln r = -2\pi HK h + C \quad (14.1)$$

where C is an integration constant.

To eliminate the integration constant we need to impose a boundary condition. In particular, we know that $h = h_e$ at $r = r_e$. Therefore

$$C = Q \ln r_e + 2\pi HK h_e \quad (14.2)$$

Substituting Eq. (14.2) into Eq. (14.1) leads to

$$h_e - h = \frac{Q}{2\pi HK} (\ln r - \ln r_e)$$

Knowing that $\ln A - \ln B = \ln\left(\frac{A}{B}\right)$ it follows that

$$h_e - h = \frac{Q}{2\pi HK} \ln\left(\frac{r}{r_e}\right)$$

By piezometric drawdown, what is meant is the extent to which the hydraulic head has been perturbed by the existence of the pumping well. Let η [L] be the piezometric drawdown in the aquifer, defined by $\eta = h_e - h$. Then

$$\eta = \frac{Q}{2\pi HK} \ln\left(\frac{r}{r_e}\right)$$

The next step is to recognize that the production well is producing water at a positive rate of Q_w . But when Q is positive, water movement is positive in the r

direction and therefore a positive Q amounts to a negative production rate. It can therefore be understood that $Q = -Q_w$ and [1, p.153]

$$\eta = \frac{Q_w}{2\pi HK} \ln \left(\frac{r_e}{r} \right)$$

Finally, it is worth to substitute the expression for the transmissivity, $T = HK$, simplifying our equation further to

$$\eta = \frac{Q_w}{2\pi T} \ln \left(\frac{r_e}{r} \right) \quad (14.3)$$

which is known as the Thiem equation.

14.3 Applying the Principle of Superposition

The Thiem equation describes piezometric drawdown around a single production well. However, because the equation represents a linear relationship between drawdown and production rate, it is possible to simulate the presence of multiple interacting wells using the principle of superposition.

The principle of superposition is the idea that, for linear systems, the net response caused by two or more simultaneous perturbations is equal to the sum of the responses that would have occurred by each perturbation individually. Note that the Thiem equation is considered a linear function in this context because η is a linear function of Q_w . The principle of superposition does not apply to non-linear systems.

The principle of superposition can be applied to the Thiem equation to study the response of different combinations of multiple production and/or injection wells as follows. Let x and y represent a Cartesian coordinate system within our laterally extensive and horizontally orientated confined aquifer. Now let (x_n, y_n) represent the coordinates of the n th production well, which is producing water at a rate of Q_{wn} . The drawdown at a location (x_0, y_0) due to the presence of the n th well by itself can be found from (recall the Thiem equation)

$$\eta_n = \frac{Q_{wn}}{2\pi T} \ln \left(\frac{r_e}{r_n} \right) \quad (14.4)$$

where

$$r_n = \sqrt{(x_0 - x_n)^2 + (y_0 - y_n)^2} \quad (14.5)$$

The drawdown, η , resulting from the composite response of N different production wells can be found from

$$\eta(x_0, y_0) = \sum_{n=1}^N \eta_n(x_0, y_0) \quad (14.6)$$

Note that injection wells can be included by incorporating additional production wells with negative production rates.

14.4 Method of Images

In what follows it will be shown that the principle of superposition can also be used to simulate the presence of fixed hydraulic head boundaries or impermeable boundaries.

14.4.1 Fixed Hydraulic Head Boundaries

Water is produced from one well at a rate of Q_p , whilst water is injected at a rate of Q_p into a neighbouring injection well (see Fig. 14.2). The production well is located at $x = a$ and $y = 0$. The injection well is located at $x = -a$ and $y = 0$.

Challenge 14.2 Obtain an expression for the drawdown due to the presence of both wells as a function of x_0 and y_0 . Also, determine the value of drawdown as a function of y_0 when $x_0 = 0$.

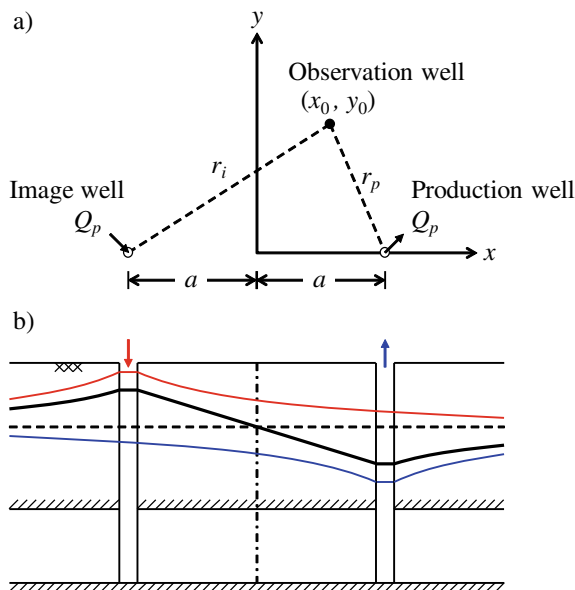


Fig. 14.2 Application of method of images to force a fixed-head boundary along the y -axis. The image well is an injection well injecting at the same rate as the production well produces. **a** Shows a plan view. **b** Shows a section. The blue line shows the piezometric surface due to the production well pumping by itself. The red line shows the piezometric surface due to the injection well pumping by itself. The horizontal dashed black line shows the level of the original unperturbed piezometric surface. The thicker black line shows the composite response of both the production well and the injection well. Note that the composite piezometric surface is unperturbed at $x = 0$

Let η_p be the drawdown due to the production well by itself such that, from the Thiem equation

$$\eta_p = \frac{Q_p}{2\pi T} \ln \left(\frac{r_e}{r_p} \right)$$

where r_p is the distance from the production well to some arbitrary point (x_0, y_0) found from (consider Eq. (14.5) when $r_n = r_p$, $x_n = a$ and $y_n = 0$)

$$r_p = \sqrt{(x_0 - a)^2 + y_0^2}$$

such that it can be said that

$$\eta_p = \frac{Q_p}{2\pi T} \ln \left(\frac{r_e}{\sqrt{(x_0 - a)^2 + y_0^2}} \right)$$

Let η_i be the drawdown due to the injection well by itself such that, from the Thiem equation (note that $Q_w = -Q_p$ in this case),

$$\eta_i = -\frac{Q_p}{2\pi T} \ln \left(\frac{r_e}{r_i} \right)$$

where r_i is the distance from the production well to some arbitrary point (x_0, y_0) found from (consider Eq. (14.5) when $r_n = r_i$, $x_n = -a$ and $y_n = 0$)

$$r_i = \sqrt{(x_0 + a)^2 + y_0^2}$$

such that it can be said that

$$\eta_i = -\frac{Q_p}{2\pi T} \ln \left(\frac{r_e}{\sqrt{(x_0 + a)^2 + y_0^2}} \right)$$

The composite response is found from [1, p.182]

$$\begin{aligned} \eta &= \eta_p + \eta_i \\ &= \frac{Q_p}{2\pi T} \left[\ln \left(\frac{r_e}{\sqrt{(x_0 - a)^2 + y_0^2}} \right) - \ln \left(\frac{r_e}{\sqrt{(x_0 + a)^2 + y_0^2}} \right) \right] \\ &= \frac{Q_p}{2\pi T} \ln \left(\frac{\sqrt{(x_0 + a)^2 + y_0^2}}{\sqrt{(x_0 - a)^2 + y_0^2}} \right) \end{aligned}$$

and for $x_0 = 0$

$$\eta(0, y_0) = \frac{Q_p}{2\pi T} \ln \left(\sqrt{\frac{a^2 + y_0^2}{a^2 + y_0^2}} \right) = \frac{Q_p}{2\pi T} \ln 1 = 0$$

So it can be seen that there is a line of zero drawdown that runs down the centre of the two wells (Fig. 14.2b). The reason is that, along the line $x_0 = 0$, water is replaced by the injection well at the same rate it is extracted by the production well.

Such a system can be used to extend the Thiem equation to account for the presence of fixed-head boundaries (equivalent to zero drawdown) associated with rivers or lakes.

Suppose we have a production well at a distance, a , from a river. The river can be treated as a zero drawdown boundary and represented by superimposing an image well, that injects at the same rate that water is produced at the production well, at a distance, a , from the other side of the river (i.e., $x_0 = -a$ as in the example above). This idea is known as the method of images.

14.4.2 Impermeable Boundaries

Two wells simultaneously produce water at a rate of Q_p (see Fig. 14.3). The first production well is located at $x = a$ and $y = 0$. The second production well is located at $x = -a$ and $y = 0$.

Challenge 14.3 Obtain an expression for the drawdown due to the presence of both wells as a function of x_0 and y_0 . Also, determine the derivative, $\partial\eta/\partial x_0$, as a function of y_0 when $x_0 = 0$.

Let η_p be the drawdown due to the first production well by itself such that, as with the previous scenario above,

$$\eta_p = \frac{Q_p}{2\pi T} \ln \left(\frac{r_e}{\sqrt{(x_0 - a)^2 + y_0^2}} \right)$$

Let η_i be the drawdown due to the second production well by itself such that, similar to the previous scenario above (but note that this time $Q_w = Q_p$),

$$\eta_i = \frac{Q_p}{2\pi T} \ln \left(\frac{r_e}{\sqrt{(x_0 + a)^2 + y_0^2}} \right)$$

The composite response is found from

$$\begin{aligned} \eta &= \eta_p + \eta_i \\ &= \frac{Q_p}{2\pi T} \ln \left(\frac{r_e}{\sqrt{(x_0 - a)^2 + y_0^2}} \right) + \frac{Q_p}{2\pi T} \ln \left(\frac{r_e}{\sqrt{(x_0 + a)^2 + y_0^2}} \right) \\ &= \frac{Q_p}{4\pi T} \ln \left(\frac{r_e^4}{[(x_0 + a)^2 + y_0^2][(x_0 - a)^2 + y_0^2]} \right) \end{aligned}$$

Now we will study $\left. \frac{\partial\eta}{\partial x_0} \right|_{x_0=0}$. To differentiate η with respect to x_0 it is worth to breakdown the above equation again to get

$$\eta = \frac{Q_p}{4\pi T} [\ln r_e^4 - \ln((x_0 + a)^2 + y_0^2) - \ln((x_0 - a)^2 + y_0^2)]$$

Noting that

$$\frac{\partial}{\partial x_0} [\ln((x_0 + a)^2 + y_0^2)] = \frac{2(x_0 + a)}{(x_0 + a)^2 + y_0^2}$$

and

$$\frac{\partial}{\partial x_0} [\ln((x_0 - a)^2 + y_0^2)] = \frac{2(x_0 - a)}{(x_0 - a)^2 + y_0^2}$$

it follows that

$$\frac{\partial \eta}{\partial x_0} = -\frac{Q_p}{4\pi T} \left[\frac{2(x_0 + a)}{(x_0 + a)^2 + y_0^2} + \frac{2(x_0 - a)}{(x_0 - a)^2 + y_0^2} \right]$$

and

$$\left. \frac{\partial \eta}{\partial x_0} \right|_{x_0=0} = 0$$

The presence of a line of zero gradient at $x_0 = 0$ (Fig. 14.3b) points towards the idea that we can use the method of images to represent an impermeable boundary. In this case, if we had a production well at a distance a from a laterally extensive

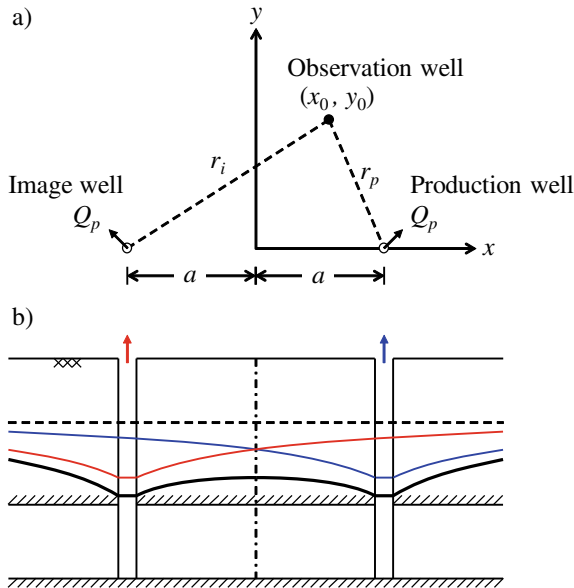


Fig. 14.3 Application of method of images to force an impermeable boundary along the y -axis. The image well is a production well producing at the same rate as the real production well. **a** Shows a plan view. **b** Shows a section. The blue line shows the piezometric surface due to the real production well pumping by itself. The red line shows the piezometric surface due to the image well pumping by itself. The horizontal dashed black line shows the level of the original unperturbed piezometric surface. The thicker black line shows the composite response of both production wells. Note that the composite piezometric surface exhibits a zero-gradient at $x = 0$

impermeable boundary, this can be imposed by superimposing the effect of an imaginary production well, producing at the same rate as the real production well, at a distance a from the other side of the impermeable boundary (i.e., $x_0 = -a$ as in the example above).

Summary

The method of images involves superimposing the effects of image wells to represent different types of boundaries when studying flow around production or injection wells using linear equations such as the Thiem equation. Image wells should be located on the other side of the boundary such that their location represents a reflection of the production wells. To represent a fixed head boundary, superimpose an image well that injects at the same rate as the production well produces. To represent an impermeable boundary, superimpose an image well that produces at the same rate as the production well.

14.5 Step-Drawdown Tests

A common way to test a well is to pump it at sequentially increasing rates. This is often referred to as a step-drawdown test because the production rate is increased in a sequence of steps (Fig. 14.4a).

When the production rate is increased the drawdown increases until a steady-state level is reached (Fig. 14.4b). According to the Thiem equation, steady-state drawdowns should plot against production rate as a straight line. However, instead it is found that drawdown follows a quadratic equation (see Fig. 14.4c), known as Jacob's equation [2]

$$\eta_w = A_J Q_w + B_J Q_w^2 \quad (14.7)$$

where η_w [L] is the drawdown in the production well, A_J [$L^{-2}T$] is referred to as a formation loss coefficient and B_J [$L^{-5}T^2$] is referred to as a well-loss coefficient.

The A_J and B_J coefficients are typically obtained by plotting η_w/Q_w against Q_w such that A_J and B_J are the intercept and slope of a best fit straight line, respectively (see Fig. 14.4d).

The value of the well-loss coefficient is traditionally associated with the quality of the production well infrastructure (see Table 14.1). However, an alternative explanation is that the associated non-linearity could be caused by non-Darcian flow (see Sect. 12.8) within the aquifer itself [4].

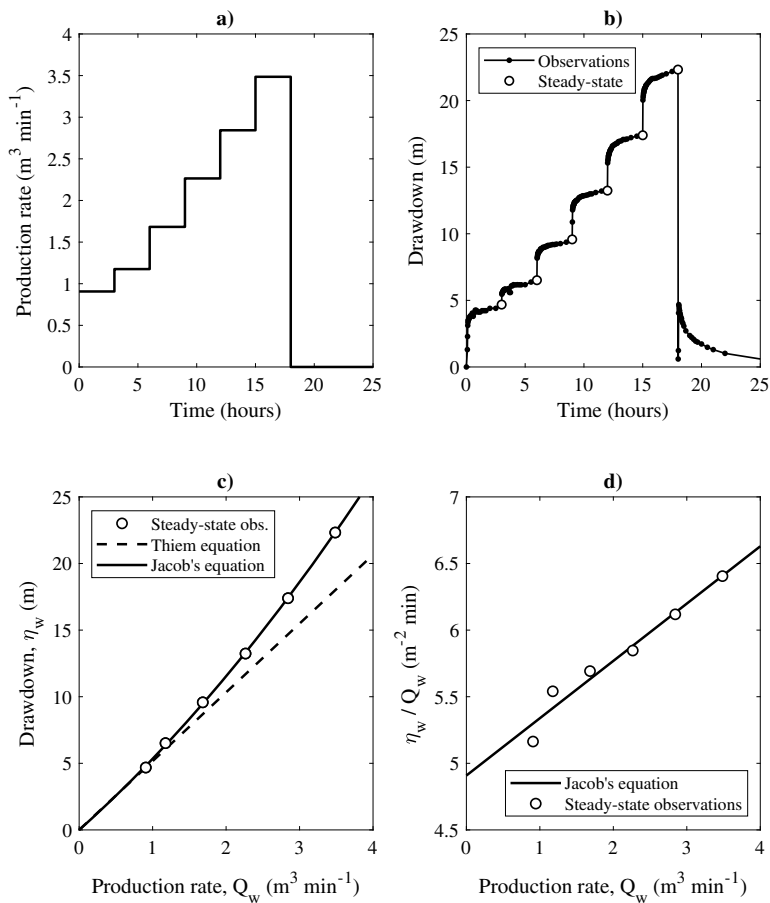


Fig. 14.4 Step-drawdown test results from a groundwater well in Saudi Arabia (observed data acquired from [3])

Table 14.1 Assessment of well-loss coefficient, B_J , from step-drawdown tests according to [5]

B_J ($\text{m}^{-5} \text{min}^2$)	Well condition
< 0.5	Properly developed and designed
0.5 to 1.0	Mild deterioration
1.0 to 5.0	Clogging is severe
> 5.0	Beyond rehabilitation

14.6 Steady-State Non-darcian Flow to a Well

Challenge 14.4 Consider again the conceptual model used to derive the Thiem equation in Sect. 14.2. Now use the Forchheimer equation (Eq. (12.26)) to determine an expression for the piezometric drawdown as a function of radial distance from the production well.

From the Forchheimer equation (Eq. (12.26)) we have that

$$\frac{\partial h}{\partial r} = -\frac{\mu q}{\rho g k} - \frac{b|q|q}{g}$$

where μ is dynamic viscosity [$\text{ML}^{-1}\text{T}^{-1}$], ρ [ML^{-3}] is fluid density, g [LT^{-2}] is gravitational acceleration, k [L^2] is permeability and b [L^{-1}] is the Forchheimer parameter.

Recognizing that $Q = Aq$, where Q [L^3T^{-1}] is the volumetric flow rate and A [L^2] is cross-sectional area, it can then be said that

$$\frac{\partial h}{\partial r} = -\frac{\mu Q}{\rho g k A} - \frac{b|Q|Q}{g A^2}$$

As before, the cross-sectional area is

$$A = 2\pi H r$$

so

$$\frac{\partial h}{\partial r} = -\frac{\mu Q}{2\pi \rho g k H r} - \frac{b|Q|Q}{(2\pi H r)^2 g}$$

Integrating both sides of the above equation with respect to r , bringing out the constant values from the integrals and changing the integral variable using the chain-rule where appropriate leads to

$$\int dh = -\frac{\mu Q}{2\pi \rho g k H} \int \frac{1}{r} dr - \frac{b|Q|Q}{(2\pi H)^2 g} \int \frac{1}{r^2} dr$$

from which it can be seen that

$$h = -\frac{\mu Q}{2\pi \rho g k H} \ln r + \frac{b|Q|Q}{(2\pi H)^2 g r} + C \quad (14.8)$$

where C is an integration constant.

To eliminate the integration constant we need to impose a boundary condition. In particular, we know that $h = h_e$ at $r = r_e$. Therefore

$$C = h_e + \frac{\mu Q}{2\pi \rho g k H} \ln r_e - \frac{b|Q|Q}{(2\pi H)^2 g r_e} \quad (14.9)$$

Substituting Eq. (14.9) into Eq. (14.8) leads to

$$h_e - h = \frac{\mu Q}{2\pi \rho g k H} \ln \left(\frac{r}{r_e} \right) - \frac{b|Q|Q}{(2\pi H)^2 g} \left(\frac{1}{r} - \frac{1}{r_e} \right)$$

Letting η [L] be the piezometric drawdown in the aquifer, defined by $\eta = h_e - h$, it can then be said that

$$\eta = \frac{\mu Q}{2\pi\rho g k H} \ln\left(\frac{r}{r_e}\right) - \frac{b|Q|Q}{(2\pi H)^2 g} \left(\frac{1}{r} - \frac{1}{r_e}\right)$$

The next step is to recognize that the production well is producing water at a positive rate of Q_w . So $Q = -Q_w$ and

$$\eta = \frac{\mu Q_w}{2\pi\rho g k H} \ln\left(\frac{r_e}{r}\right) + \frac{bQ_w^2}{(2\pi H)^2 g} \left(\frac{1}{r} - \frac{1}{r_e}\right) \quad (14.10)$$

Finally, it is worth to substitute the expression for the hydraulic conductivity (Eq. (12.23)), $K = \frac{\rho g k}{\mu}$, and transmissivity, $T = HK$, for further simplification such that it can be said that

$$\eta = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r}\right) + \frac{b}{g} \left(\frac{Q_w}{2\pi H}\right)^2 \left(\frac{1}{r} - \frac{1}{r_e}\right) \quad (14.11)$$

which is a non-Darcian form of the Thiem equation.

Comparison with Jacob's Equation

Noting that $\eta = \eta_w$ when $r = r_w$, where r_w is the production well radius, it further follows that

$$\eta_w = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r_w}\right) + \frac{b}{g} \left(\frac{Q_w}{2\pi H}\right)^2 \left(\frac{1}{r_w} - \frac{1}{r_e}\right)$$

which, by comparison with Jacob's equation (Eq. (14.7)), suggests that the formation loss coefficient and the well loss coefficient are found from (similar to [4])

$$A_J = \frac{1}{2\pi T} \ln\left(\frac{r_e}{r_w}\right) \quad \text{and} \quad B_J = \frac{b}{g} \left(\frac{1}{2\pi H}\right)^2 \left(\frac{1}{r_w} - \frac{1}{r_e}\right) \quad (14.12)$$

Substituting the above expression for the well-loss coefficient back into Eq. (14.11) leads to

$$\eta = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r}\right) + B_J Q_w^2 \left(\frac{r_e - r}{r_e - r_w}\right) \frac{r_w}{r}$$

from which it can be understood that the effect of the non-Darcian well-losses becomes decreasingly significant with increasing radial distance from the production well. This is because the fluid velocities are becoming smaller with increasing distance from the well.

14.7 Problem Sheet

Problem 14.1 (see Worked Solution 14.1)

A production well, of 0.1 m diameter, produces water from a confined aquifer at a constant rate of $0.074 \text{ m}^3\text{s}^{-1}$. The piezometric drawdown is monitored in two observation wells located 6 m and 46 m from the production well, respectively. The drawdown in the nearest observation well is 1.82 m whereas the drawdown in the well furthest away is 0.40 m. Use the Thiem equation to calculate the transmissivity and radius of influence of the aquifer along with the drawdown in the production well.

Problem 14.2 (see Worked Solution 14.2)

Consider again the scenario from the previous problem. Now $0.037 \text{ m}^3\text{s}^{-1}$ is produced from the original production well whilst an additional $0.037 \text{ m}^3\text{s}^{-1}$ is produced from the observation well located 6 m away. Determine the resulting drawdown in both production wells.

Problem 14.3 (see Worked Solution 14.3)

A chocolate factory is currently producing $285 \text{ m}^3\text{day}^{-1}$ from a pumping well situated 1.5 km from a river. The production well fully penetrates a confined aquifer of 15 m thickness with a hydraulic conductivity of 0.0002 m s^{-1} . The aquifer is known to be hydraulically connected to the river. The Environment Agency (EA) has stipulated that beyond 2 km from the well, the piezometric surface in the aquifer must not be lowered by more than 0.5 m. Estimate the maximum drawdown 2 km from the well and forecast whether the EA's stipulation is being satisfied.

Problem 14.4 (see Worked Solution 14.4)

A solar thermal plant situated on the outskirts of Los Angeles is seeking a new water supply for its cooling towers. The current plan is to produce water from an extensive confined aquifer that lies beneath the plant location. A regional hydrogeological report suggests the aquifer has a transmissivity of around $1300 \text{ m}^2\text{day}^{-1}$. However, of concern is that the aquifer is bounded by a laterally extensive vertically oriented impermeable fault zone, which lies 1800 m from the proposed production well location. The Environment Protection Agency has stipulated that drawdown should not exceed 15 cm within 100 m of the fault zone. Assuming a radius of influence of 3000

m, estimate the maximum allowable water production rate that can be achieved from the proposed production well.

Problem 14.5 (see Worked Solution 14.5)

As part of a drought mitigation programme, a water company is planning to produce water from a previously abandoned 0.1 m diameter production well. A step-drawdown test is performed to assess feasibility. The following results are obtained:

Production rate ($\text{m}^3\text{min}^{-1}$)	0.139	0.278	0.417	0.556
Final drawdown (cm)	91.5	197	315	447

- (a) Use the Jacob equation to determine the formation loss coefficient and the well-loss coefficient.
- (b) Calculate the transmissivity of the aquifer assuming a radius of influence of 8 km.

14.8 Worked Solutions

Worked Solution 14.1 (see Problem 14.1)

From the Thiem equation we have that

$$\eta = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r}\right)$$

where η is drawdown, Q_w is production rate, T is transmissivity, r_e is the radius of influence and r is radial distance from the production well.

In this case we have results from two drawdown measurements, η_1 and η_2 , from locations r_1 and r_2 , respectively, such that it can be said that

$$\eta_1 = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r_1}\right)$$

and

$$\eta_2 = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r_2}\right)$$

From the data given, we have that the radius of the well, $r_w = 0.05$ m, $Q_w = 0.074$ m^3s^{-1} , $r_1 = 6$ m, $r_2 = 46$ m, $\eta_1 = 1.82$ m and $\eta_2 = 0.40$ m. It follows that:

$$T = \frac{Q_w}{2\pi(\eta_1 - \eta_2)} \ln\left(\frac{r_2}{r_1}\right) = 0.01689 = 0.0169 \text{ m}^2 \text{ s}^{-1}$$

$$r_e = r_1 \exp\left(\frac{2\pi T \eta_1}{Q_w}\right) = 81.60 = 81.6 \text{ m}$$

and

$$\eta_w = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r_w}\right) = 5.158 = 5.16 \text{ m}$$

where η_w is the drawdown in the well.

Worked Solution 14.2 (see Problem 14.2)

The principle of superposition can be used to represent the presence of multiple wells.

First determine the drawdown in the original production well assuming that it produces by itself

$$\eta_w = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r_w}\right) = \frac{0.037}{2\pi \times 0.01689} \ln\left(\frac{81.60}{0.05}\right) = 2.579 \text{ m}$$

Next determine the drawdown in the original production well assuming that the new production well is producing by itself

$$\eta = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r}\right) = \frac{0.037}{2\pi \times 0.01689} \ln\left(\frac{81.60}{6}\right) = 0.9100 \text{ m}$$

According to the principle of superposition, the drawdown expected in the production well when both wells are pumping simultaneously can be found by adding together the two individual responses. So the drawdown in the original production well will be $2.579 + 0.9100 = 3.489 = 3.49 \text{ m}$. The drawdown in the other production well will also be 3.49 m because both wells are pumping at the same rate.

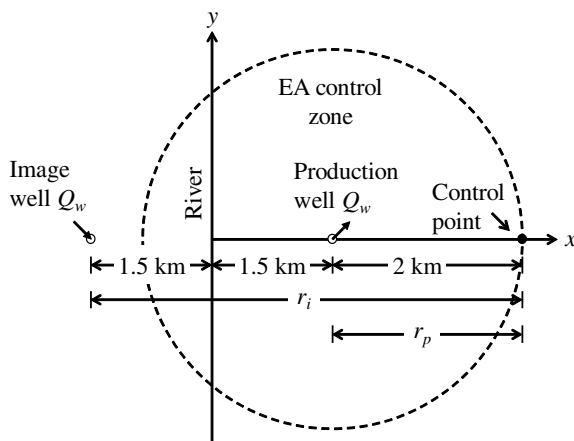
It is interesting to see that the same amount of water is being produced from the aquifer in both Problems 14.1 and 14.2. However, by distributing the production between two wells located 6 m apart, the piezometric drawdown has been reduced by 32.4%.

Worked Solution 14.3 (see Problem 14.3)

Solving this problem involves applying the method of images. The river can be treated as a fixed-head boundary. To represent the fixed-head boundary, the image well needs to do the opposite of what the actual well is doing. In this case the actual well is a production well so the image well needs to be an injection well.

We are interested in verifying that the drawdown does not exceed 0.5 m within a 2 km radius of the production well. This zone is shown as a dashed circle in Fig. 14.5. The drawdown will vary along the circle starting from zero at the river and then reaching a maximum value at the furthestest point from the river, which is denoted as the control point in Fig. 14.5. First we need to calculate the drawdown at the control

Fig. 14.5 Plan view of a production well with an image well present to represent a fixed-head boundary associated with a river



point due to the production well by itself and then the image well by itself, both using the Thiem equation. Finally, we will add the two drawdowns together to determine the drawdown at the control point due to the production well in the presence of the river.

The drawdown due to the production well is found from

$$\eta_p = \frac{Q_w}{2\pi T} \ln \left(\frac{r_e}{r_p} \right)$$

The drawdown due to the image well is found from (notice the negative sign needed because this well is injecting)

$$\eta_i = -\frac{Q_w}{2\pi T} \ln \left(\frac{r_e}{r_i} \right)$$

The drawdown due to the production well in the presence of the river is found from

$$\begin{aligned} \eta &= \eta_p + \eta_i \\ &= \frac{Q_w}{2\pi T} \ln \left(\frac{r_e}{r_p} \right) - \frac{Q_w}{2\pi T} \ln \left(\frac{r_e}{r_i} \right) \\ &= \frac{Q_w}{2\pi T} \ln \left(\frac{r_i}{r_p} \right) \end{aligned}$$

From the data provided in Problem 14.3:

$$Q_w = 285 \text{ m}^3 \text{ day}^{-1},$$

$$r_i = 3000 + 2000 = 5000 \text{ m},$$

$$r_p = 2000 \text{ m}$$

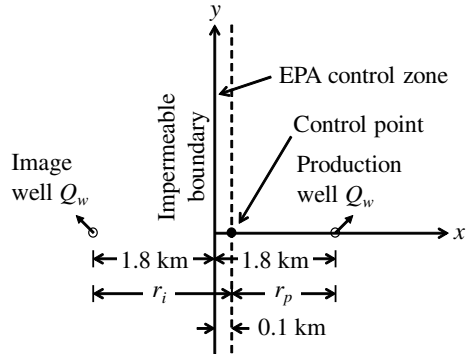
$$T = KH = 0.0002 \times 15 = 0.003 \text{ m}^2 \text{ s}^{-1} = 259.2 \text{ m}^2 \text{ day}^{-1}$$

It follows that

$$\eta = \frac{285}{2\pi \times 259.2} \ln \left(\frac{5000}{2000} \right) = 0.1604 = 0.160 \text{ m}$$

which is less than 0.5 m so the scheme should be satisfactory.

Fig. 14.6 Plan view of a production well with an image well present to represent an impermeable boundary associated with a fault zone



Worked Solution 14.4 (see Problem 14.4)

We need to use the method of images again. However, this time, the image well needs to be a production well because we are trying to represent an impermeable boundary.

We are interested in verifying that the drawdown does not exceed 0.15 m within a 100 m of the fault zone. The area of interest is bounded by a dashed line in Fig. 14.6. The drawdown will increase with decreasing distance from the production well. The location of maximum drawdown within the control zone is labelled as the control point in Fig. 14.6. As before, we need to determine an equation for the drawdown at the control point due to the production well by itself and then due to the image well by itself, both using the Thiem equation. We then need to add the two drawdowns together to determine an equation for the drawdown at the control point due to the production well in the presence of the impermeable boundary. This equation can be rearranged to determine the production rate that would give rise to a composite drawdown of 0.15 m.

The drawdown due to the production well is

$$\eta_p = \frac{Q_w}{2\pi T} \ln \left(\frac{r_e}{r_p} \right)$$

The drawdown due to the image well is (notice there is no negative sign here because the image well is also producing)

$$\eta_i = \frac{Q_w}{2\pi T} \ln \left(\frac{r_e}{r_i} \right)$$

The drawdown due to the production well in the presence of the impermeable boundary is

$$\begin{aligned}\eta &= \eta_p + \eta_i \\ &= \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r_p}\right) + \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r_i}\right) \\ &= \frac{Q_w}{2\pi T} \ln\left(\frac{r_e^2}{r_p r_i}\right)\end{aligned}$$

From the data provided in Problem 14.4:

$$\begin{aligned}\eta &= 0.15 \text{ m,} \\ T &= 1300 \text{ m}^2\text{day}^{-1} \\ r_e &= 3000 \text{ m,} \\ r_i &= 1800 + 100 = 1900 \text{ m,} \\ r_p &= 1800 - 100 = 1700 \text{ m}\end{aligned}$$

It therefore follows that

$$Q_w = \frac{2\pi T \eta}{\ln\left(\frac{r_e^2}{r_p r_i}\right)} = \frac{2\pi \times 1300 \times 0.15}{\ln\left(\frac{3000^2}{1700 \times 1900}\right)} = 1196 = 1190 \text{ m}^3\text{day}^{-1}$$

Worked Solution 14.5 (see Problem 14.5)

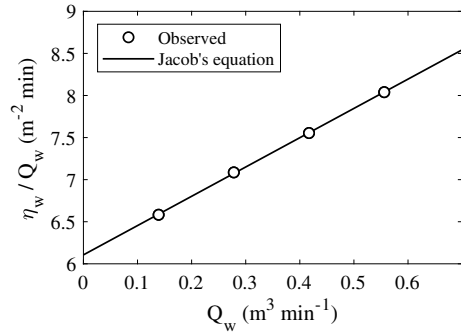
(a) The first step is to divide the drawdown data, η_w , by the production rate, Q_w :

$Q_w \text{ (m}^3\text{min}^{-1}\text{)}$	0.139	0.278	0.417	0.556
$\eta_w \text{ (m)}$	0.915	1.97	3.15	4.47
$\eta_w/Q_w \text{ (m}^{-2}\text{min)}$	6.583	7.086	7.554	8.040

The formation loss and well-loss parameters can be obtained by linear regression using the following MATLAB code:

```
%Use linear regression to find Aj and Bj
%that satisfy etaW/Qw=Aj+Bj*Qw.
%etaW (m)is drawdown in the well
%Qw (m^3 min^-1)is the production rate
%Aj (m^-2 min) is the formation loss coefficient
%Bj (m^-5 min^2) is the well-loss coefficient
X=[ones(size(Qw)) Qw]\(etaW./Qw);
Aj=X(1)
Bj=X(2)
```


Fig. 14.7 Analysis of results from a step-drawdown test



Alternatively, we can plot η_w / Q_w against Q_w and fit a straight line through the data (see Fig. 14.7). The formation loss coefficient, A_J , is found from the zero-intercept of the straight line, which in this case is $6.11 \text{ m}^{-2} \text{min}$.

The well-loss coefficient, B_J , is found from the slope of the straight line and is $3.48 \text{ m}^{-5} \text{min}^2$.

(b) Recall from Eq. (14.12) that

$$A_J = \frac{1}{2\pi T} \ln \left(\frac{r_e}{r_w} \right)$$

From the data in the question we have that $r_e = 8000 \text{ m}$ and $r_w = 0.05 \text{ m}$. Therefore the transmissivity of the aquifer is

$$T = \frac{1}{2\pi A_J} \ln \left(\frac{r_e}{r_w} \right) = \frac{1}{2\pi \times 6.11} \ln \left(\frac{8000}{0.05} \right) = 0.312 \text{ m}^2 \text{min}^{-1}.$$

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Abstract

This chapter focuses on the inclusion of fluid compressibility and rock compressibility to form a partial differential equation describing transient groundwater flow. The concepts of fluid compressibility and rock compressibility are explained. A transient mass conservation equation is derived by a control-volume approach. An expression for the specific storage coefficient is derived by application of the product rule and chain rule. A comparison is made between storativity for confined aquifers and specific yield for unconfined aquifers. A similarity transform is used to derive a complementary error function solution describing one-dimensional transient flow in a confined aquifer. Practical applications are presented through a problem sheet with worked solutions.

Notation

A	Cross-sectional area of sample [L^2].
c_F	Fluid compressibility [$M^{-1}LT^2$].
c_R	Rock compressibility [$M^{-1}LT^2$].
g	Gravitational acceleration [LT^{-2}].
h	Hydraulic head [L].
h_i	Initial hydraulic head [L].
h_0	Boundary hydraulic head [L].
H	Formation thickness [L].
K	Hydraulic conductivity [LT^{-1}].
L	Length of sample [L].
m_w	Mass of water per unit volume of rock [ML^{-3}].
M	Mass of water particles [M].
p	Pressure [$ML^{-1}T^{-2}$].
q	Darcy flux [LT^{-1}].
Q	Flow rate [L^3T^{-1}].

S	Storativity [-].
S_s	Specific storage [L^{-1}].
S_y	Specific yield [-].
t	Time [T].
T	Transmissivity [L^2T^{-1}].
u	Dependent variable transform [$L^{-1}T$].
V	Volume of a rigid tank [L^3].
V_S	Volume of solid material [L^3].
V_T	Total volume of sample [L^3].
V_V	Volume of voids [L^3].
V_W	Volume of water [L^3].
x	Distance in the x -direction [L].
y	Distance in the y -direction [L].
z	Elevation [L].
α	Similarity transform exponent [-].
α_B	Biot coefficient [-].
β	Similarity transform exponent [-].
ζ	Dimensionless similarity transform [-].
ξ	Similarity transform [$L^\alpha T^\beta$].
ρ	Fluid density [ML^{-3}].
σ_e	Effective stress [$ML^{-1}T^{-2}$].
σ_t	Total stress [$ML^{-1}T^{-2}$].
ϕ	Porosity [-].

15.1 Introduction

Under steady-state conditions, mass conservation dictates that, over a designated time-period, any mass of fluid entering a control-volume equals the mass of fluid leaving the control-volume. Under transient conditions (i.e., when steady-state conditions do not apply), we have instead that, over a designated time-period, any mass of fluid entering a control-volume equals the mass of fluid leaving the control-volume plus a change in mass of fluid stored within the control-volume.

In seeking to develop a set of equations to describe groundwater flow under transient conditions we need to develop an understanding of where fluid is stored within a porous medium. Of course, the fluid is stored within the volume of voids. However, if the pore-space is already filled with fluid, how is it possible to store more fluid? Alternatively, if the pore-space remains completely filled with fluid following fluid extraction, where did the extracted fluid come from?

In fact, more fluid can be accommodated by an already filled pore-space by squeezing the existing fluid particles closer together. Squeezing the fluid particles closer together leads to an increase in fluid density, which in turn leads to an increase in fluid pressure. The fluid pressure is applied isotropically to the face of the rock grains that make up the porous medium of concern. An increase in fluid pressure leads to

a pushing apart of the rock grains and a consequential expansion of the pore-space. The resulting increase in porosity provides additional capacity to store more fluid.

When fluid is extracted from a porous medium but the pore-space remains fully saturated, the newly available space within the porous medium is taken over by the remaining fluid particles moving away from each other (i.e., a reduction in fluid density), which leads to a reduction in fluid pressure. The reduction in fluid pressure also leads to the rock grains closing in on each other and a consequential reduction in the volume of available pore-space.

The outline of this chapter is as follows: The concepts of fluid compressibility and rock compressibility are introduced. A mass conservation equation for transient groundwater flow is derived. Darcy's law, fluid compressibility and rock compressibility are used to transform this mass conservation equation into a diffusion equation where hydraulic head is the primary dependent variable. This leads to the introduction of three new aquifer properties: specific storage coefficient, storativity and specific yield. An analytical solution is then derived to describe transient one-dimensional groundwater flow in a semi-infinite, homogeneous and confined aquifer.

15.2 Fluid Compressibility

Consider a rigid tank of volume, V [L^3], initially containing a mass of water particles, M_0 [M] (Fig. 15.1a). An additional mass of fluid, δM [M], is injected into the tank. Consequently the pressure in the tank increases from an initial pressure, p_0 [$ML^{-1}T^{-2}$], to a final pressure of $p_0 + \delta p$. There are now more fluid particles in the tank and these are closer together (Fig. 15.1b). Therefore the fluid density has increased from an initial value, ρ_0 [ML^{-3}], to a final value of $\rho_0 + \delta \rho$, both defined as follows:

$$\rho_0 = \frac{M_0}{V}$$

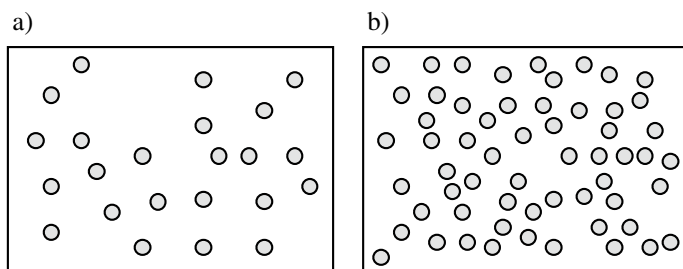


Fig. 15.1 **a** A tank containing some fluid particles. **b** The same tank after the pressure has been increased by injecting more fluid. There are now more fluid particles in the tank so the particles are closer together; the fluid density has increased

$$\rho_0 + \delta\rho = \frac{M_0 + \delta M}{V}$$

and so

$$\delta\rho = \frac{\delta M}{V}$$

Fluid compressibility, c_F [$M^{-1}LT^2$], is a parameter used to describe how fluid density changes with pressure and is defined by

$$c_F = \frac{1}{\rho_0 + \delta\rho/2} \frac{\delta\rho}{\delta p}$$

or for an infinitesimal change in pressure

$$c_F = \frac{1}{\rho} \frac{\partial\rho}{\partial p}. \quad (15.1)$$

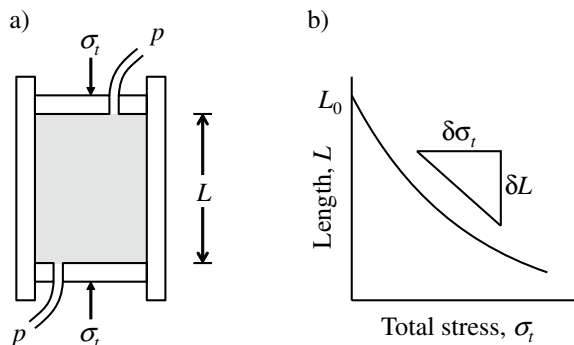
15.3 Rock Compressibility

Consider a cylindrical sample of porous material of initial length, L_0 [L], and cross-sectional area, A [L^2] (Fig. 15.2a). The sample is encased within a rigid cylindrical sleeve and confined between two loading plates such that the sample is placed in compression due to a vertical total stress, σ_t [$ML^{-1}T^{-2}$]. The sample is fully saturated with fluid at a pressure, p [$ML^{-1}T^{-2}$], which is maintained at a constant value within the sample by two pressure relief pipes. The total stress applied is increased in a sequence of steps, $\delta\sigma_t$ [$ML^{-1}T^{-2}$]. Following an incremental increase in total stress, the fluid pressure temporarily increases and then decreases back to the maintained value due to the relief pipes. Once this has occurred the reduction in sample length, δL [L], is measured and recorded (Fig. 15.2b).

The bulk compressibility of the sample, hereafter referred to as the rock compressibility, c_R [$M^{-1}LT^2$], is recorded as follows

$$c_R = \frac{1}{L_0} \frac{\delta L}{\delta\sigma_t}$$

Fig. 15.2 **a** Schematic of loading cell for measuring rock compressibility. **b** Plot of sample length against total stress from loading cell experiments. (adapted from [1, p. 55])



Because the sample is laterally confined by the rigid sleeve, the cross-sectional area of the sample remains constant. Noting that the total volume of the sample, $V_T = AL$, it can be understood that c_R also satisfies the relationship

$$c_R = \frac{1}{V_{T0}} \frac{\delta V_T}{\delta \sigma_t}$$

where V_{T0} [L^3] is the initial volume of the sample.

The total stress is related to the effective stress, σ_e [$ML^{-1}T^{-2}$], by the relationship

$$\sigma_e = \sigma_t - \alpha_B p$$

where α_B [-] is known as the Biot coefficient. Furthermore, because the experiment described above is maintained at constant pressure, it can be said that $\delta \sigma_e = \delta \sigma_t$ and therefore

$$c_R = \frac{1}{V_{T0}} \frac{\delta V_T}{\delta \sigma_e}$$

In continuous form

$$c_R = -\frac{1}{V_T} \frac{\partial V_T}{\partial \sigma_e}$$

where the negative sign comes about because δV_T represented a loss in total volume in this case. Some typical values of rock compressibility are given in Table 15.1.

The total volume is related to the volume of voids, V_V [L^3] (where the fluid is stored), by $V_T = V_V + V_S$, where V_S [L^3] is the volume of solid material contained within the porous medium. For hydrogeology applications, it is often assumed that the solid material is incompressible, such that $dV_S = 0$ and $\alpha_B = 1$ [1, p. 54]. Furthermore, although the experiment described above involves changing σ_t and keeping p constant, hydrogeologists often extrapolate the rock compressibility parameter to conditions where σ_t is assumed constant and p is allowed to vary. Under such conditions $d\sigma_e = -dp$ and

$$c_R = \frac{1}{V_T} \frac{\partial V_V}{\partial p} \quad (15.2)$$

See [2] for more detail about the general case when $\alpha_B \in [0, 1]$.

Table 15.1 Rock compressibilities (c_R) for different formations along with the compressibility of water (c_F) [1, p. 55]

Formation	Compressibility (Pa^{-1})
Clay	$10^{-6} - 10^{-8}$
Sand	$10^{-7} - 10^{-9}$
Gravel	$10^{-8} - 10^{-10}$
Jointed rock	$10^{-8} - 10^{-10}$
Sound rock	$10^{-9} - 10^{-11}$
Water	4.4×10^{-10}

15.4 Mass Conservation in a Control-Volume

Here we will apply mass conservation in a control-volume (CV) of aquifer formation to develop an equation to describe groundwater flow under transient conditions.

The CV has dimensions of δx , δy and δz (Fig. 15.3). The mass of fluid stored in the CV is found from $\delta x \delta y \delta z m_w$, where m_w [ML^{-3}] is the mass of fluid per unit volume of rock.

Challenge 15.1 Use the expressions describing the inputs and outputs of the CV to derive a partial differential equation for transient mass conservation in groundwater systems.

Under transient conditions, mass conservation dictates that over a designated time-period, any mass of fluid entering a CV equals the mass of fluid leaving the CV plus a change in mass of fluid stored within the control-volume.

The mass of fluid entering the CV is

$$\delta y \delta z \delta t \rho q_x + \delta x \delta z \delta t \rho q_y + \delta x \delta y \delta t \rho q_z$$

where q_x [LT^{-1}], q_y [LT^{-1}] and q_z [LT^{-1}] are the Darcy fluxes in the x , y and z directions, respectively.

The mass of fluid leaving the CV is

$$\delta y \delta z \delta t [\rho q_x + \delta(\rho q_x)] + \delta x \delta z \delta t [\rho q_y + \delta(\rho q_y)] + \delta x \delta y \delta t [\rho q_z + \delta(\rho q_z)]$$

The resulting change in the mass of fluid stored within the CV is

$$\delta x \delta y \delta z \delta m_w$$

Mass conservation therefore dictates that

$$\begin{aligned} 0 = & \delta y \delta z \delta t \rho q_x + \delta x \delta z \delta t \rho q_y + \delta x \delta y \delta t \rho q_z \\ & - \delta y \delta z \delta t [\rho q_x + \delta(\rho q_x)] - \delta x \delta z \delta t [\rho q_y + \delta(\rho q_y)] \\ & - \delta x \delta y \delta t [\rho q_z + \delta(\rho q_z)] - \delta x \delta y \delta z \delta m_w \end{aligned}$$

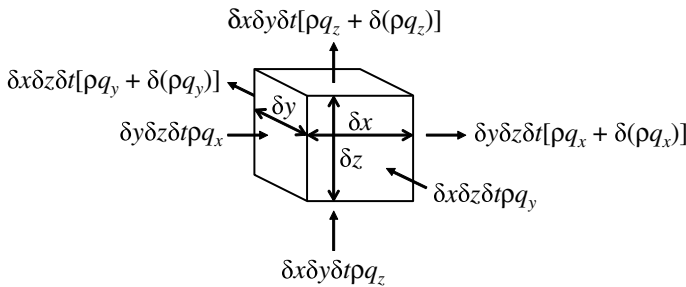


Fig. 15.3 Mass conservation for a control-volume

which can be simplified to get

$$\frac{\delta m_W}{\delta t} = -\frac{\delta(\rho q_x)}{\delta x} - \frac{\delta(\rho q_y)}{\delta y} - \frac{\delta(\rho q_z)}{\delta z}$$

If we now consider an infinitesimal time-period and an infinitesimal CV, this reduces further to the following partial differential equation

$$\frac{\partial m_W}{\partial t} = -\frac{\partial(\rho q_x)}{\partial x} - \frac{\partial(\rho q_y)}{\partial y} - \frac{\partial(\rho q_z)}{\partial z}$$

or in vector-calculus notation

$$\frac{\partial m_W}{\partial t} = -\nabla \cdot (\rho \mathbf{q}) \quad (15.3)$$

where

$$\mathbf{q} = \begin{bmatrix} q_x \\ q_y \\ q_z \end{bmatrix}.$$

15.4.1 Writing in Terms of Hydraulic Head

For anisotropic hydraulic conductivity, Darcy's law gives that

$$q_x = -K_x \frac{\partial h}{\partial x}, \quad q_y = -K_y \frac{\partial h}{\partial y}, \quad q_z = -K_z \frac{\partial h}{\partial z}$$

where K_x [LT^{-1}], K_y [LT^{-1}] and K_z [LT^{-1}] are hydraulic conductivity in the x , y and z directions, respectively, and h [L] is hydraulic head.

In vector-calculus notation, this takes the form

$$\mathbf{q} = -\mathbf{K} \nabla h \quad (15.4)$$

where

$$\mathbf{K} = \begin{bmatrix} K_x & 0 & 0 \\ 0 & K_y & 0 \\ 0 & 0 & K_z \end{bmatrix}$$

Substituting Eq. (15.4) into Eq. (15.3) leads to

$$\frac{\partial m_W}{\partial t} = \nabla \cdot (\rho \mathbf{K} \nabla h) \quad (15.5)$$

It is therefore convenient to write the time-derivative in terms of hydraulic head.

Challenge 15.2 Use the definitions of fluid compressibility and rock compressibility, given by Eqs. (15.1) and (15.2), to write the time-derivative in Eq. (15.5) in terms of hydraulic head.

Recall from Eqs. (15.1) and (15.2) that

$$c_F = \frac{1}{\rho} \frac{\partial \rho}{\partial p} \quad \text{and} \quad c_R = \frac{1}{V_T} \frac{\partial V_V}{\partial p}$$

where c_F is the fluid compressibility, ρ is the fluid density, p is fluid pressure, c_R is the rock compressibility, V_T is the total volume of porous material being studied and V_V is the volume of voids contained within that volume.

The relevance here is that the m_W term in Eq. (15.5) is mass of fluid per unit volume of rock. It follows that

$$\frac{\partial m_W}{\partial t} = \frac{1}{V_T} \frac{\partial (\rho V_V)}{\partial t}$$

Application of the product rule leads to

$$\frac{\partial m_W}{\partial t} = \frac{V_V}{V_T} \frac{\partial \rho}{\partial t} + \frac{\rho}{V_T} \frac{\partial V_V}{\partial t}$$

Given that both V_V and ρ are functions of pressure, the chain rule can be used to state that

$$\frac{\partial m_W}{\partial t} = \left(\frac{V_V}{V_T} \frac{\partial \rho}{\partial p} + \frac{\rho}{V_T} \frac{\partial V_V}{\partial p} \right) \frac{\partial p}{\partial t}$$

Substituting the definitions for fluid and rock compressibility then leads to

$$\frac{\partial m_W}{\partial t} = \rho (\phi c_F + c_R) \frac{\partial p}{\partial t} \quad (15.6)$$

where $\phi = \frac{V_V}{V_T}$ is the porosity of the material.

Recall that hydraulic head, h , is related to pressure by

$$h = \frac{p}{\rho g} + z$$

where g [LT^{-2}] is gravitational acceleration.

So $p = \rho g(h - z)$ and $\frac{\partial p}{\partial h} = \rho g$.

Applying the chain-rule again to Eq. (15.6) therefore leads to

$$\frac{\partial m_W}{\partial t} = \rho^2 g (\phi c_F + c_R) \frac{\partial h}{\partial t} \quad (15.7)$$

Equating Eqs. (15.5) and (15.7) leads to

$$\rho^2 g (\phi c_F + c_R) \frac{\partial h}{\partial t} = \nabla \cdot (\rho \mathbf{K} \nabla h). \quad (15.8)$$

15.4.2 Writing as a Diffusion Equation

The spatial variations of fluid density are small in the context of groundwater modelling. Consequently density is typically assumed to be spatially uniform such that Eq. (15.8) reduces to

$$\rho g (\phi c_F + c_R) \frac{\partial h}{\partial t} = \nabla \cdot (\mathbf{K} \nabla h) \quad (15.9)$$

Note that if the aquifer is homogeneous and isotropic (i.e., S_s and K are uniform and non-directional), Eq. (15.9) reduces to a diffusion equation

$$\rho g (\phi c_F + c_R) \frac{\partial h}{\partial t} = K \left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} \right) = K \nabla^2 h.$$

15.5 Storage Coefficients

15.5.1 Specific Storage Coefficient

The coefficients on the left-hand-side of Eq. (15.9) are often lumped together into a single coefficient known as the specific storage coefficient, S_s [L^{-1}] [1, p. 59]:

$$S_s = \rho g (\phi c_F + c_R) \quad (15.10)$$

such that

$$S_s \frac{\partial h}{\partial t} = \nabla \cdot (\mathbf{K} \nabla h) \quad (15.11)$$

The specific storage coefficient represents the volume of water released per unit volume of aquifer as a result of a unit decline in a piezometric surface. The water arises from the small reduction in fluid density and aquifer porosity which collectively result from a drop in fluid pressure.

15.5.2 Storativity

Consider a confined aquifer of formation thickness, H . In this case, Eq. (15.11) can be integrated with respect to z to get

$$S \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left(T_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T_y \frac{\partial h}{\partial y} \right)$$

where the transmissivities in the x and y direction are found from $T_x = H K_x$ and $T_y = H K_y$, respectively, and S [-] is known as the storativity, found from $S = H S_s$.

The storativity of a confined aquifer represents the volume of water released per unit area over the entire aquifer thickness as a result of a unit decline in piezometric surface. Again, the water arises from the small reduction in fluid density and aquifer porosity which collectively result from the drop in fluid pressure.

15.5.3 Specific Yield

A related equation for an unconfined aquifer is

$$S_y \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left(K_x h \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y h \frac{\partial h}{\partial y} \right)$$

where S_y [-] is known as the specific yield.

The specific yield of an unconfined aquifer represents the volume of water released per unit area over the entire aquifer thickness as a result of a unit fall in the water table elevation. The water arises from the draining of pores as the water table is lowered. The specific yield is similar to but smaller than the porosity of the formation (see Table 15.2). This is because not all the water present in the pore-space can drain by gravity, which will be discussed further in Chap. 17.

Table 15.2 Porosity, ϕ , specific yield, S_y , and hydraulic conductivity, K , for a range of geological formations [3, pp. 38, 51 and 93]

	ϕ (%)	S_y (%)	K (m day ⁻¹)
Gravel, coarse	28	23	150
Gravel, medium	32	24	270
Gravel, fine	34	25	450
Sand, coarse	39	27	45
Sand, medium	39	28	12
Sand, fine	43	23	2.5
Silt	46	8	0.08
Clay	42	3	0.0002
Sandstone, fine grained	33	21	0.2
Sandstone, medium grained	37	27	3.1
Limestone	30	14	0.94
Dune sand	45	38	20
Loess	49	18	0.08
Peat	92	44	5.7
Schist	38	26	0.2
Till, predominantly silt	34	6	0.49
Till, predominantly sand	31	16	30
Tuff	41	21	0.2

15.6 Solution by Similarity Transform

Many one-dimensional partial differential equations (PDE) are self-similar, which means they can be reduced to an ordinary differential equation (ODE) with respect to an appropriate similarity transform. Once transformed to an ODE, the PDE can be solved using methods already developed for solving ODEs. Here we will use a similarity transform to derive an analytical solution for transient one-dimensional groundwater flow in a semi-infinite, homogeneous and confined aquifer.

The first step is to transform the PDE into a second-order ODE using a similarity transform. A dependent variable transform is then used to transform the second-order ODE into a first-order ODE. This latter equation can be solved by separation of variables and integration. The resulting analytical solution takes the form of a complementary error function.

15.6.1 Application of an Independent Variable Transform

A PDE in x and t is said to be self-similar if it is possible to change the independent variables in the denominator of all the partial derivatives to the generalized independent variable transform

$$\xi = x^\alpha t^\beta \quad (15.12)$$

and choose values of α and β such that x and t are eliminated from the PDE as well as the associated initial condition and boundary conditions.

Here we will consider the governing equation for one-dimensional groundwater flow in a semi-infinite and homogeneous confined aquifer

$$S \frac{\partial h}{\partial t} - T \frac{\partial^2 h}{\partial x^2} = 0 \quad (15.13)$$

subjected to the initial and boundary conditions:

$$\begin{aligned} h &= h_i, \quad x \geq 0, \quad t = 0 \\ h &= h_0, \quad x = 0, \quad t > 0 \\ h &= h_i, \quad x \rightarrow \infty, \quad t > 0 \end{aligned} \quad (15.14)$$

where h_i and h_0 are initial and boundary hydraulic heads, respectively.

Challenge 15.3 Substitute the generalized independent variable transform, Eq.(15.12), into Eq.(15.13), determine values for α and β such that x and t are eliminated and show that the problem, defined by Eqs.(15.13) and (15.14), is self-similar.

Application of the chain rule to Eq.(15.13) leads to

$$S \frac{\partial \xi}{\partial t} \frac{\partial h}{\partial \xi} - T \frac{\partial}{\partial x} \left(\frac{\partial \xi}{\partial x} \frac{\partial h}{\partial \xi} \right) = 0 \quad (15.15)$$

then application of the product rule to the second term in Eq. (15.15) yields

$$S \frac{\partial \xi}{\partial t} \frac{\partial h}{\partial \xi} - T \left[\frac{\partial^2 \xi}{\partial x^2} \frac{\partial h}{\partial \xi} + \frac{\partial \xi}{\partial x} \frac{\partial}{\partial x} \left(\frac{\partial h}{\partial \xi} \right) \right] = 0$$

and finally application of the chain rule again to the last term leads to

$$S \frac{\partial \xi}{\partial t} \frac{\partial h}{\partial \xi} - T \left[\frac{\partial^2 \xi}{\partial x^2} \frac{\partial h}{\partial \xi} + \left(\frac{\partial \xi}{\partial x} \right)^2 \frac{\partial^2 h}{\partial \xi^2} \right] = 0 \quad (15.16)$$

From Eq. (15.12):

$$\begin{aligned} \frac{\partial \xi}{\partial t} &= \beta x^\alpha t^{\beta-1} = \frac{\beta \xi}{t} \\ \frac{\partial \xi}{\partial x} &= \alpha x^{\alpha-1} t^\beta = \frac{\alpha \xi}{x} \\ \frac{\partial^2 \xi}{\partial x^2} &= \alpha(\alpha-1)x^{\alpha-2}t^\beta = \frac{\alpha(\alpha-1)\xi}{x^2} \end{aligned}$$

which, when substituted into Eq. (15.16), lead to

$$S \frac{\beta \xi}{t} \frac{\partial h}{\partial \xi} - T \left(\alpha(\alpha-1) \frac{\xi}{x^2} \frac{\partial h}{\partial \xi} + \frac{\alpha^2 \xi^2}{x^2} \frac{\partial^2 h}{\partial \xi^2} \right) = 0 \quad (15.17)$$

The problem is self-similar if it is possible to choose values of α and β such that all the x and t terms are eliminated.

Multiplying both sides of Eq. (15.17) by x^2 it can be seen that

$$S \frac{\beta \xi x^2}{t} \frac{\partial h}{\partial \xi} - T \left(\alpha(\alpha-1) \xi \frac{\partial h}{\partial \xi} + \alpha^2 \xi^2 \frac{\partial^2 h}{\partial \xi^2} \right) = 0$$

Recalling that $\xi = x^\alpha t^\beta$, it is now apparent that all the x and t terms are eliminated when $\alpha = 2$ and $\beta = -1$ such that $\xi = x^2 t^{-1}$. Setting $\alpha = 2$ and $\beta = -1$ leads to

$$\left(S + \frac{2T}{\xi} \right) \frac{\partial h}{\partial \xi} + 4T \frac{\partial^2 h}{\partial \xi^2} = 0 \quad (15.18)$$

which is a linear, second-order, ODE in ξ .

Also note that the initial and boundary conditions, given earlier in Eq. (15.14), reduce to

$$\begin{aligned} h &= h_i, \quad \xi \rightarrow \infty \\ h &= h_0, \quad \xi = 0 \end{aligned} \quad (15.19)$$

so the problem is self-similar.

15.6.2 Application of a Dependent Variable Transform

The ODE in Eq. (15.18) remains difficult to solve. At this stage it is useful to consider the following dependent variable transform

$$u = \frac{\partial h}{\partial \xi} \quad (15.20)$$

with the aim of transforming Eq. (15.18) from being a second-order ODE to an easier to solve, first-order ODE.

Challenge 15.4 Substitute the dependent variable transform, Eq. (15.20), into Eq. (15.18), solve for u and then obtain a solution for h in terms of an integral function of ξ .

Substituting Eq. (15.20) into Eq. (15.18) leads to

$$\left(S + \frac{2T}{\xi}\right)u + 4T \frac{\partial u}{\partial \xi} = 0 \quad (15.21)$$

Separating variables we then have

$$\int \left(S + \frac{2T}{\xi}\right) d\xi = -4T \int \frac{1}{u} du$$

which leads to

$$S\xi + 2T \ln \xi = -4T \ln u + A_1$$

where A_1 is an integration constant yet to be defined.

After some further rearrangement, it can be shown that

$$u = \xi^{-1/2} \exp\left(\frac{A_1 - S\xi}{4T}\right) = \exp\left(\frac{A_1}{4T}\right) \xi^{-1/2} \exp\left(-\frac{S\xi}{4T}\right)$$

Invoking again Eq. (15.20), we have that

$$\frac{\partial h}{\partial \xi} = \exp\left(\frac{A_1}{4T}\right) \xi^{-1/2} \exp\left(-\frac{S\xi}{4T}\right)$$

and integrating both sides with respect to ξ leads to:

$$h = \exp\left(\frac{A_1}{4T}\right) \int \xi^{-1/2} \exp\left(-\frac{S\xi}{4T}\right) d\xi. \quad (15.22)$$

15.6.3 Substituting the Complementary Error Function

The complementary error function, $\text{erfc}(\zeta)$, is defined by

$$\text{erfc}(\zeta) = \frac{2}{\sqrt{\pi}} \int_{\zeta}^{\infty} e^{-\zeta^2} d\zeta \quad (15.23)$$

and has the following properties: $\text{erfc}(0) = 1$ and $\text{erfc}(\infty) = 0$.

Challenge 15.5 Substitute the complementary error function into Eq. (15.22) and determine expressions for the two resulting integration constants such that the initial and boundary conditions provided in Eq. (15.19) are satisfied.

Comparing Eqs. (15.22) and (15.23) suggests that we should try to make the substitution

$$\zeta^2 = \frac{S\xi}{4T}$$

from which it follows that

$$\xi = \frac{4T\zeta^2}{S} \quad \text{and} \quad \frac{\partial \xi}{\partial \zeta} = \frac{8T\zeta}{S} = 4 \left(\frac{T\xi}{S} \right)^{1/2}$$

It can therefore be understood that

$$h = 4 \left(\frac{T}{S} \right)^{1/2} \exp \left(\frac{A_1}{4T} \right) \int e^{-\zeta^2} d\zeta$$

It is now possible to substitute the complementary error function to get

$$h = 2 \left(\frac{\pi T}{S} \right)^{1/2} \exp \left(\frac{A_1}{4T} \right) \text{erfc}(\zeta) + A_2$$

where A_2 is another integration constant.

Recalling that $\xi = x^2 t^{-1}$ it follows that

$$\zeta^2 = \frac{Sx^2}{4Tt}$$

and the initial and boundary conditions given in Eq. (15.19) transform to

$$\begin{aligned} h &= h_i, \quad \zeta \rightarrow \infty \\ h &= h_0, \quad \zeta = 0 \end{aligned}$$

Noting that $\text{erfc}(\infty) = 0$ it can be determined that $A_2 = h_i$. Furthermore, noting that $\text{erfc}(0) = 1$ it follows that

$$2 \left(\frac{\pi T}{S} \right)^{1/2} \exp \left(\frac{A_1}{4T} \right) = h_0 - h_i$$

Finally it can be said that the analytical solution to the problem defined by Eqs. (15.13) and (15.14) is [4, p. 21]

$$\frac{h - h_i}{h_0 - h_i} = \text{erfc}(\zeta) = \text{erfc} \left(\sqrt{\frac{Sx^2}{4Tt}} \right). \quad (15.24)$$

15.7 Problem Sheet

Problem 15.1 (see Worked Solution 15.1)

Calculate the quantity of water required to raise the water table of an unconfined aquifer by 180 cm over an area of 1 km^2 , assuming the aquifer has a specific yield of 0.057.

Problem 15.2 (see Worked Solution 15.2)

Following a sequence of field tests, the storativity of a confined aquifer is thought to be around 5.2×10^{-4} . Assuming the thickness and porosity of the aquifer to be 60 m and 0.23, respectively, estimate the rock compressibility (i.e., c_R).

Problem 15.3 (see Worked Solution 15.3)

The specific storage coefficient of a 40 m thick confined aquifer is $4.2 \times 10^{-5} \text{ m}^{-1}$. Calculate the quantity of water needed to be removed to lower the piezometric surface by 350 cm over an area of 1 km^2 .

Problem 15.4 (see Worked Solution 15.4)

A semi-infinite, homogeneous and confined aquifer is bounded by a lake. Initially the hydraulic head in both the lake and the aquifer is at a uniform value of 40 mAOD. An earthquake causes the water level in the lake to instantaneously reduce by 10 m. Determine the spatial distribution of hydraulic head within the aquifer up to a distance of 20 km from the lake for 1 day, 10 days and 100 days after the earthquake.

(a) Assume the aquifer is comprised of medium grained sand with a rock compressibility of 10^{-8} Pa^{-1} , a porosity of 0.39 and a hydraulic conductivity of 12 m day^{-1} .

(b) Assume the aquifer is comprised of medium grained gravel with a rock compressibility of 10^{-9} Pa^{-1} , a porosity of 0.32 and a hydraulic conductivity of 270 m day^{-1} .

15.8 Worked Solutions

Worked Solution 15.1 (see Problem 15.1)

Recall that the specific yield, S_y , is the volume of water released per unit area as a result of a unit fall in the water table elevation. The quantity of water required, V_W , to raise the water table by a distance, Δh , over an area, A , is therefore found from

$$V_W = AS_y \Delta h$$

From the information given in Problem 15.1 we have that $A = 10^6 \text{ m}^2$, $S_y = 0.057$ and $\Delta h = 1.80 \text{ m}$. Therefore

$$V_W = 10^6 \times 0.057 \times 1.80 = 1.026 \times 10^5 \text{ m}^3 = 102.6 \text{ ML}$$

So the quantity of water required is 103 ML.

Worked Solution 15.2 (see Problem 15.2)

Recall that the storativity, $S = HS_s$, where H is the formation thickness and S_s is the specific storage coefficient found from

$$S_s = \rho g(\phi c_F + c_R)$$

where ρ is fluid density, $g = 9.81 \text{ m s}^{-2}$, ϕ is porosity, c_F is fluid compressibility and c_R is the rock compressibility. It follows that

$$c_R = \frac{S}{\rho g H} - \phi c_F$$

From the information given in Problem 15.2 we have that $S = 5.2 \times 10^{-4}$, $H = 60 \text{ m}$ and $\phi = 0.23$. For water, $\rho = 1000 \text{ kg m}^{-3}$ and $c_F = 4.4 \times 10^{-10} \text{ Pa}^{-1}$. Therefore

$$c_R = \frac{5.2 \times 10^{-4}}{1000 \times 9.81 \times 60} - 0.23 \times 4.4 \times 10^{-10} = 7.823 \times 10^{-10} \text{ Pa}^{-1}$$

So the rock compressibility is $7.82 \times 10^{-10} \text{ Pa}^{-1}$.

Worked Solution 15.3 (see Problem 15.3)

Similar to as for Problem 15.1, it can be said that

$$V_W = AHS_s \Delta h$$

where H is the aquifer thickness and S_s is the specific storage coefficient.

From the information given, we have that $A = 10^6 \text{ m}^2$, $H = 40 \text{ m}$, $S_s = 4.2 \times 10^{-5} \text{ m}^{-1}$ and $\Delta h = 3.50 \text{ m}$. Therefore

$$V_W = 10^6 \times 40 \times 4.2 \times 10^{-5} \times 3.50 = 5880 \text{ m}^3 = 5.88 \text{ ML}$$

So the quantity of water removed is 5.88 ML.

Worked Solution 15.4 (see Problem 15.4)

This problem can be addressed using Eq. (15.24). Note that although Eq. (15.24) requires information about transmissivity, T , and storativity, S , information about the thickness of the aquifer, H , is not required because $T/S = (HK)/(HS_s) = K/S_s$ where K is the hydraulic conductivity and S_s is the specific storage coefficient.

Information is given in Problem 15.4 about hydraulic conductivity. However for the specific storage coefficient we need to use the equation, $S_s = \rho g(\phi C_F + C_R)$.

(a) For the sand:

$$K = 12 \text{ m day}^{-1}$$

$$S_s = 1000 \times 9.81 \times (0.39 \times 4.4 \times 10^{-10} + 10^{-8}) = 9.978 \times 10^{-5} \text{ m}^{-1}$$

(b) For the gravel:

$$K = 270 \text{ m day}^{-1}$$

$$S_s = 1000 \times 9.81 \times (0.32 \times 4.4 \times 10^{-10} + 10^{-9}) = 1.119 \times 10^{-5} \text{ m}^{-1}$$

Below is a MATLAB script to implement Eq. (15.24) and plot the desired results:

```
h0=30; %Boundary hydraulic head (mAOD)
hi=40; %Initial hydraulic head (mAOD)
x=linspace(0,20e3,100)'; %Distance (m)
t=[1 10 100]; %Time (days)
%Hydraulic conductivity (m/day)
K=[12 270];
%Specific storage coefficient (m-1)
Ss=[9.978e-5 1.119e-5];
figure(1);clf
MYtitle{1}='a) Sand';
MYtitle{2}='b) Gravel';
for n=1:2
%Determine hydraulic head
zeta=sqrt(Ss(n)*x.^2/4/K(n)./t);
h=(h0-hi)*erfc(zeta)+hi;
subplot(1,2,n)
plot(x/1000,h) %Plot results
xlabel('Distance (km)')
ylabel('Hydraulic head (mAOD)')
legend('1 day','10 day','100 day')
title(MYtitle{n})
end
```

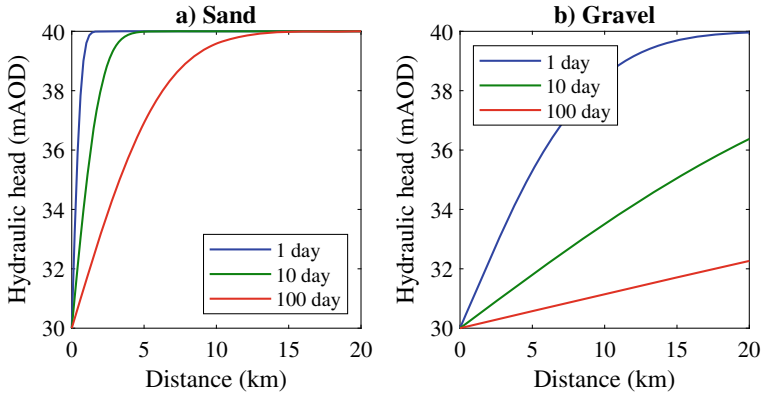


Fig. 15.4 Plots of hydraulic head against distance for different times and different aquifer material

Graphs showing the results are given in Fig. 15.4. Notice that the pressure perturbation resulting from the lake level decline takes much longer to penetrate the sand aquifer as compared to the gravel aquifer. This is because the gravel aquifer has a higher hydraulic conductivity and a smaller rock compressibility, leading to a larger hydraulic diffusivity (i.e., a larger K/S_s ratio).

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Abstract

This chapter is concerned with the derivation and application of analytical solutions for describing transient groundwater flow around production and injection wells. A transient radial flow equation, describing one-dimensional groundwater flow around a pumping well in a confined aquifer, is derived by combining a control-volume approach with the specific storage coefficient concept. A similarity transform is used to derive an important exponential integral solution known as the Theis solution. A large-time approximation, known as Jacob's approximation, is obtained using a series expansion of the exponential integral function. Jacob's approximation is equated with the Theim equation to study how a radius of influence grows with time. Non-Darcy effects are incorporated using the Forchheimer equation. It is shown how to use Jacob's approximation to estimate aquifer properties from pumping test data including both drawdown and recovery phases. Practical applications are presented through a problem sheet with worked solutions.

Notation

A	Cross-sectional area [L^2].
b	Forchheimer coefficient [L^{-1}].
c	Intercept of a straight line.
c_F	Fluid compressibility [$M^{-1}LT^2$].
c_R	Rock compressibility [$M^{-1}LT^2$].
$E_1(x)$	Exponential integral function [-].
g	Gravitational acceleration [LT^{-2}].
h	Hydraulic head [L].
h_e	Unperturbed hydraulic head [L].
H	Formation thickness [L].
k	Permeability [L^2].

K	Hydraulic conductivity [LT^{-1}].
m	Slope of a straight line.
m_w	Mass of water per unit volume of rock [ML^{-3}].
p	Pressure [$\text{ML}^{-1}\text{T}^{-2}$].
q	Darcy flux [LT^{-1}].
Q	Flow rate [L^3T^{-1}].
Q_w	Production rate [L^3T^{-1}].
r	Radial distance from well [L].
r_e	Radius of influence [L].
S	Storativity [-].
S_s	Specific storage [L^{-1}].
t	Time [T].
t_0	Duration of water production [T].
t_R	Transformed time for recovery analysis [T].
T	Transmissivity [L^2T^{-1}].
$W(t)$	Well function [L]
α	Similarity transform exponent [-].
β	Similarity transform exponent [-].
γ	Euler-Mascheroni constant [-].
ζ	Dimensionless similarity transform [-].
η	Piezometric drawdown [L].
η_0	Drawdown at time when production is terminated [L].
η_i	Drawdown due to an injection well [L].
η_p	Drawdown due to a production well [L].
η_R	Transformed drawdown for recovery analysis [L].
μ	Dynamic viscosity [$\text{ML}^{-1}\text{T}^{-1}$].
ξ	Similarity transform [$\text{L}^\alpha\text{T}^\beta$].
ρ	Fluid density [ML^{-3}].
ϕ	Porosity [-].

16.1 Introduction

In the Chap. 15 we derived a transient mass conservation equation for fluid flow in porous media. In particular, we learnt about a new physical property, the storativity, which represents the volume of fluid released from a unit-area of aquifer subjected to a unit decline in hydraulic head. In Chap. 14 we looked at how we can determine aquifer transmissivity by studying the steady-state component of a step-drawdown test. In this chapter we will look at how the storativity can be determined, for a given aquifer, by studying the transient portion of such a pumping test.

First we derive a transient mass conservation statement to describe fluid flow in a radially symmetric flow field around a production well or injection well. The resulting partial differential equation is solved using a similarity transform, giving rise to an analytical solution in terms of an exponential integral function. The derived

analytical solution describes how the piezometric drawdown around a constant-rate production well changes with time. A series expansion form of the exponential integral function is exploited to enable the analytical solution to be fitted to transient drawdown observations by linear regression, resulting in the determination of the transmissivity and storativity of an aquifer of concern. Finally, the principle of superposition is applied to enable additional estimates of aquifer transmissivity and storativity to be determined by studying how an aquifer recovers after groundwater production, from a pumping well, is terminated.

16.2 Mass Conservation with Radial Symmetry

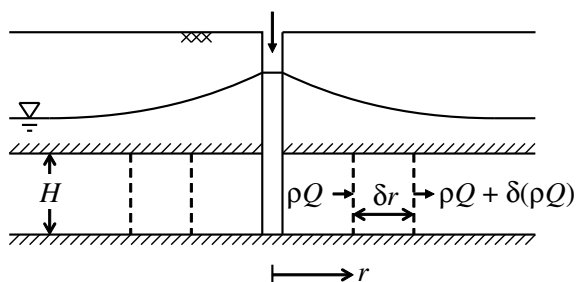
Consider a fluid injection well in a homogeneous confined aquifer of uniform thickness, H [L], as shown in Fig. 16.1. Water flows through the aquifer away from the well. Initially the injection well is not flowing and the aquifer is hydrostatic. The well then starts to inject and a perturbation in hydraulic head moves through the aquifer as more water is injected. The volumetric flow rate within the aquifer, Q [L^3T^{-1}], is not steady-state or spatially uniform with radial distance from the well.

Here we will look at mass conservation within a control-volume (CV) (see Fig. 16.1), of radial length, δr [L], and thickness, H , to develop an equation to describe groundwater flow under transient conditions in a one-dimensional radially symmetric flow field.

Challenge 16.1 Use the expressions describing the input and output of the CV, shown in Fig. 16.1, to derive a partial differential equation for transient mass conservation in a one-dimensional radially symmetric flow field.

Under transient conditions, mass conservation dictates that over a designated time-period, δt [T], any mass of fluid entering a CV equals the mass of fluid leaving the CV plus a change in mass of fluid stored within the CV.

Fig. 16.1 Schematic diagram of confined aquifer control-volume in a radially symmetric flow field



The mass of fluid entering the CV is

$$\delta t \rho Q$$

where ρ [ML⁻³] is the fluid density.

The mass of fluid leaving the CV is

$$\delta t [\rho Q + \delta(\rho Q)]$$

The resulting change in the mass of fluid stored within the CV is

$$\pi [(r + \delta r)^2 - r^2] H \delta m_W = \pi (2r\delta r + \delta r^2) H \delta m_W$$

where m_W [ML⁻³] is a measure of the mass of water per unit volume of rock.

Mass conservation therefore dictates that

$$0 = \delta t \rho Q - \delta t [\rho Q + \delta(\rho Q)] - \pi (2r\delta r + \delta r^2) H \delta m_W$$

which simplifies to get

$$\frac{\delta m_W}{\delta t} = - \frac{\delta(\rho Q)}{\pi (2r\delta r + \delta r^2) H}$$

For an infinitesimal time-period, δt , and an infinitesimal change in radial distance, δr , it follows that

$$\frac{\partial m_W}{\partial t} = - \frac{1}{2\pi H r} \frac{\partial(\rho Q)}{\partial r} \quad (16.1)$$

Challenge 16.2 Use Darcy's law and expressions for fluid compressibility and rock compressibility to re-write Eq. (16.1) with hydraulic head as the only dependent variable.

From Darcy's law we have that

$$Q = -AK \frac{\partial h}{\partial r}$$

where A [L²] is the flowing cross-sectional area, K [LT⁻¹] is hydraulic conductivity and h [L] is hydraulic head. In this case, the cross-sectional area is found from $A = 2\pi H r$.

Substituting both of the above expressions into Eq. (16.1) leads to

$$\frac{\partial m_W}{\partial t} = \frac{K}{r} \frac{\partial}{\partial r} \left(\rho r \frac{\partial h}{\partial r} \right)$$

Note that H and K are assumed to be spatially uniform so they can come outside of the derivative and H cancels out.

Using the definitions of fluid compressibility, c_F , and rock compressibility, c_R , it was shown in the previous chapter that (recall Eq.(15.7))

$$\frac{\partial m_W}{\partial t} = \rho S_s \frac{\partial h}{\partial t}$$

where S_s [L^{-1}] is the specific storage coefficient found from

$$S_s = \rho g (\phi c_F + c_R)$$

It therefore follows that

$$\rho S_s \frac{\partial h}{\partial t} = \frac{K}{r} \frac{\partial}{\partial r} \left(\rho r \frac{\partial h}{\partial r} \right). \quad (16.2)$$

16.3 Solution by Similarity Transform

Now consider the case where the hydraulic head is initially at a uniform value, h_e [L], but the pumping well is used to produce water at a constant rate, Q_w [$L^3 T^{-1}$]. It is further assumed that the fluid density can be treated as spatially uniform, the aquifer is semi-infinite and the production well has an infinitesimally small radius. It follows that

$$S \frac{\partial h}{\partial t} = -\frac{1}{2\pi r} \frac{\partial Q}{\partial r} \quad (16.3)$$

where $S = HS_s$ [-] is the storativity of the aquifer.

Darcy's law gives us

$$Q = -2\pi T r \frac{\partial h}{\partial r} \quad (16.4)$$

where $T = HK$ [$L^2 T^{-1}$] is the transmissivity of the aquifer.

The initial and boundary conditions can be written as:

$$\begin{aligned} h &= h_e, & r &\geq 0, & t &= 0 \\ Q &= -Q_w, & r &= 0, & t &> 0 \\ h &= h_e, & r &\rightarrow \infty, & t &> 0 \end{aligned} \quad (16.5)$$

Challenge 16.3 Substitute the generalized similarity transform, $\xi = r^\alpha t^\beta$, into Eq. (16.3) and determine values for α and β such that r and t are eliminated and the problem, including the initial and boundary conditions given in Eq. (16.5), is demonstrated to be self-similar.

Consider the generalized similarity transform

$$\xi = r^\alpha t^\beta \quad (16.6)$$

where α and β are yet to be defined. Application of the chain rule to Eq. (16.3) leads to

$$S \frac{\partial \xi}{\partial t} \frac{\partial h}{\partial \xi} = -\frac{1}{2\pi r} \frac{\partial \xi}{\partial r} \frac{\partial Q}{\partial \xi} \quad (16.7)$$

Partial differentiation of ξ gives us

$$\frac{\partial \xi}{\partial t} = \beta r^\alpha t^{\beta-1} = \frac{\beta \xi}{t} \quad \text{and} \quad \frac{\partial \xi}{\partial r} = \alpha r^{\alpha-1} t^\beta = \frac{\alpha \xi}{r}$$

which on substitution into Eq. (16.7) leads to

$$\frac{S\beta\xi}{t} \frac{\partial h}{\partial \xi} = -\frac{\alpha\xi}{2\pi r^2} \frac{\partial Q}{\partial \xi}$$

The problem is thought to be self-similar if it is possible to choose values of α and β such that all the r and t terms are eliminated. Recalling that $\xi = r^\alpha t^\beta$, it is now apparent that all the r and t terms are eliminated when $\alpha = 2$ and $\beta = -1$ such that $\xi = r^2 t^{-1}$. Setting $\alpha = 2$ and $\beta = -1$ leads to

$$\xi \frac{\partial h}{\partial \xi} = \frac{1}{\pi S} \frac{\partial Q}{\partial \xi} \quad (16.8)$$

Also note that the initial and boundary conditions, given earlier in Eq. (16.5), reduce to

$$\begin{aligned} h &= h_e, & \xi &\rightarrow \infty \\ Q &= -Q_w, & \xi &= 0 \end{aligned} \quad (16.9)$$

so the problem looks like it might be self-similar. However, we also need to look at Eq. (16.4).

Challenge 16.4 Apply the similarity transform (Eq. (16.6)) to Eq. (16.4), substitute the result into Eq. (16.8) and derive an analytical solution for Q .

Applying the chain-rule to Eq. (16.4) gives us

$$Q = -2\pi T r \frac{\partial \xi}{\partial r} \frac{\partial h}{\partial \xi} = -2\pi T r \frac{\alpha \xi}{r} \frac{\partial h}{\partial \xi} = -4\pi T \xi \frac{\partial h}{\partial \xi}$$

from which it follows that

$$\xi \frac{\partial h}{\partial \xi} = -\frac{Q}{4\pi T} \quad (16.10)$$

Equating Eqs. (16.8) and (16.10) then leads to

$$-\frac{Q}{4\pi T} = \frac{1}{\pi S} \frac{\partial Q}{\partial \xi}$$

Separating the Q -factors and ξ -factors and integrating both sides with respect to ξ gives us

$$-\frac{S}{4T} \int d\xi = \int \frac{1}{Q} dQ$$

which leads to

$$-\frac{S\xi}{4T} = \ln Q + A_1$$

where A_1 is an integration constant.

Recall that $Q = -Q_w$ when $\xi = 0$. Therefore $A_1 = -\ln(-Q_w)$ and

$$Q = -Q_w \exp\left(-\frac{S\xi}{4T}\right) \quad (16.11)$$

Challenge 16.5 Substitute Eq. (16.11) into Eq. (16.10) and obtain an integral equation for h .

Substituting Eq. (16.11) into Eq. (16.10) leads to

$$\xi \frac{\partial h}{\partial \xi} = \frac{Q_w}{4\pi T} \exp\left(-\frac{S\xi}{4T}\right)$$

from which it can be said that

$$h = \int \frac{Q_w}{4\pi T \xi} \exp\left(-\frac{S\xi}{4T}\right) d\xi. \quad (16.12)$$

16.3.1 Substituting the Exponential Integral Function

The exponential integral function, $E_1(\zeta)$, is defined by

$$E_1(\zeta) = \int_{\zeta}^{\infty} \frac{e^{-\zeta}}{\zeta} d\zeta \quad (16.13)$$

and has the following properties: $E_1(0) = \infty$ and $E_1(\infty) = 0$.

Challenge 16.6 Substitute the exponential integral function into Eq. (16.12) and determine the resulting integration constant such that the initial and boundary conditions provided in Eq. (16.9) are satisfied.

Comparing Eqs. (16.12) and (16.13) suggests that we should try to make the substitution

$$\zeta = \frac{S\xi}{4T}$$

from which it follows that $\xi = \frac{4T\zeta}{S}$, $\frac{\partial \xi}{\partial \zeta} = \frac{4T}{S}$ and therefore

$$h = \int \frac{Q_w}{4\pi T \zeta} e^{-\zeta} d\zeta$$

Looking at Eq. (16.13) it can be seen that we need to have some limits so let us say that

$$h = - \int_{\zeta}^{\infty} \frac{Q_w}{4\pi T \zeta} e^{-\zeta} d\zeta + A_2$$

where A_2 is another integration constant. Note that the negative sign is needed because ζ is specified as the lower limit of the integral. It is now possible to substitute the exponential integral function to get

$$h = - \frac{Q_w}{4\pi T} E_1(\zeta) + A_2$$

Recalling that $\xi = r^2 t^{-1}$, it can be said that

$$\zeta = \frac{Sr^2}{4Tt}$$

and the initial and boundary conditions given in Eq. (16.5) transform to

$$\begin{aligned} h &= h_e, & \zeta &\rightarrow \infty \\ Q &= -Q_w, & \zeta &= 0 \end{aligned}$$

Noting $E_1(\infty) = 0$, it can be understood that $A_2 = h_e$. The analytical solution to the problem defined by Eqs. (16.3) and (16.5) is therefore

$$h_e - h = \frac{Q_w}{4\pi T} E_1\left(\frac{Sr^2}{4Tt}\right)$$

Recall from Chap. 14 that $h_e - h = \eta$ where η [L] is referred to as the piezometric drawdown. It further follows that [1]

$$\eta = \frac{Q_w}{4\pi T} E_1\left(\frac{Sr^2}{4Tt}\right) \quad (16.14)$$

which is often referred as the Theis Solution.

16.3.2 Large-Time Approximation

The exponential integral can be approximated using a series expansion [2, p. 229]

$$E_1(\zeta) = -\gamma - \ln \zeta + O(\zeta) \quad (16.15)$$

where $\gamma = 0.5772$ is the Euler-Mascheroni constant.

Substituting Eq. (16.15) into Eq. (16.14) leads to [3]

$$\eta = \frac{Q_w}{4\pi T} \left[\ln\left(\frac{4Tt}{Sr^2}\right) - \gamma \right] + O\left(\frac{Sr^2}{4Tt}\right) \quad (16.16)$$

which is often referred to as Jacob's approximation. Notice that the truncation error (i.e., the $O(\zeta)$ term) becomes small when $t \gg Sr^2/(4T)$.

16.3.3 Transient Radius of Influence

Recall the Thiem equation for steady-state flow to a well in a confined aquifer (Eq. (14.3))

$$\eta = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r}\right)$$

where r_e is the radius of influence.

Challenge 16.7 By comparing the Thiem equation with the Jacob approximation (Eq. (16.16)), derive an equation to describe how the radius of influence of a production well increases with time.

Assuming that r_e is a transient parameter, the Thiem equation can be equated directly with Eq. (16.16) and solved for r_e . Equating the two equations leads to

$$\frac{Q_w}{4\pi T} \left[\ln\left(\frac{4Tt}{Sr^2}\right) - \gamma \right] + O\left(\frac{Sr^2}{4Tt}\right) = \frac{Q_w}{2\pi T} \ln\left(\frac{r_e}{r}\right)$$

Providing a sufficient amount of time has passed (i.e., $t \gg Sr^2/(4T)$) the truncation error can be ignored and common factors can be eliminated such that

$$\ln\left(\frac{4Tt}{Sr^2}\right) - \gamma = 2 \ln\left(\frac{r_e}{r}\right)$$

Bringing γ within the $\ln$ term on the left-hand-side leads to

$$\frac{1}{2} \ln\left(\frac{4Te^{-\gamma}t}{Sr^2}\right) = \ln\left(\frac{r_e}{r}\right)$$

which means that

$$\left(\frac{4Te^{-\gamma}t}{Sr^2}\right)^{1/2} = \frac{r_e}{r}$$

and therefore

$$r_e = \left(\frac{4Te^{-\gamma}t}{S}\right)^{1/2} = 1.499 \left(\frac{Tt}{S}\right)^{1/2}. \quad (16.17)$$

16.3.4 Incorporation of Non-darcy Effects

The above analysis assumes that groundwater flow is adequately described by Darcy's law. However, because the fluid velocities around a pumping well can be very high, non-Darcian effects are likely to be important and the Forchheimer equation will provide a more accurate description. Revisiting the above analysis using the Forchheimer equation is beyond the scope of this text. Nevertheless, it can be shown that when the Forchheimer equation (Eq. (12.26)) is used, Eq. (16.16) becomes [4]

$$\eta = \frac{Q_w}{4\pi T} \left[\ln\left(\frac{4Tt}{Sr^2}\right) - \gamma \right] + \left(\frac{Q_w}{2\pi H}\right)^2 \frac{b}{gr} + O\left(\frac{Sr^2}{4Tt}\right) \quad (16.18)$$

where b [L^{-1}] is the Forchheimer coefficient and g [LT^{-2}] is gravitational acceleration.

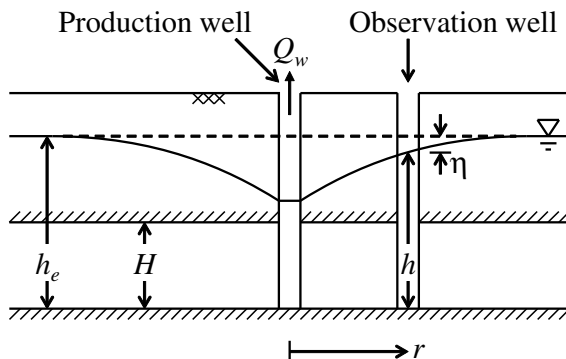
Relaxing some of the other limiting assumptions leads to much more complicated expressions for drawdown. See [5] for problems involving partially penetrating production wells (i.e., wells that do not produce water from the entire vertical extent of the aquifer). See [6] and [7] for problems involving unconfined aquifers as opposed to confined aquifers.

16.4 Pumping Test Analysis

Aquifers are notoriously heterogeneous with permeability being a property that can vary over orders of magnitude within a single geological formation. Consequently, obtaining permeability measurements from core-samples provides limited insight about how an aquifer will behave as a whole. Therefore, hydrogeologists prefer to measure larger scale properties such as transmissivity, T , and storativity, S , by inverse modelling data from field-scale pumping test experiments.

The step-drawdown test, we looked at previously in Chap. 14, is an example of a pumping test experiment. Water is produced from a pumping well and piezometric drawdown in the aquifer is simultaneously monitored and recorded. A groundwater flow model is then calibrated to the drawdown observations to obtain estimates of T and S . To overcome problems associated with non-Darcian well-losses, drawdown observations are often simultaneously recorded in a nearby observation well (Fig. 16.2). The advantage here is that the observation well should be sufficiently far away from the production well such that the fluid velocities are small enough to allow Darcy's law to be a good approximation for the flow processes taking place. This means that only a single production rate need be considered.

Fig. 16.2 Location of an observation well during a pumping test



16.4.1 Analysis of Drawdown Data

Recall Jacob's approximation (Eq. (16.16)). After some further rearrangement it can be said that

$$\eta = \frac{Q_w}{4\pi T} \ln t + \frac{Q_w}{4\pi T} \left[\ln \left(\frac{4T}{Sr^2} \right) - \gamma \right] + O \left(\frac{Sr^2}{4Tt} \right) \quad (16.19)$$

This means that if we plot drawdown observations from an observation well against the natural log of time after the production well commenced water production at a single constant rate, we should be able to exploit linear regression and fit a straight line through the data (once $t \gg Sr^2/(4T)$, where r now represents the distance between the observation well and the production well)

$$\eta = m \ln t + c \quad (16.20)$$

where m and c represent the slope and y-axis intercept of the fitted straight line, respectively.

Challenge 16.8 Derive expressions for transmissivity, T , and storativity, S , in terms of the slope, m , and y-axis intercept, c , for a best fit line through time-drawdown data plotted on log-linear axes.

By comparing Eqs. (16.19) and (16.20) it can be understood that

$$m = \frac{Q_w}{4\pi T} \quad \text{and} \quad c = \frac{Q_w}{4\pi T} \left[\ln \left(\frac{4T}{Sr^2} \right) - \gamma \right]$$

It follows that measurements of T and S , for an aquifer being studied, can be obtained from

$$T = \frac{Q_w}{4\pi m} \quad \text{and} \quad S = \frac{Q_w}{\pi m r^2} \exp \left(-\frac{c}{m} - \gamma \right) \quad (16.21)$$

Figure 16.3b shows Jacob's approximation fitted as a best fit line through the last ten drawdown data points from a USDI pumping test example [8]. Drawdown values using the Theis solution are also shown, which can be seen to closely match the early-time drawdown observations not used for fitting in this case.

16.4.2 Analysis of Recovery Data

Once water production has ceased, the piezometric surface gradually recovers back to its original uniform state. The recovery of the piezometric surface is also recorded and can be independently analysed for measurement of aquifer transmissivity and storativity. This analysis can also be performed using the Theis solution or Jacob's approximation. Because both equations represent drawdown as a linear function

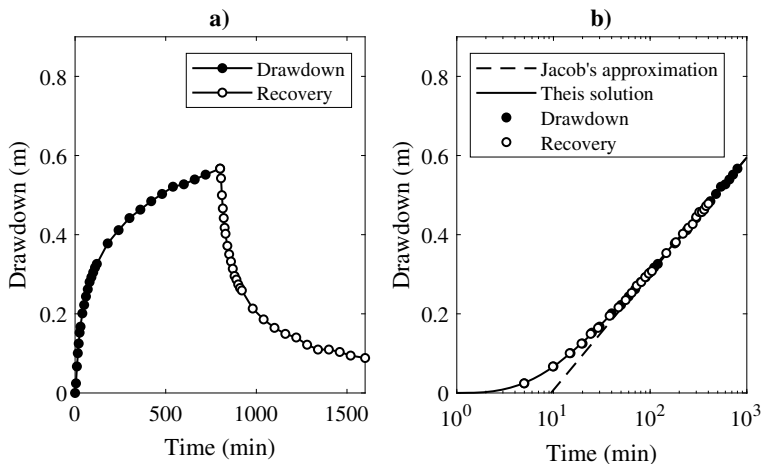


Fig. 16.3 Drawdown and recovery data from an observation well during a pumping test near Las Vegas (data acquired from [8, pp. 256–257])

of production rate, it is possible to simulate the recovery using the principle of superposition.

Consider again the Theis solution (Eq. (16.14)). Let $W(t)$ be a well function defined by

$$W(t) = \begin{cases} 0, & t \leq 0 \\ \frac{Q_w}{4\pi T} E_1\left(\frac{Sr^2}{4Tt}\right), & t > 0 \end{cases} \quad (16.22)$$

Let η_p [L], be the piezometric drawdown due to a pumping well producing water at a constant rate, Q_w , with the pump switched on at $t = 0$. It can be said that

$$\eta_p = W(t) \quad (16.23)$$

Let η_i [L], be the piezometric drawdown due to a pumping well injecting water at a constant rate, Q_w , with the pump switched on at $t = t_0$. It can be said that

$$\eta_i = -W(t - t_0) \quad (16.24)$$

Let η [L] be the piezometric drawdown due to a pumping well producing water at a constant rate, Q_w , for $t \in [0, t_0]$, with the pump switched off thereafter. Using the principle of superposition it can be said that

$$\eta = \eta_p + \eta_i \quad (16.25)$$

Challenge 16.9 Replace the Theis solution in Eq. (16.22) with Jacob's approximation (Eq. (16.16)) and derive an explicit equation for the recovery of the piezometric surface for $t > t_0$ using Eq. (16.25).

Replacing the Theis solution in Eq.(16.22) with Jacob's approximation (Eq. (16.16)), Eqs. (16.23) and (16.24) become

$$\eta_p = \frac{Q_w}{4\pi T} \left[\ln \left(\frac{4Tt}{Sr^2} \right) - \gamma \right], \quad t > t_0$$

and

$$\eta_i = -\frac{Q_w}{4\pi T} \left[\ln \left(\frac{4T(t-t_0)}{Sr^2} \right) - \gamma \right], \quad t > t_0$$

respectively.

From Eq. (16.25) it follows that

$$\eta = \frac{Q_w}{4\pi T} \left[\ln \left(\frac{4Tt}{Sr^2} \right) - \gamma \right] - \frac{Q_w}{4\pi T} \left[\ln \left(\frac{4T(t-t_0)}{Sr^2} \right) - \gamma \right], \quad t > t_0$$

which reduces further to obtain

$$\eta = \frac{Q_w}{4\pi T} \ln \left(\frac{t}{t-t_0} \right), \quad t > t_0 \quad (16.26)$$

from which it appears that recovery data only contains information about the transmissivity and is independent of storativity.

Challenge 16.10 Let η_0 be the drawdown at the time the production well is switched off, i.e., $\eta_0 = W(t_0)$. Use Jacob's approximation to determine an expression for $\eta_0 - \eta$ for $t > t_0$.

Let

$$\eta_0 \equiv W(t_0) = \frac{Q_w}{4\pi T} \left[\ln \left(\frac{4Tt_0}{Sr^2} \right) - \gamma \right]$$

From Eq. (16.26) it follows that

$$\eta_0 - \eta = \frac{Q_w}{4\pi T} \left[\ln \left(\frac{4Tt_0}{Sr^2} \right) - \gamma \right] - \frac{Q_w}{4\pi T} \ln \left(\frac{t}{t-t_0} \right), \quad t > t_0$$

and therefore [9]

$$\eta_R = \frac{Q_w}{4\pi T} \left[\ln \left(\frac{4Tt_R}{Sr^2} \right) - \gamma \right], \quad t_R > 0 \quad (16.27)$$

where

$$\eta_R = \eta_0 - \eta \quad \text{and} \quad t_R = \frac{t_0(t-t_0)}{t} \quad (16.28)$$

from which it can be seen that recovery data indeed contains information about storativity providing the drawdown at the end of production is known. Furthermore, comparing Eq. (16.27) with Eq. (16.16) shows that if the recovery data is plotted in terms of η_R and t_R it can be analysed in exactly the same way as when studying drawdown data, (i.e., η and t during the production phase).

Figure 16.3b shows the recovery data from the USDI [8] pumping test example plotted, using the transformations given in Eq. (16.28), alongside the drawdown data from the same test. It can be seen that the transformed recovery data almost perfectly matches the drawdown test. Nevertheless, pumping test parameters obtained from drawdown and recovery data often exhibit substantial differences in practice [10].

16.5 Problem Sheet

Problem 16.1 (see Worked Solution 16.1)

A pumping well produces water at a constant rate of 2.8 ML day^{-1} for 15 h from a 70 m thick confined aquifer. The permeability, porosity and rock compressibility of the aquifer are $3.7 \times 10^{-12} \text{ m}^2$, 0.15 and 10^{-8} Pa^{-1} , respectively. The production well is 0.1 m in diameter and there is an observation well 20 m from the production well.

- (a) Use Jacob's approximation (Eq. (16.16)) to determine the piezometric drawdown in both the production well and the observation well after 15 h of production.
- (b) Determine the radius of influence for the production well after 15 h.
- (c) Determine the Forchheimer parameter, b , for this aquifer using Geertsma's correlation (Eq. (12.27)) and then recalculate the drawdowns in the production well and the observation well using the Forchheimer equation extension to Jacob's approximation given by Eq. (16.18).

Problem 16.2 (see Worked Solution 16.2)

An observation well is located 50 m East of a pumping well producing at a constant rate of 1.5 ML day^{-1} . The water is produced from a confined aquifer with a transmissivity of $750 \text{ m}^2 \text{ day}^{-1}$ and a storativity of 0.0015.

- (a) Use the Theis solution (Eq. (16.14)) to plot piezometric drawdown in the observation well as a function of time, after the commencement of groundwater production, for one day.
- (b) Use the method of images to show a plot of observation well drawdown against time in the presence of an impermeable boundary running North-South at a distance of 200 m West of the production well.
- (c) Use the method of images to show a plot of observation well drawdown against time in the presence of a fixed-head boundary running North-South at a distance of 200 m West of the production well.

Problem 16.3 (see Worked Solution 16.3)

Revisit the scenario described in Problem 16.2 and use the principle of superposition to plot observation well drawdown as a function of time for one day but assuming that the production well is switched off after 0.4 days.

Problem 16.4 (see Worked Solution 16.4)

A pumping well produces water from a confined aquifer at a constant rate of $1 \text{ m}^3 \text{ min}^{-1}$ for 180 min. The following set of piezometric drawdown measurements are made in an observation well, 50 m away from the production well:

Time (min)	10	40	80	120	180
Drawdown (m)	0.20	0.39	0.49	0.56	0.62
Time (min)	190	220	260	300	360
Drawdown (m)	0.43	0.25	0.18	0.14	0.11

- (a) Use the drawdown data obtained during the production period to estimate the transmissivity and storativity of the aquifer.
- (b) Use the drawdown data obtained during the recovery period (after the pumping well has ceased production) to estimate the transmissivity and storativity of the aquifer.

16.6 Worked Solutions**Worked Solution 16.1** (see Problem 16.1)

- (a) The Jacob approximation reads as follows:

$$\eta = \frac{Q_w}{4\pi T} \left[\ln \left(\frac{4Tt}{Sr^2} \right) - 0.57721 \right]$$

First we need to determine the transmissivity, T , and storativity, S , of the aquifer.

Considering Eqs. (12.23) and (15.10) it can be said that

$$T = KH = \frac{\rho g k H}{\mu} \quad \text{and} \quad S = S_s H = \rho g (\phi c_F + c_R) H$$

The formation thickness, H , permeability, k , porosity, ϕ , and rock compressibility, c_R , are 70 m, $3.7 \times 10^{-12} \text{ m}^2$, 0.15 and 10^{-8} Pa^{-1} , respectively. Noting $g = 9.81 \text{ ms}^{-2}$ and that the density, ρ , viscosity, μ , and compressibility, c_R , of water are 1000 kg m^{-3} , 10^{-3} Pa s and $4.4 \times 10^{-10} \text{ Pa}^{-1}$, respectively, we therefore have that:

$$T = \frac{1000 \times 9.81 \times 3.7 \times 10^{-12} \times 70}{10^{-3}} = 2.541 \times 10^{-3} \text{ m}^2 \text{ s}^{-1}$$

and

$$S = 1000 \times 9.81 \times (0.15 \times 4.4 \times 10^{-10} + 10^{-8}) \times 70 = 6.912 \times 10^{-3}$$

We also know that the production rate, $Q_w = 2800 \div (24 \times 60^2) = 0.03241 \text{ m}^3\text{s}^{-1}$ and the time of interest is $15 \times 60^2 = 54000 \text{ s}$.

The piezometric drawdown can now be determined using Jacob's approximation. For the drawdown in the production well, $r = 0.05 \text{ m}$ (the radius of the well) so

$$\eta = 1.015 \times \left[\ln \left(\frac{79400}{0.05^2} \right) - 0.5772 \right] = 16.95 = 17.0 \text{ m}$$

For the drawdown in the observation well, $r = 20 \text{ m}$ so

$$\eta = 1.015 \times \left[\ln \left(\frac{79400}{20^2} \right) - 0.5772 \right] = 4.784 = 4.78 \text{ m}$$

(b) The radius of influence can be determined from Eq. (16.17):

$$\begin{aligned} r_e &= 1.499 \left(\frac{Tt}{S} \right)^{1/2} \\ &= 1.499 \times \left(\frac{2.541 \times 10^{-3} \times 54000}{6.912 \times 10^{-3}} \right)^{1/2} = 211 \text{ m} \end{aligned}$$

(c) From Eq. (16.18) we have that

$$\eta = \frac{Q_w}{4\pi T} \left[\ln \left(\frac{4Tt}{Sr^2} \right) - 0.57721 \right] + \left(\frac{Q_w}{2\pi H} \right)^2 \frac{b}{gr}$$

where b is found from Eq. (12.27):

$$\begin{aligned} b &= 0.005k^{-0.5}\phi^{-5.5} \\ &= 0.005 \times (3.7 \times 10^{-12})^{-0.5} \times 0.15^{-5.5} \\ &= 8.838 \times 10^7 \text{ m}^{-1} \end{aligned}$$

from which it follows that for the production well

$$\eta = 16.95 + \frac{0.04891}{0.05} = 17.9 \text{ m}$$

and the for the observation well

$$\eta = 4.784 + \frac{0.04891}{20} = 4.79 \text{ m}$$

This is a good example showing how non-Darcy effects are less important for interpreting measurements from the observation well.

Worked Solution 16.2 (see Problem 16.2)

The following MATLAB code produces the requested plots:

```
%Use the Theis solution and the method
%of images to plot drawdown in an
%observation well in proximity to a
%production well and an impermeable
%boundary or a fixed-head boundary.
Qw=1500; %Production rate (m3/day)
S=0.0015; %Storativity (-)
T=750; %Transmissivity (m2/day)
r=50; %Distance to observation well (m)
a=200; %Distance to boundary (m)
%Specify times to evaluate for (days)
t=linspace(0,1,300)';
%Drawdown due to production well
etaP=Qw/4/pi/T*expint(S*r^2/4/T./t);
%Drawdown due to image well
etaI=Qw/4/pi/T*expint(S*(r+2*a)^2/4/T./t);
%Plot results
figure
plot(t,[etaP etaP+etaI etaP-etaI])
xlabel('Time (days)')
ylabel('Drawdown (m)')
legend('a) Infinite aquifer',...
'b) Impermeable boundary',...
'c) Fixed-head boundary')
```

The resulting graphs are shown in Fig. 16.4.

Worked Solution 16.3 (see Problem 16.3)

The following MATLAB code produces the requested plot:

```
%Use the Theis solution and the
%principle of superposition to plot
%drawdown and recovery in an
%observation well in proximity to a
%production well pumping for 0.4 days.
Qw=1500; %Production rate (m3/day)
S=0.0015; %Storativity (-)
T=750; %Transmissivity (m2/day)
r=50; %Distance to observation well (m)
```

Fig. 16.4 Plots of drawdown against time for aquifers with different boundary conditions

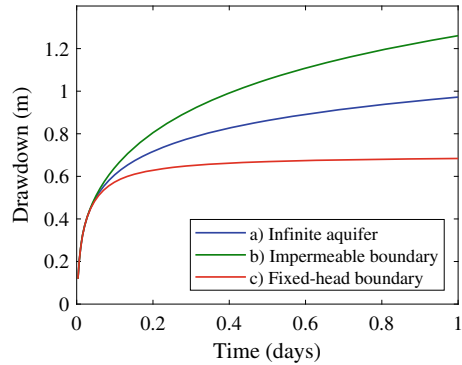
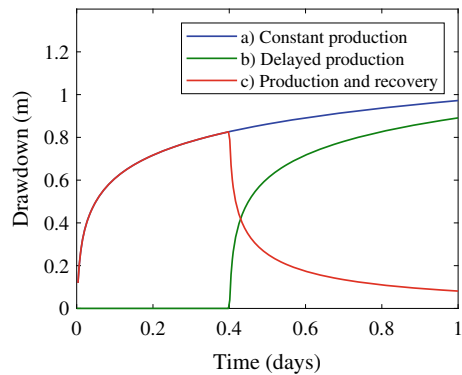


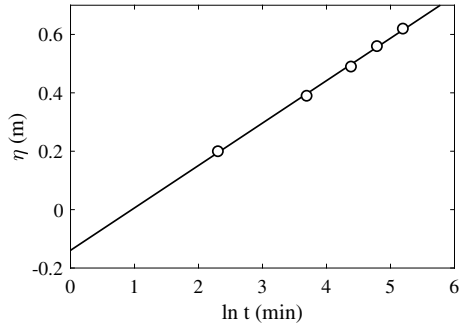
Fig. 16.5 Demonstration showing the use of the principle superposition to simulate the recovery period after a pumping test



```
t0=0.4; %Duration of pumping (days)
%Specify times to evaluate for
t=linspace(0,1,300)';
%Drawdown due to production well
etaP=Qw/4/pi/T*expint(S*r^2/4/T./t);
%Drawdown due to delayed production well
etaI=Qw/4/pi/T*expint(S*r^2/4/T./(t-t0));
etaI(t<t0)=0;
%Plot results
figure
plot(t,[etaP etaI etaP-etaI])
xlabel('Time (days)')
ylabel('Drawdown (m)')
legend('a) Constant production',...
       'b) Delayed production',...
       'c) Production and recovery')
```

The resulting graphs are shown in Fig. 16.5.

Fig. 16.6 Fitting Jacob's approximation to drawdown data



Worked Solution 16.4 (see Problem 16.4)

(a) The first step is to calculate the natural log of time:

t (min)	10	40	80	120	180
η (m)	0.20	0.39	0.49	0.56	0.62
$\ln t$ (min)	2.303	3.689	4.382	4.787	5.193

We then need to plot drawdown against the natural log of time and fit a straight line through the data to find the y-axis intercept and slope (see Fig. 16.6).

The y-axis intercept, $c = -0.1394$, and the slope, $m = 0.1453$. From Eq. (16.21):

$$T = \frac{Q_w}{4\pi m} = \frac{1}{4 \times \pi \times 0.1453} = 0.548 \text{ m}^2 \text{ min}^{-1}$$

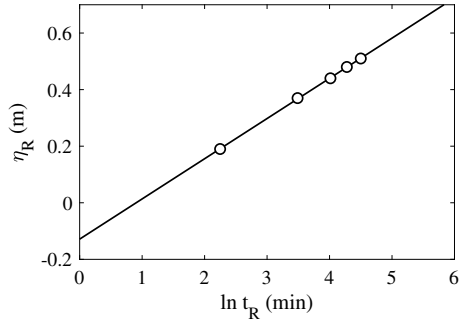
and

$$\begin{aligned} S &= \frac{Q_w}{\pi m r^2} \exp\left(-\frac{c}{m} - \gamma\right) \\ &= \frac{1}{\pi \times 0.1453 \times 50^2} \exp\left(\frac{0.1394}{0.1453} - 0.5772\right) \\ &= 0.00128 \end{aligned}$$

(b) The first step is to calculate η_R and $\ln t_R$ using Eq. (16.28). In this case $t_0 = 180$ min and $\eta_0 = 0.62$ m. It follows that:

t (min)	190	220	260	300	360
η (m)	0.43	0.25	0.18	0.14	0.11
t_R (min)	9.474	32.73	55.38	72.00	90.00
η_R (m)	0.19	0.37	0.44	0.48	0.51
$\ln t_R$ (min)	2.249	3.488	4.014	4.277	4.500

Fig. 16.7 Fitting Jacob's approximation to recovery data



We then need to plot drawdown against the natural log of time and fit a straight line through the data to find the y-axis intercept and slope (see Fig. 16.7). The y-axis intercept, $c = -0.1285$, and the slope, $m = 0.1421$. From Eq. (16.21):

$$T = \frac{Q_w}{4\pi m} = \frac{1}{4 \times \pi \times 0.1421} = 0.560 \text{ m}^2 \text{ min}^{-1}$$

and

$$\begin{aligned} S &= \frac{Q_w}{\pi m r^2} \exp\left(-\frac{c}{m} - \gamma\right) \\ &= \frac{1}{\pi \times 0.1421 \times 50^2} \exp\left(\frac{0.1285}{0.1421} - 0.57721\right) \\ &= 0.00124. \end{aligned}$$

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Abstract

This chapter focuses on the development of mathematical equations to describe water movement in the vadose zone (the subsurface region above the water table otherwise referred to as the unsaturated zone). The concepts of negative pressure head, surface tension, wettability and air-entry pressure are explained. Empirical functions are presented for describing how moisture content and hydraulic conductivity reduce with increasingly negative pressure head. These are combined with the previously derived transient groundwater flow equation, leading to the development of Richards' equation for water movement in partially saturated porous media. A specific capacity function is derived by combining a soil moisture characteristic curve with the specific storage coefficient. It is explained how to estimate runoff and infiltration rates from rainfall data and infiltration capacity functions. Theoretical infiltration capacity functions, the Green and Ampt solution and the Philip equation, are derived from Richards' equation by imposing a sharp wetting front assumption. Various methods are explained and compared for obtaining in situ field measurements for moisture content and negative pressure head. Quantitative methods are presented for determining soil moisture deficit and depth to zero flux plane. Practical applications are presented through a problem sheet with worked solutions.

Notation

- A Cross-sectional area [L^2].
 C Specific moisture capacity [L^{-1}].
 c_R Rock compressibility [$M^{-1}LT^2$].
 c_F Fluid compressibility [$M^{-1}LT^2$].
 D Cylindrical capillary tube diameter [L].

f	Infiltration capacity [LT^{-1}].
F	Volume of water infiltrated through a unit area of land surface [L].
g	Gravitational acceleration [LT^{-2}].
h	Hydraulic head [L].
K	Hydraulic conductivity [LT^{-1}].
K_0	Hydraulic conductivity at the land surface [LT^{-1}].
K_i	Initial hydraulic conductivity [LT^{-1}].
K_s	Saturated hydraulic conductivity [LT^{-1}].
L	Length of sample or depth [L].
L_f	Depth of wetting front [L].
m	Empirical exponent for the S_e function [-].
m_W	Mass of water per unit volume of rock [ML^{-3}].
p	Pressure [$\text{ML}^{-1}\text{T}^{-2}$].
p_e	Air-entry pressure [$\text{ML}^{-1}\text{T}^{-2}$].
p_A	Air pressure [$\text{ML}^{-1}\text{T}^{-2}$].
p_W	Water pressure [$\text{ML}^{-1}\text{T}^{-2}$].
q	Darcy flux [LT^{-1}].
Q	Flow rate [L^3T^{-1}].
s	Distance in the direction of flow [L].
S	Sorptivity [$\text{LT}^{-1/2}$].
S_e	Effective saturation [-].
S_s	Specific storage coefficient [L^{-1}].
t	Time [T].
V_R	Volume of voids containing the residual moisture content [L^3].
V_T	Volume of porous material [L^3].
V_V	Volume of voids [L^3].
V_W	Volume of water present in pore-space [L^3].
z	Elevation [L].
z_0	Elevation of the land surface [L].
z_f	Elevation of a sharp wetting front [L].
α	Pressure head scaling parameter for the S_e function [L^{-1}].
γ_{st}	Surface tension [MT^{-2}].
η	Empirical exponent for the K function [-].
θ	Moisture content [-].
θ_0	Moisture content at the land surface [-].
θ_i	Initial moisture content [-].
θ_r	Residual moisture content [-].
θ_s	Saturated moisture content [-].
Θ	Contact angle [-].
λ	Similarity transform [$\text{LT}^{-1/2}$].
ρ	Fluid density [ML^{-3}].
ϕ	Porosity [-].
ψ	Pressure head [L].
ψ_0	Pressure head at the land surface [L].

ψ_e	Air-entry pressure head [L].
ψ_i	Initial pressure head [L].
ψ_{wt}	Elevation of the water table [L].

17.1 Introduction

The vadose zone represents the subsurface region above the water table. The vadose zone is important in hydrology because it controls how much rainfall infiltrates the land surface, how much water evaporates or transpires back to the atmosphere and how much water drains down to underlying aquifers. In previous chapters, we learnt how to use Darcy's law to describe water movement in the saturated zone. In this chapter we extend these ideas to model water movement in unsaturated porous media. We will derive some simple models to predict infiltration rates and explore different field methods for observing water movement within the vadose zone.

The chapter is structured as follows: First we develop key concepts, including negative pressure head, surface tension and relationships between moisture content, hydraulic conductivity and pressure head. Our transient groundwater flow equation is then extended to account for partial water saturation. We then make a sharp wetting front assumption, enabling the derivation of an important analytical solution used to estimate infiltration and surface runoff. We study different measurement methods for observing moisture content and negative pressure head, in the context of a case-study from Berkshire in the UK. Finally, some practical exercises are provided involving estimation of infiltration rates, runoff rates, soil moisture deficits and the direction of fluid movement within the vadose zone.

17.2 Basic Principles

17.2.1 Negative Pressure Heads

The pore-space beneath the water table (the saturated zone) is completely filled with water. The pore-space above the water table (the vadose zone or unsaturated zone) is partially filled with water and air. The amount of water present in the vadose zone can be quantitatively described by its moisture content, θ , defined by

$$\theta = \frac{V_W}{V_T}$$

where V_T [L³] is the volume of a portion of porous material and V_W [L³] is the volume of water present in its pore-space.

The continuous presence of water in the vadose zone means that the concept of groundwater hydraulic head can be extended up to the land surface. An interesting phenomenon is observed by considering a hydrostatic profile, as shown in Fig. 17.1.

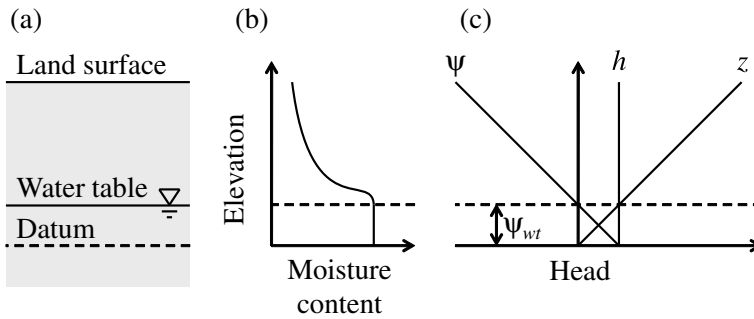


Fig. 17.1 **a** Schematic diagram of a water table below a land surface. **b** A hypothetical moisture content profile for a hydrostatic homogeneous soil column with a water table. **c** Plots of hydraulic head, h , pressure head, ψ , and elevation head, z , against elevation, z , for a hydrostatic profile with a water table located at $z = \psi_{wt}$

Assuming a homogeneous porous medium, the moisture content will be constant within the saturated zone and equal to the porosity of the porous medium. Above the water table, the moisture content continuously declines with elevation (Fig. 17.1b).

Let our datum for elevation head, z [L], be a distance, ψ_{wt} [L], below the water table. The pressure head, ψ [L], at the datum will therefore be ψ_{wt} . Under hydrostatic conditions, there is no hydraulic head gradient, and the hydraulic head, $h = \psi_{wt}$ throughout the vertical profile under consideration. Recalling that $h = \psi + z$, it follows that (Fig. 17.1c)

$$\psi = \psi_{wt} - z$$

At the water table, the pressure head is zero ($\psi(z = \psi_{wt}) = 0$). Above the water table, the pressure head will be negative. Negative pressure heads are a defining characteristic of the vadose zone.

17.2.2 Surface Tension and Wettability

Water in the vadose zone is held against gravity by surface tension. Consider a liquid-gas interface (Fig. 17.2a). Molecules of liquid are more attracted to each other than they are to gas molecules at the interface. This gives rise to a tension force that develops along the interface. The property, surface tension, γ_{st} [MT^{-2}], represents the tension force per unit length of gas-liquid-solid interface. Surface tension is dependent on the interaction characteristics of the two fluids of concern. It is independent of any solid involved with the interface. The surface tension of water in air at 20°C is $7.27 \times 10^{-2} \text{ N m}^{-1}$ [1, p. 40].

Consider two fluid phases in the presence of a solid surface. It is often the case that one fluid phase has a stronger affinity with the solid surface than the other. This fluid is known as the wetting fluid and is said to have a preferential wettability for that surface.

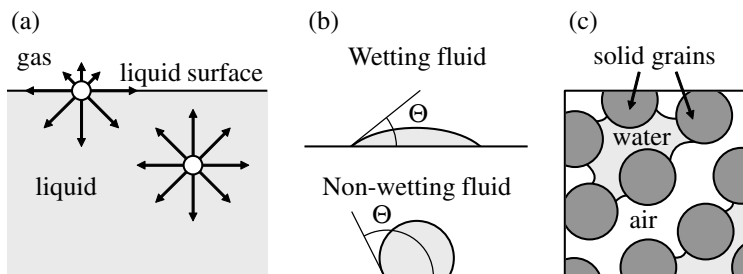


Fig. 17.2 Schematic diagrams showing: **a** how molecular attractions at a liquid-gas interface give rise to a surface in tension; **b** the contact angle, Θ , for globules of wetting fluid and non-wetting fluid on a solid surface; **c** how globules of water in an unsaturated water-wet porous medium arrange themselves with concave water-air interfaces

A globule of wetting fluid will spread out on a solid surface. In contrast, a globule of non-wetting fluid will hold in on itself. The wettability of a fluid-solid combination can be quantified in terms of a contact angle, Θ (Fig. 17.2b). A low contact angle implies that a fluid has high wettability and vice versa.

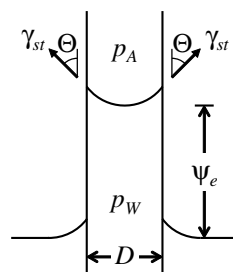
Many soils and rocks are often assumed to be water wet, with a water contact angle close to zero. This gives rise to the idea that water is held within the pores with a concave water-air interface (Fig. 17.2c).

17.2.3 Air-Entry Pressure of a Capillary Tube

As stated above, the pressure head within the vadose zone is negative. The surface tension effect within a porous medium gives rise to a strong relationship between moisture content and pressure head.

To gain further insight we will consider the surface tension that develops in a cylindrical capillary tube of diameter, D [L]. When such a tube is placed in a basin of water, the water will rise up the capillary tube to an elevation, ψ_e [L], above the surrounding water surface (Fig. 17.3). The column of water is held against gravity due to surface tension, γ_{st} . The wettability of the water within the tube is such that the water surface intersects the walls of the tube at an angle of Θ to the vertical (the contact angle).

Fig. 17.3 Schematic diagram of a capillary tube



Challenge 17.1 Use a vertical force balance to determine a relationship between the water column height, ψ_e , and the diameter of the capillary tube, D .

The force holding the column of water up is due to the vertical component of the surface tension,

$$\pi D \gamma_{st} \cos \Theta$$

At the same time, the column of water is pulled down by its weight,

$$\frac{\pi D^2 \psi_e \rho g}{4}$$

where ρ [ML^{-3}] is the density of the water and g [LT^{-2}] is gravitational acceleration.

Since the column of water is static

$$\pi D \gamma_{st} \cos \Theta = \frac{\pi D^2 \psi_e \rho g}{4}$$

and therefore

$$\psi_e = \frac{4 \gamma_{st} \cos \Theta}{D \rho g}$$

Let p_A [$\text{ML}^{-1}\text{T}^{-2}$] and p_W [$\text{ML}^{-1}\text{T}^{-2}$] be the pressure in the air and water, respectively. It is possible to push the water out of the tube by increasing the air pressure such that $p_A > p_W + p_e$, where $p_e = \rho g \psi_e = 4 \gamma_{st} \cos \Theta / D$ is referred to as the air-entry pressure. Notice that the smaller the capillary tube diameter, the harder it is to move the water out.

The pressure, p [$\text{ML}^{-1}\text{T}^{-2}$], in our equation for pressure head, $\psi = p/(\rho g)$, is not an absolute pressure but instead the water pressure relative to the local air pressure, i.e., $p = p_W - p_A$. It follows that $\psi = (p_W - p_A)/(\rho g)$. Furthermore, it can be said that the water held by surface tension in a capillary tube will drain when $\psi < -\psi_e$.

A porous medium can be thought of as a bundle of capillary tubes with some random distribution of pore-sizes. Each pore will hold water against gravity until the pressure head drops below a negative critical level, inversely proportional to its diameter. This implies that if we drain a saturated soil sample, the largest pores empty first and the smallest pores empty last. Conversely, if we fill a dry soil sample with water, the smallest pores fill with water first and the largest pores last.

17.2.4 Soil Moisture Characteristic Curve

The soil moisture characteristic curve describes the relationship between moisture content, θ , and pressure head, ψ , for a given porous medium. There are many ways to obtain soil moisture characteristic curves [2]. For brevity, we will focus on the pressure plate method.

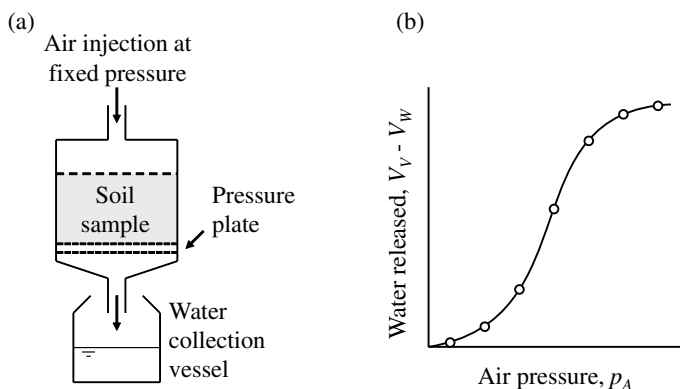


Fig. 17.4 Schematic diagram of a pressure plate apparatus for obtaining a soil moisture characteristic curve

A soil sample is saturated with water and placed into a pressure cell with a pressure plate at the base (Fig. 17.4a). The pressure plate comprises a ceramic porous material with a known air-entry pressure.

The underside of the pressure plate is maintained at atmospheric conditions. Air is injected into the pressure cell at a fixed pressure (greater than atmospheric pressure) such that water is displaced from the soil sample through the pressure plate, into a water collection vessel below.

Once water ceases to drain from the pressure cell, the volume of water is recorded and the air pressure is increased to a new value, and a subsequent release of water is measured, and so on (Fig. 17.4b).

Providing the air pressure, p_A does not exceed the air-entry pressure, p_e , of the ceramic pressure plate, only water is able to leave the pressure cell. The air-entry pressure of the pressure plate must be larger than the maximum air pressure to be applied in the experiment, for the results to be valid.

At the end of the experiment, the soil sample is removed and the remaining moisture content is determined by a gravimetric method. The results of the experiment can be used to determine how the moisture content changed with air pressure. The fact that the underside of the pressure plate is maintained at atmospheric conditions implies that the water pressure, p_W , is the same as the atmospheric pressure. A set of corresponding pressure heads, ψ , can therefore be calculated from the air pressure values, and the soil moisture characteristic curve can be determined.

Figure 17.5a shows example soil moisture characteristic curves for three different materials. The sandstone can be seen to significantly reduce its moisture content over a narrow interval of negative pressure head. This suggests that it has a well-sorted pore-size distribution. Notice that the moisture content does not drop below 0.15. This lower level of moisture content is referred to as the residual moisture content. The clay has a much higher porosity and is poorly sorted. The silt loam provides an intermediate response between the sandstone and the clay.

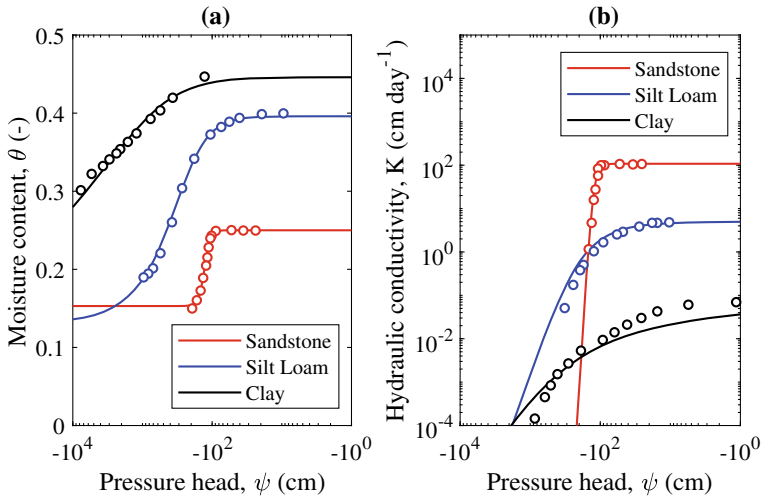


Fig. 17.5 Soil moisture characteristic curves and unsaturated hydraulic conductivity for three different porous media (data acquired from [3])

17.2.5 Unsaturated Hydraulic Conductivity

Given that the moisture content of a porous medium declines with reducing pressure head it can be understood that the hydraulic conductivity will also reduce. Unsaturated hydraulic conductivity can be obtained using a modified permeameter that takes advantage of pressure plates. A schematic diagram of such a scheme is presented in Fig. 17.6a.

A saturated soil sample is enclosed within a cylindrical casing bounded above and below by pressure plates. Both the inlet and outlet of the pressure cell are connected to separate fixed head devices, which are located below so as to impose negative pressure head conditions. The pressure plates make a hydraulic connection between water filled pores and the water filled inlet and outlet tubes. Water is therefore sucked from the inlet by a syphoning effect and then transported through the soil sample to the outlet. The cylindrical casing is perforated with small holes to enable the air-phase within the porous medium to remain at atmospheric conditions. Once a steady-state flow rate, Q [L^3T^{-1}], is observed, the hydraulic conductivity, K [LT^{-1}] of the sample can be obtained using a rearrangement of Darcy's law.

Recall Darcy's law (Eq. (12.5))

$$\frac{Q}{A} = -K \frac{\partial h}{\partial s} = -K \left(\frac{\partial \psi}{\partial s} + \frac{\partial z}{\partial s} \right) = -K \left(\frac{\psi_2 - \psi_1}{L} - 1 \right)$$

where A [L^2] is the cross-sectional area of the soil sample, s [L] is distance in the direction of flow, L [L] is the thickness of the soil sample, ψ_1 [L] is the pressure head at the top of the soil sample and ψ_2 [L] is the pressure head at the base.

Note that if $\psi_1 = \psi_2$, then $Q = K$. The boundary pressure heads can be progressively decreased to obtain different associated values of unsaturated hydraulic

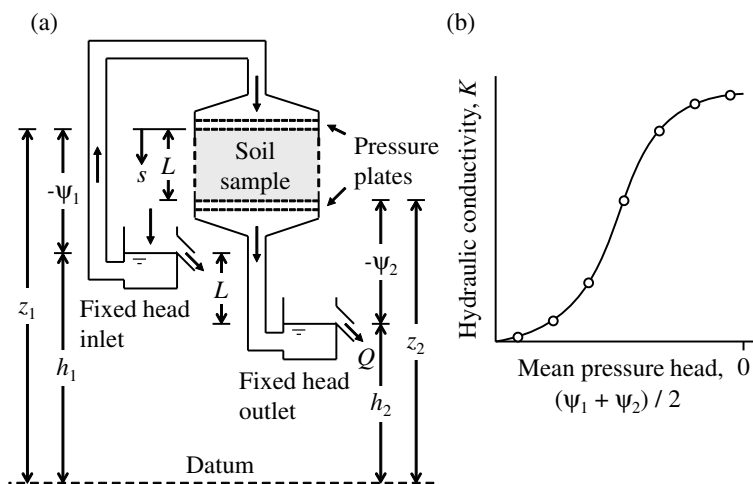


Fig. 17.6 Schematic diagram of a steady-state measuring device for unsaturated hydraulic conductivity. Note that the cylindrical casing of the soil samples requires additional holes to maintain an atmospheric air pressure within the pore-space

conductivity (see Fig. 17.6b). As the pressure reduces the moisture content reduces and air is sucked into the pore-space through the holes in the cylindrical casing, such that the air-pressure is maintained at atmospheric conditions.

Figure 17.5b shows some example unsaturated hydraulic conductivity curves for three different porous media. Hydraulic conductivity non-linearly decreases with decreasing pressure head and moisture content. This is because the largest pores de-water first and therefore the most permeable pathways are lost at the beginning of a drainage cycle. Furthermore, as more pores are de-watered, remaining water filled pathways become blocked by air. Consequently there is a residual moisture content that is effectively impermeable, which can only be moved by vapour diffusion or film flow (see [4]).

17.2.6 Empirical Functions

A commonly used set of empirical functions for soil moisture characteristic curves and unsaturated hydraulic conductivity, due to [3], include:

$$\theta = (\theta_s - \theta_r)S_e + \theta_r$$

$$K = K_s S_e^\eta [1 - (1 - S_e^{1/m})^m]^2$$

where S_e [-] is referred to as the effective saturation, found from

$$S_e = \left(1 + |\alpha \psi|^{1/(1-m)}\right)^{-m}$$

and θ_s [-] is the saturated moisture content, θ_r [-] is the residual moisture content, K_s [LT⁻¹] is the saturated hydraulic conductivity, α [L⁻¹] is an empirical pressure

head scaling parameter, m [–] is an empirical exponent characterising the pore-size distribution and η is an empirical exponent characterising the tortuosity of flow pathways.

At saturation (i.e., $\psi \geq 0$), $S_e = 1$, $\theta = \theta_s$ and $K = K_s$. At residual saturation (i.e., $\psi \rightarrow -\infty$), $S_e = 0$, $\theta = \theta_r$ and $K = 0$. Examples of such functions are plotted as solid lines alongside the experimental data shown in Fig. 17.5.

Values for θ_s , θ_r , K_s , α , m and η can be predicted for a given soil texture using a pedotransfer function, for example, the ROSETTA database [5]. The ROSETTA database uses an artificial neural network to interpolate experimental results from several thousand soil samples. Soil texture concerns the percentage of clay, silt and sand in a given soil. Particles less than 0.002 mm in diameter are considered clay particles. Particles greater than 0.05 mm in diameter are considered sand particles. Any particles with diameters between 0.002 and 0.05 mm are classified as silt particles.

17.3 Richards' Equation

Consider the transient groundwater flow equation (Eq. (15.5))

$$\frac{\partial m_w}{\partial t} = \nabla \cdot (\rho \mathbf{K} \nabla h)$$

where m_w [ML^{-3}] is the mass of water per unit volume of rock or soil, t [T] is time, ρ [ML^{-3}] is the fluid density, $\mathbf{K}$ [LT^{-1}] is the hydraulic conductivity tensor and h [L] is hydraulic head.

For groundwater flow in the saturated zone we sought to write the above PDE in a form such that h was the only dependent variable. This gave rise to the specific storage coefficient, S_s [L^{-1}]. However, for unsaturated conditions, $\mathbf{K}$ is a function of pressure head, ψ . Therefore, it is convenient to find a new form that is written with ψ as the only dependent variable.

Recall that $h = \psi + z$. Therefore

$$\frac{\partial m_w}{\partial t} = \nabla \cdot \left[\rho \mathbf{K} \left(\nabla \psi + \hat{\mathbf{k}} \right) \right]$$

where

$$\hat{\mathbf{k}} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

17.3.1 Pressure Head Formulation

The left-hand-side of the above equation can be written with ψ as the dependent variable by introducing another function, the specific moisture capacity, $C(\psi)$ [L^{-1}],

whereby

$$\rho C(\psi) \frac{\partial \psi}{\partial t} = \nabla \cdot \left[\rho \mathbf{K} (\nabla \psi + \hat{\mathbf{k}}) \right] \quad (17.1)$$

which is known as the pressure head formulation of Richards' equation.

Both C and $\mathbf{K}$ are non-linear functions of ψ . The specific moisture capacity, $C(\psi)$ [L^{-1}], represents the volume of water released per unit volume of soil (or rock) as a result of a unit decline in pressure head. Mathematically, it can be stated that

$$C(\psi) = \frac{1}{\rho} \frac{\partial m_W}{\partial \psi}. \quad (17.2)$$

17.3.2 Specific Moisture Capacity

We can derive an expression for the specific moisture capacity, $C(\psi)$, in terms of the specific storage coefficient, S_s , previously discussed in Sect. 15.5.1.

Recall the definitions of fluid compressibility, c_F [M^{-1}LT^2], and rock compressibility, c_R [M^{-1}LT^2]:

$$c_F = \frac{1}{\rho} \frac{\partial \rho}{\partial p} \quad \text{and} \quad c_R = \frac{1}{V_T} \frac{\partial V_V}{\partial p}$$

where V_T [L^3] is the total volume of porous material being studied and V_V [L^3] is the volume of voids contained within the material.

The relevance here is that

$$\theta = (\theta_s - \theta_r) S_e + \theta_r$$

where $\theta = V_W/V_T$ and V_W [L^3] is the volume of water contained within the voids.

Let us define V_R as the volume of voids containing the residual moisture content, such that $\theta_r = V_R/V_T$. Note that $\theta_s \equiv \phi = V_V/V_T$, where ϕ [-] is the porosity of the porous medium. It follows that

$$V_W = (V_V - V_R) S_e + V_R \quad (17.3)$$

It is further assumed that V_R/V_V is constant. A consequence of this assumption is that

$$\frac{\partial V_R}{\partial V_V} = \frac{V_R}{V_V}$$

and therefore

$$\frac{1}{V_T} \frac{\partial V_R}{\partial p} = \left(\frac{V_R}{V_V} \right) \frac{1}{V_T} \frac{\partial V_V}{\partial p} \quad (17.4)$$

Challenge 17.2 Use the above information and apply similar procedures to those in Sect. 15.4.1 to derive a relationship between $C(\psi)$, S_s , ϕ , θ , θ_s , θ_r and $\partial S_e / \partial \psi$.

Given Eq. (17.2) and that $m_W = \rho V_W / V_T$, it follows that

$$C(\psi) = \frac{1}{\rho V_T} \frac{\partial(\rho V_W)}{\partial \psi}$$

Substituting Eq. (17.3) and applying the product rule leads to

$$C(\psi) = \frac{\theta}{\rho} \frac{\partial \rho}{\partial \psi} + \frac{1}{V_T} \left[\left(\frac{\partial V_V}{\partial \psi} - \frac{\partial V_R}{\partial \psi} \right) S_e + \frac{\partial V_R}{\partial \psi} \right] + (\theta_s - \theta_r) \frac{\partial S_e}{\partial \psi}$$

Recall that $\frac{\partial p}{\partial \psi} = \rho g$ so

$$C(\psi) = \rho g \left\{ \frac{\theta}{\rho} \frac{\partial \rho}{\partial p} + \frac{1}{V_T} \left[\left(\frac{\partial V_V}{\partial p} - \frac{\partial V_R}{\partial p} \right) S_e + \frac{\partial V_R}{\partial p} \right] \right\} + (\theta_s - \theta_r) \frac{\partial S_e}{\partial \psi}$$

Imposing the assumption about the compressibility of the residual moisture content pore-space, given in Eq. (17.4), it follows that

$$C(\psi) = \rho g \left\{ \frac{\theta}{\rho} \frac{\partial \rho}{\partial p} + \left[\frac{(V_V - V_R) S_e + V_R}{V_V} \right] \frac{1}{V_T} \frac{\partial V_V}{\partial p} \right\} + (\theta_s - \theta_r) \frac{\partial S_e}{\partial \psi}$$

Substituting the expressions for fluid compressibility, rock compressibility, porosity and moisture content then yields

$$C(\psi) = \frac{\theta S_s}{\phi} + (\theta_s - \theta_r) \frac{\partial S_e}{\partial \psi}$$

where (recall Eq. (15.10))

$$S_s = \rho g (\phi c_F + c_R)$$

Note that $C(\psi \geq 0) = S_s$.

17.3.3 Moisture Content Formulation

The water and rock are sometimes assumed to be incompressible, in which case, Eq. (15.5) reduces directly to

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \left[\mathbf{K} (\nabla \psi + \hat{\mathbf{k}}) \right] \quad (17.5)$$

which is known as the moisture content formulation of Richards' equation.

17.4 Infiltration Modelling

The infiltration rate is the rate at which water passes into the soil from the land surface. The maximum infiltration rate that can be accommodated by a given soil at a given time is referred to as the infiltration capacity. Surface runoff can be determined from the excess rainfall that does not infiltrate the soil for a given rainfall event.

Imagine applying water to initially dry soil at a constant supply rate (see Fig. 17.7). At the beginning, all the water infiltrates the soil. Eventually, ponding occurs and the infiltration rate will reduce as the near-surface pore-space is used up. Finally the infiltration rate reaches a steady-state rate, which is dependent on the hydraulic conductivity of the soil.

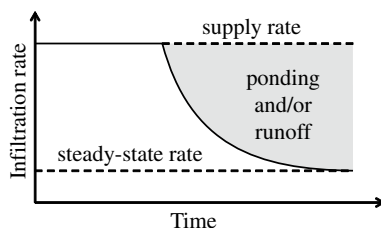


Fig. 17.7 Schematic plot of infiltration rate against time for a constant supply rate

17.4.1 Infiltration Capacity

Figure 17.8 shows some simple examples of how a theoretical infiltration capacity curve can be used to determine volumes of infiltration and surface runoff for a given rainfall event.

Infiltration capacity represents a theoretical infiltration rate that would occur if an initially dry soil surface was suddenly inundated by a shallow water body, held at a constant water depth, indefinitely. Initially the infiltration capacity is very high due to the presence of abundant near-surface pore-space to accommodate the infiltrating water. Infiltration capacity declines, non-linearly with time, as the pore-space is continuously used up. The steady-state rate represents gravity drainage of water

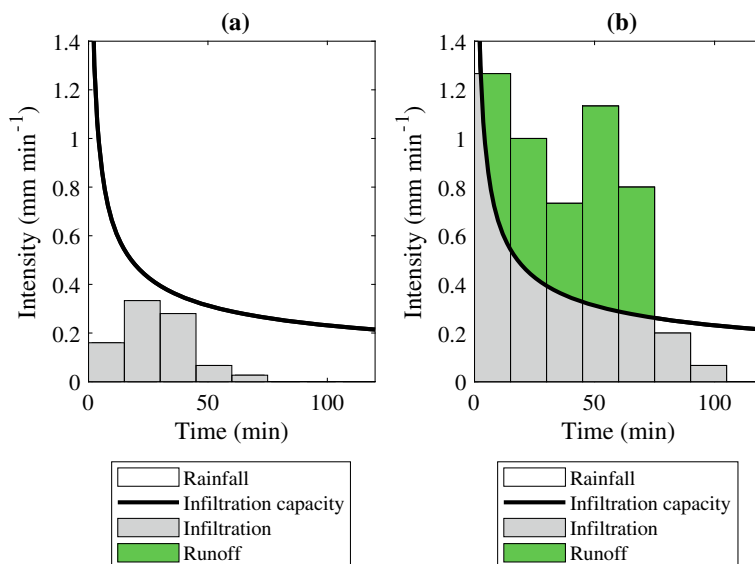


Fig. 17.8 Infiltration examples. **a** Rainfall is less than infiltration capacity so all rainfall becomes infiltration. **b** Rainfall is greater than infiltration capacity at the beginning and some surface runoff develops (the green shaded area)

from the near-surface pore-space, which will continue to occur after the near-surface pore-space has reached saturation.

In Fig. 17.8a, the rainfall rate is always less than the infiltration capacity. Therefore there is no expected runoff and the actual infiltration rate is expected to be equal to the rainfall rate.

In Fig. 17.8b, the rainfall rate initially exceeds the infiltration capacity. During this period, the infiltration rate equals the infiltration capacity and the excess rainfall forms surface runoff (the green shaded area). However, towards the end of the rainfall event, the rainfall rate is less than the infiltration capacity. For this latter period, there is no expected runoff and the actual infiltration rate is expected to be equal to the rainfall rate.

In the event that rainfall is initially less than infiltration capacity but then exceeds infiltration capacity, later on during the rainfall event, a complicated procedure, known as time compression, is required to determine the infiltration and runoff volumes (see [6, p. 164]).

17.4.2 Sharp Wetting Front Assumption

Below we will use Richards' equation to obtain an analytical solution for infiltration capacity using a sharp wetting front assumption. The soil is assumed to be homogeneous and initially dry with a uniform moisture content. The land surface is then exposed to a fixed pressure head condition such that infiltration occurs and a sharp wetting front migrates downwards through the soil profile.

Flow is one-dimensional and the water and soil are assumed to be incompressible such that

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} \quad (17.6)$$

where the Darcy flux, q [LT^{-1}], is found from Darcy's law

$$q = -K \left(\frac{\partial \psi}{\partial z} + 1 \right) \quad (17.7)$$

The relevant initial and boundary conditions are:

$$\begin{aligned} \psi &= \psi_i, \quad z \leq z_0 \quad t = 0 \\ \psi &= \psi_0, \quad z = z_0 \quad t > 0 \end{aligned}$$

where z_0 [L] is the elevation of the land surface, ψ_i [L] is the initial pressure head and ψ_0 [L] is the land surface pressure head.

Let z_f be the elevation of a sharp wetting front below the land surface (see Fig. 17.9) such that

$$\psi = \begin{cases} \psi_0, & z \in (z_f, z_0] \\ \psi_i, & z \leq z_f \end{cases}$$

It follows that

$$\theta = \begin{cases} \theta_0, & z \in (z_f, z_0] \\ \theta_i, & z \leq z_f \end{cases} \quad \text{and} \quad K = \begin{cases} K_0, & z \in (z_f, z_0] \\ K_i, & z \leq z_f \end{cases}$$

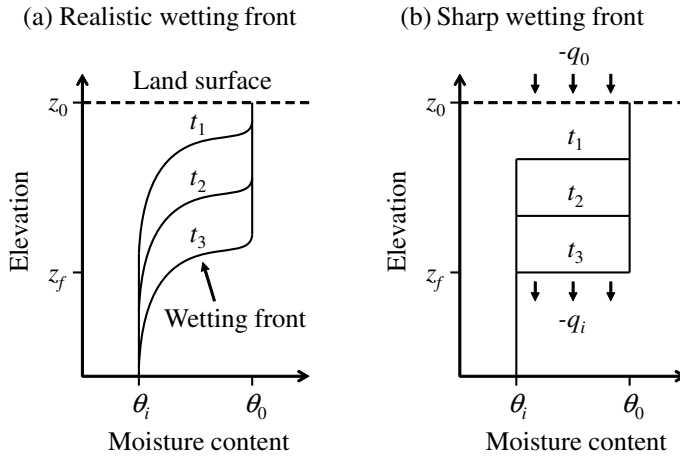


Fig. 17.9 Schematic diagram comparing a realistic wetting front with a sharp wetting front

where $\theta_0 = \theta(\psi_0)$, $\theta_i = \theta(\psi_i)$, $K_0 = K(\psi_0)$ and $K_i = K(\psi_i)$.

It is further assumed that

$$q = \begin{cases} q_0, & z \in (z_f, z_0] \\ q_i, & z \leq z_f \end{cases}$$

Let $L_f = z_0 - z_f$ be the depth of the wetting front. The volume of water that has infiltrated through a unit area of land surface, F [L], at time, t , is found from

$$F \equiv - \int_0^t q_0 dt = (\theta_0 - \theta_i) L_f - \int_0^t q_i dt \quad (17.8)$$

In what follows we will determine an analytical solution for L_f such that Eq. (17.8) can be differentiated with respect to time, to obtain an expression for q_0 , as a function of time. The infiltration rate, $f = -q_0$, is analogous to the infiltration capacity, we discussed previously.

First we will derive an expression for q_0 in terms of z_f . Then we will obtain a differential equation for L_f , which can be solved implicitly. We will make an additional assumption such that an explicit solution for L_f is found. An expression for q_0 is then determined as an explicit function of time.

Challenge 17.3 Determine expressions for q_0 and q_i using Darcy's law.

Integrating both sides of Darcy's law (Eq. (17.7)) leads to

$$\int_{z_f}^{z_0} q dz = - \int_{\psi_i}^{\psi_0} K d\psi - \int_{z_f}^{z_0} K dz$$

Noting that $q = q_0$ and $K = K_0$ for $z \in (z_f, z_0]$, it follows that

$$q_0 = -K_0 \left(\frac{\psi_0 - \psi_i}{z_0 - z_f} + 1 \right) \quad (17.9)$$

Noting that $K = K_i$ and $\psi = \psi_i$ for $z \leq z_f$, it further follows that

$$\int_0^{z_f} q_i dz = - \int_{\psi_i}^{\psi_i} K d\psi - \int_0^{z_f} K_i dz$$

and

$$q_i = -K_i \quad (17.10)$$

Challenge 17.4 Integrate both sides of Eq. (17.6) with respect to z from z_f to z_0 and derive an ordinary differential equation for L_f with respect to time.

Integrating both sides of Eq. (17.6) with respect to z leads to

$$\int_{z_f}^{z_0} \frac{\partial \theta}{\partial t} dz = - \int_{z_f}^{z_0} \frac{\partial q}{\partial z} dz \quad (17.11)$$

Considering Eqs. (17.9) and (17.10)

$$- \int_{z_f}^{z_0} \frac{\partial q}{\partial z} dz = q_i - q_0 = K_0 \left(\frac{\psi_0 - \psi_i}{z_0 - z_f} + 1 \right) - K_i \quad (17.12)$$

Now consider Leibniz's theorem for differentiation of an integral [7, p. 11]

$$\frac{d}{dt} \int_{z_f}^{z_0} \theta(z, t) dz = \int_{z_f}^{z_0} \frac{\partial \theta}{\partial t} dz + \theta(z_0, t) \frac{dz_0}{dt} - \theta(z_f, t) \frac{dz_f}{dt}$$

Noting that z_0 is constant, $\theta(z \in (z_f, z_0], t) = \theta_0$ and $\theta(z_f, t) = \theta_i$, it follows that

$$\int_{z_f}^{z_0} \frac{\partial \theta}{\partial t} dz = \frac{d}{dt} \int_{z_f}^{z_0} \theta_0 dz + \theta_i \frac{dz_f}{dt} = -(\theta_0 - \theta_i) \frac{dz_f}{dt}$$

Letting $L_f = z_0 - z_f$ it follows that

$$\int_{z_f}^{z_0} \frac{\partial \theta}{\partial t} dz = (\theta_0 - \theta_i) \frac{dL_f}{dt} \quad (17.13)$$

Substituting Eqs. (17.12) and (17.13) into Eq. (17.11) leads to

$$(\theta_0 - \theta_i) \frac{dL_f}{dt} = K_0 \left(\frac{\psi_0 - \psi_i}{L_f} + 1 \right) - K_i \quad (17.14)$$

17.4.3 Implicit Solution for L_f

Challenge 17.5 Given that $L_f = 0$ when $t = 0$, derive an implicit solution for L_f .

Rearranging Eq. (17.14) leads to

$$\frac{dL_f}{dt} = \frac{K_0(\psi_0 - \psi_i) + (K_0 - K_i)L_f}{(\theta_0 - \theta_i)L_f}$$

To tidy things up, let $\delta\theta = \theta_0 - \theta_i$, $\delta\psi = \psi_0 - \psi_i$ and $\delta K = K_0 - K_i$ such that

$$\frac{dL_f}{dt} = \frac{K_0\delta\psi + \delta K L_f}{\delta\theta L_f} \quad (17.15)$$

Equation (17.15) can be further simplified by making the substitution

$$U = \frac{K_0\delta\psi + \delta K L_f}{\delta\theta} \quad (17.16)$$

such that

$$L_f \frac{dL_f}{dU} \frac{dU}{dt} = U \quad (17.17)$$

From Eq. (17.16) we have

$$\frac{dU}{dL_f} = \frac{\delta K}{\delta\theta} \quad \text{and} \quad L_f = \frac{\delta\theta}{\delta K} \left(U - K_0 \frac{\delta\psi}{\delta\theta} \right)$$

which on substitution into Eq. (17.17) leads to

$$\left(\frac{\delta\theta}{\delta K} \right)^2 \left(U - K_0 \frac{\delta\psi}{\delta\theta} \right) \frac{dU}{dt} = U \quad (17.18)$$

Separating variables and integrating both sides with respect to t leads to

$$\int \left(1 - \frac{K_0}{U} \frac{\delta\psi}{\delta\theta} \right) dU = \int \left(\frac{\delta K}{\delta\theta} \right)^2 dt$$

and therefore

$$U - K_0 \frac{\delta\psi}{\delta\theta} \ln U = \left(\frac{\delta K}{\delta\theta} \right)^2 t + A_0$$

where A_0 is an integration constant.

Reversing the substitution in Eq. (17.16) then yields

$$\frac{K_0\delta\psi + \delta K L_f}{\delta\theta} - K_0 \frac{\delta\psi}{\delta\theta} \ln \left(\frac{K_0\delta\psi + \delta K L_f}{\delta\theta} \right) = \left(\frac{\delta K}{\delta\theta} \right)^2 t + A_0$$

Recall that $L_f = 0$ at $t = 0$. Therefore

$$A_0 = K_0 \frac{\delta\psi}{\delta\theta} - K_0 \frac{\delta\psi}{\delta\theta} \ln \left(K_0 \frac{\delta\psi}{\delta\theta} \right)$$

and

$$1 - \frac{\delta\psi}{\delta K} \frac{K_0}{L_f} \ln \left(1 + \frac{\delta K}{\delta\psi} \frac{L_f}{K_0} \right) = \frac{\delta K}{\delta\theta} \frac{t}{L_f} \quad (17.19)$$

which is known as the Green and Ampt solution [8].

17.4.4 The Philip Equation

The problem with the above equation is that L_f , for a given t , must be obtained by iterative solution.

Challenge 17.6 Obtain an explicit solution for L_f for the special case when $\delta K \rightarrow 0$. Hint: $\frac{1}{x} \ln(1+x) = 1 - \frac{x}{2} + \frac{x^2}{3} + O(x^3)$

Expanding the $\frac{1}{x} \ln(1+x)$ term, in Eq. (17.19), about $x = 0$ leads to

$$1 - 1 + \frac{1}{2} \frac{\delta K}{\delta \psi} \frac{L_f}{K_0} - \frac{1}{3} \left(\frac{\delta K}{\delta \psi} \frac{L_f}{K_0} \right)^2 + O(\delta K^3) = \frac{\delta K}{\delta \theta} \frac{t}{L_f}$$

and therefore

$$\frac{L_f}{2K_0\delta\psi} + O(\delta K) = \frac{t}{\delta\theta L_f}$$

which can be rearranged to get

$$L_f = \sqrt{\frac{2K_0\delta\psi t}{\delta\theta}} + O(\delta K^{1/2}) \quad (17.20)$$

Challenge 17.7 Use Eqs. (17.8) and (17.20) to derive an expression for the volume of water that has infiltrated through a unit area of land surface, F [L], after time, t . Afterwards, differentiate your expression for F with respect to t to obtain an expression for the infiltration rate, f .

Recall Eq. (17.8), for the volume of water that has infiltrated through a unit area of land surface, F [L], at time, t :

$$F = \delta\theta L_f - \int_0^t q_i dt$$

Note that $q_i = -K_i$, which is constant. Furthermore, because we have assumed $\delta K = 0$, $K_i = K_0$. Therefore

$$F = \delta\theta L_f + K_0 t \quad (17.21)$$

Substituting Eq. (17.20) into Eq. (17.21) leads to

$$F = S t^{1/2} + K_0 t \quad (17.22)$$

where S [$LT^{-1/2}$] is referred to as the sorptivity, found from (in this case)

$$S = \sqrt{2K_0\delta\psi\delta\theta} \quad (17.23)$$

The infiltration rate, f [LT^{-1}], is obtained by differentiating Eq. (17.22) with respect to time to get

$$f(t) \equiv \frac{dF}{dt} = \frac{S t^{-1/2}}{2} + K_0 \quad (17.24)$$

which is often referred to as the Philip equation.

We have derived Eq. (17.24) using a sharp wetting front assumption. However, [9] showed that Eq. (17.24) applies more generally, providing the sorptivity is found from

$$S = \int_{\theta_i}^{\theta_0} \lambda(\theta) d\theta \quad (17.25)$$

where $\lambda = Lt^{-1/2}$ is a Boltzmann transform. For a fast and accurate procedure to evaluate Eq. (17.25), see [10].

17.5 Field Measurements

In this section we will look at some common methods for acquiring field measurements of soil moisture content and negative pressure head.

17.5.1 Measuring Moisture Content

17.5.1.1 Neutron Method

The neutron method is the most established method of measuring in situ soil moisture content. A neutron probe contains a fast neutron emitting radioactive source and a slow neutron counter. Hydrogen atoms in water slow down fast moving neutrons. Detection of slow moving neutrons in the presence of a neutron probe is therefore indicative of water. In situ measurements of moisture content can be determined from the slow neutron counter using an empirical relationship between moisture content and slow neutron count.

Prior to using a neutron probe, a vertical access tube must be augured into the soil. The neutron probe is then lowered into the access tube, using a cable, to obtain measurements of moisture content at different depths below the soil surface. Measurements are typically taken at intervals of 10–30 cm to soil depths of up to 5 m. Typical access tubes are around 50 mm in diameter and are made of aluminium or plastic. A commonly used radioactive source is Americium–beryllium, which has a half-life of 458 years. See [11] for more detail.

The main disadvantage of neutron probes concerns the use of radioactive substances, which require significant health and safety precautions. Consequently, neutron probes cannot be left unattended with automatic loggers. Although the use of an access tube allows high spatial resolution in measurements, the absence of automatic loggers prohibits high temporal resolution.

17.5.1.2 Dielectric Methods

An increasingly widespread alternative is to use dielectric methods for soil moisture content measurement. A dielectric is an electrical insulator. In the presence of an

electrical field, a dielectric will store energy. Permittivity is a measure of a material's capability to store energy in this way. Relative permittivity is a dimensionless quantity relating how many times more energy a material can store as compared to a vacuum.

Importantly, the relative permittivity of water is 78 whereas the relative permittivity of dry soil and air are much lower at 6 and 1, respectively [11]. Consequently, a calibration relationship between relative permittivity of unsaturated soils and soil moisture content can be determined. Measurements of permittivity can then be translated to measurements of in situ soil moisture content.

Total domain reflectometry (TDR), impedance techniques and capacitance technique are three different but commonly used dielectric methods for measuring soil moisture content [11]. The advantage of dielectric methods as compared to the neutron method is that they are cheaper and safer to use. In particular, dielectric probes can be left unattended and automatically logged to obtain high temporal resolution in situ measurements. A disadvantage is that calibration relationships between relative permittivity and soil moisture content are not robust and should be uniquely obtained for each installation. This is often achieved by supplementing data with a sparse set of neutron probe measurements.

17.5.2 Measuring Negative Pressure Head

17.5.2.1 Tensiometer

Tensiometers provide a direct means of measuring in situ negative pressure head. A tensiometer comprises a pressurised water-filled tube with a porous cup at the end. A pressure transducer is used to measure water pressure within the tensiometer. The tensiometer is installed within the soil at a depth where pressure head measurement is required. The porous cup is embedded into the soil such that hydraulic contact is made between the water in the tensiometer and water in the soil. Where electrical pressure transducers are used, the pressure head can be continuously recorded using an automatic logger.

Because unsaturated soil has a negative pressure head, water is sucked out of the tensiometer through the porous cup into the soil until the pressure in the tensiometer is the same as the pressure in the soil. A negative pressure head is recorded. If the soil experiences an increase in moisture content (due to infiltration for instance), water will migrate back into the tensiometer until pressure equilibrium is again reached, and a corresponding increase in pressure head will be observed [12].

An issue is that soil water, sucked into the tensiometer during wetter periods, contains high levels of dissolved gas. When the pressure in the tensiometer reduces below -85 kPa, air bubbles form and block instrument tubing, making further measurements unreliable [12]. The tensiometer must then be manually purged by replacing the water with degassed water. Consequently tensiometers are unsuitable for measuring pressure heads less than -8.66 m.

17.5.2.2 Porous Material Sensors

Porous material sensors are preferred to tensiometers for very dry conditions. Porous material sensors comprise a porous block with an embedded electrical moisture content sensor embedded within the block. The porous block is embedded within the soil where the pressure head measurement is required. Water is sucked into the porous block from the soil until the water pressure in the block is the same as that of the soil. The moisture content of the block is continuously monitored and recorded using an automatic logger. The moisture content data is then translated to pressure head using a pre-calibrated relationship between porous block moisture content and pressure head.

A well established porous material sensor is the equitensiometer, which uses a TDR moisture content sensor within a proprietary porous material [12]. A significant limitation is that moisture content of porous media tends to become insensitive to changes in pressure head as saturation is approached. Consequently porous material sensors are found to provide unreliable measurements during very wet conditions. The best option is to use a combination of tensiometers and equitensiometers to capture both very wet and very dry conditions.

17.5.3 Comparison of Field Measurements

Fig. 17.10a shows a comparison of moisture content measurements obtained using both the dielectric method and the neutron method. These data were both obtained at one meter depth from a grass crop site in Berkshire, UK. See [13] for more details about the installation. The dielectric results closely follow the neutron probe data because the latter data was used to develop the calibration relationship between moisture content and permittivity at this location. The advantage of the dielectric measurements is that they enable us to observe moisture content at a much finer temporal resolution.

Figure 17.10b shows a comparison of pressure head measurements obtained using both an equitensiometer and a tensiometer. These data were also obtained at one metre depth from the same grass crop site in Berkshire (see, [13]). For intermediate pressure head values, i.e. $\psi \in (-8.6 \text{ m}, -1 \text{ m})$, both instruments yield very similar results. For $\psi > -1 \text{ m}$, the equitensiometer provides unreliable results because the moisture content of the porous block used is insensitive to pressure head in this range. For $\psi < -8.6 \text{ m}$, the tensiometer provides unreliable results because of air bubble formation from water in the tensiometer. However, by combining measurements from both instruments it is possible to observe pressure head over the full practical range.

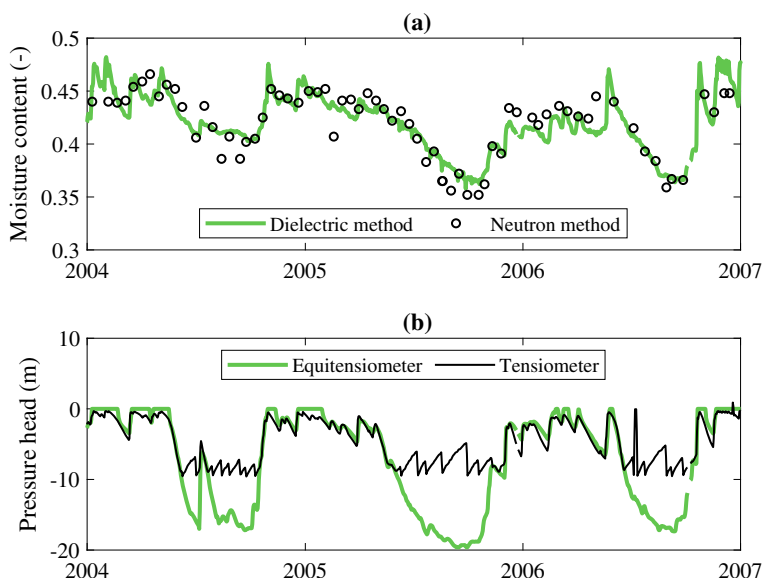


Fig. 17.10 **a** Comparison of the dielectric method and neutron method for measuring moisture content. **b** Comparison of equitensiometer and tensiometer measurements of pressure head. This data was acquired from [14]

17.5.4 Soil Moisture Deficit and the Zero Flux Plane

Figure 17.11a shows moisture content measurements taken at four different depths from the same location in Berkshire. The measurement at 10 cm depth shows strong fluctuations. The notable summer decline in moisture content is largely driven by evapotranspiration. Increases in moisture content are driven by the infiltration of individual rainfall events. Moisture content fluctuations become attenuated and smoothed out with depth. Very little fluctuation is observed at 290 cm depth because infiltrating water is mostly held in the top one metre of the soil.

Figure 17.11b shows hydraulic head measurements taken at four different depths. Hydraulic head is calculated from pressure head results by adding the elevation of each pressure head probe. The datum is taken to be at the land surface in this case. This hydraulic head record has been compiled from a combination of equitensiometer and tensiometer measurements. Because of the relationship between moisture content and pressure head, hydraulic heads progressively reduce as the soil dries out in the summer.

Further insight can be obtained by studying the hydraulic gradients between the four pressure head probes (Fig. 17.11c). A positive gradient implies downward flow. A negative gradient implies upward flow. At 350 cm, it can be seen that fluid persistently moves downwards, due to gravity drainage, throughout the year. At 250 cm depth, water moves downwards in the winter but upwards during the summer, due to evapotranspiration. At 150 cm depth, water moves downwards in the winter, upwards

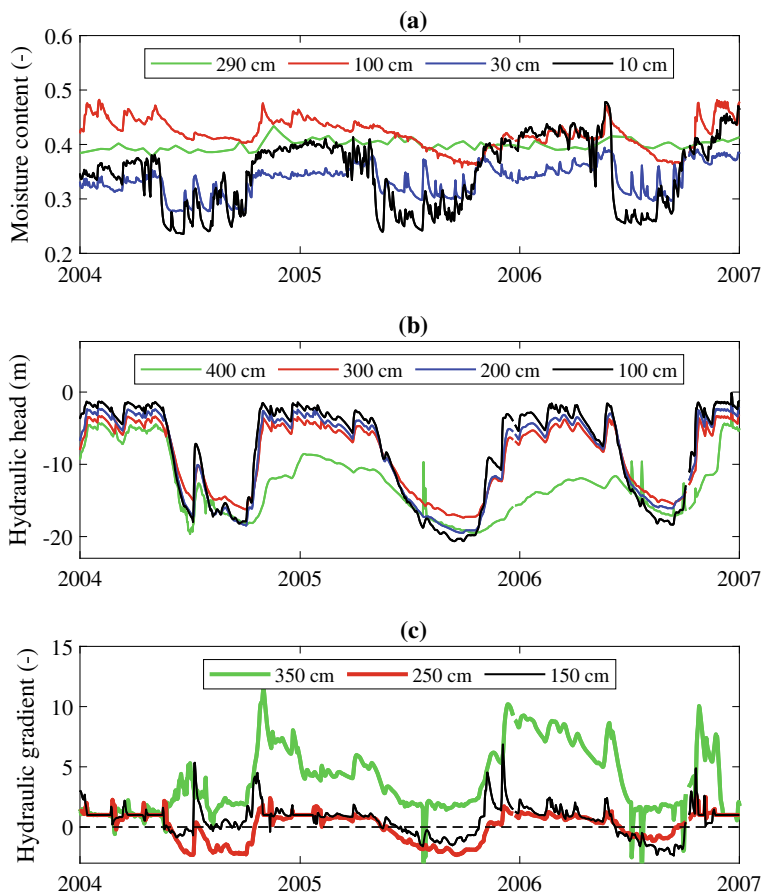


Fig. 17.11 Vadose zone hydrology in Berkshire. **a** Plots of moisture content at different depths. **b** Plots of hydraulic head at different depths. **c** Plots of hydraulic gradient at different depths (positive gradients imply downwards flow). The depths of the measurements are given in the legends. Moisture content and pressure head data used to develop these plots were acquired from [14]

for most of the summer, but sometimes downwards during the summer when there are excessively heavy rainfall events.

The moisture content data can be integrated with respect to elevation to obtain a depth of water stored in the measured region, i.e., the top 400 cm in this case. A plot of storage depth, based on the measurements given in Fig. 17.11a, is shown in Fig. 17.12b. Corresponding rainfall and potential evapotranspiration rates are shown in Fig. 17.12a. The storage depth increases and recedes with each rainfall event and progressively dries out during the summer as the evapotranspiration increases.

The storage column appears never to exceed 1750 mm in this case. This upper level is referred to as the field capacity. The field capacity is commonly defined as the amount of water held in soil after excess water has drained away and the

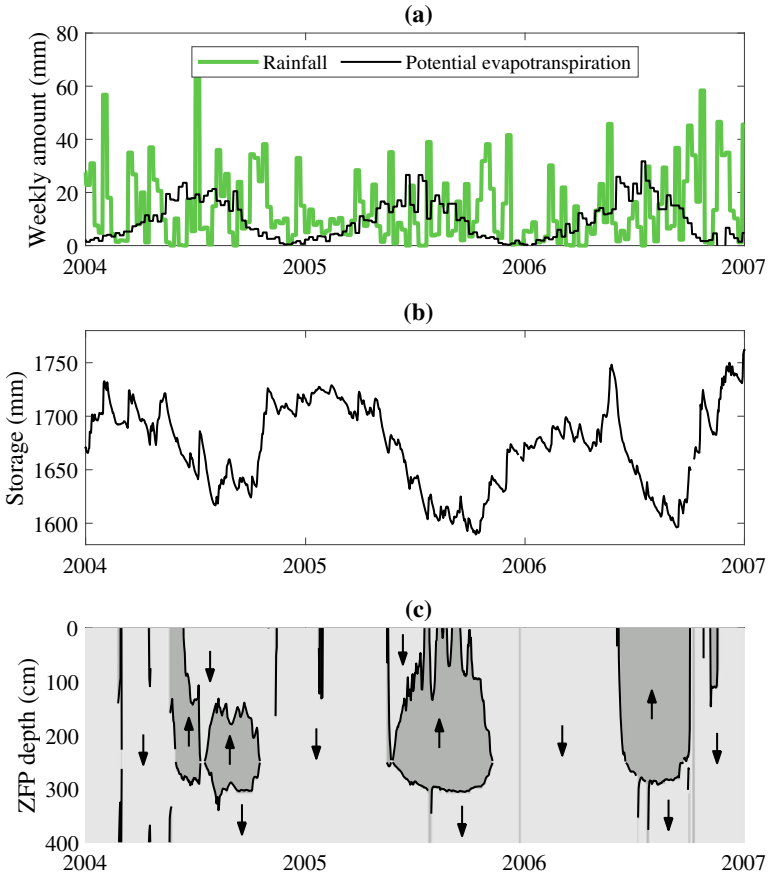


Fig. 17.12 Vadose zone hydrology in Berkshire. **a** Rainfall and potential evapotranspiration. **b** Total water stored in the top 400 cm of vadose zone. **c** Depth of the zero-flux-plane (ZFP) showing how the direction of flow changes with time and depth. Rainfall data, weather station data (used to determine potential evapotranspiration), moisture content data (used to determine storage depth) and pressure head data (used to determine ZFP depth) were acquired from [14]

rate of downward movement has materially decreased. The difference between the field capacity and the current storage level is referred to as the soil moisture deficit (SMD). The SMD is highest in the summer and lowest in the winter. A common misconception is that drainage does not occur when the SMD is greater than zero [15].

In principle, the hydraulic gradient data in Fig. 17.11c can be used to determine the evaporation and drainage rates. However, this is normally not possible due to uncertainty about the hydraulic conductivity. Nevertheless, additional insight can be obtained by determining the depth to which a zero hydraulic gradient occurs. This depth is referred to as a zero flux plane (ZFP).

The depth to the ZFP, based on a linear interpolation of the hydraulic gradient data in Fig. 17.11c, is shown in Fig. 17.12c. Often there are two ZFP. The lower ZFP is a divergent ZFP, where flow diverges upwards and downwards, away from the ZFP. The upper ZFP is a convergent ZFP, where flow converges upwards and downwards, towards the ZFP. The divergent ZFP is caused by evapotranspiration. The convergent ZFP is caused by rainfall events that occur in the presence of a divergent ZFP. Continuous infiltration through the entire soil profile mostly occurs during the winter. In the winter of 2006, continuous infiltration through the soil profile occurs despite the SMD being greater than zero throughout the year.

Many attempts have been made to use numerical solutions of Richards' equation to predict moisture content and hydraulic head responses due to the rainfall and evapotranspiration. Such models are considered useful to help manage groundwater resources and pollution control. Assumptions of homogeneous properties are inadequate in this context due to high natural variabilities in saturated and residual moisture content [16]. However, homogeneous Richards' equation models can provide a realistic representation of the natural system when studied in terms of storage levels and ZFP depth [15, 17].

17.6 Problem Sheet

Problem 17.1 (see Worked Solution 17.1)

The following consecutive depths of rainfall are measured at 15 min intervals: 25 mm, 21 mm, 4 mm and 2 mm. Prior to the storm, the moisture content and pressure head of the nearby soil are observed to be 0.131 and -86 cm, respectively. The saturated moisture content and hydraulic conductivity are 0.396 and 4.96 cm day^{-1} , respectively. Assume a sharp wetting front develops during infiltration and apply the Philip equation, for infiltration capacity, to estimate the depth of surface runoff and infiltration that occurs at the end of each 15 min interval.

Problem 17.2 (see Worked Solution 17.2)

A field site is instrumented with a neutron probe access tube and four equitensiometers. Moisture content and pressure head measurements are presented in Tables 17.1 and 17.2, respectively.

- Estimate the soil moisture deficit for each month and plot your results against time.
- Estimate the depth to any zero flux planes, where they exist, and plot your results against time.

Table 17.1 Moisture content measurements from Problem 17.2

Depth (cm)	10	30	100	290
Month	Moisture content (–)			
1	0.457	0.387	0.449	0.414
2	0.360	0.341	0.480	0.391
3	0.393	0.345	0.431	0.402
4	0.364	0.330	0.446	0.389
5	0.378	0.349	0.456	0.379
6	0.259	0.278	0.430	0.393
7	0.264	0.285	0.411	0.384
8	0.241	0.278	0.414	0.386
9	0.295	0.294	0.412	0.389
10	0.269	0.280	0.403	0.395
11	0.385	0.348	0.474	0.406
12	0.391	0.344	0.447	0.420

Table 17.2 Pressure head measurements from Problem 17.2

Depth (cm)	100	200	300	400
Month	Pressure head (m)			
1	-1.11	-0.963	-1.11	-8.20
2	-0.319	-0.319	-0.319	-0.319
3	-2.81	-2.77	-2.59	-5.80
4	-1.00	-1.00	-1.00	-1.41
5	-0.544	-0.544	-0.544	-0.557
6	-6.74	-5.19	-3.98	-4.76
7	-15.8	-14.4	-11.2	-13.6
8	-13.7	-12.8	-10.6	-11.2
9	-14.5	-14.1	-11.6	-12.9
10	-17.0	-16.4	-13.2	-14.1
11	-0.552	-0.552	-0.727	-11.40
12	-1.23	-1.72	-1.48	-7.77

(c) Plot hydraulic head against depth for the months of April (month 4), July (month 7) and September (month 9). Also mark on the location of your estimated zero flux plane depths.

17.7 Worked Solutions

Worked Solution 17.1 (see Problem 17.1)

Considering Fig. 17.8, we need to determine the infiltration capacity for each 15 min interval and then work out how much rain can infiltrate. Any remaining rainfall is assumed to become surface runoff. From the information given, $\theta_i = 0.131$, $\psi_i = -86$ cm, $\theta_s = 0.396$ and $K_s = 4.96$ cm day⁻¹.

The Philip equation equation for infiltration capacity, f [LT⁻¹], is found from Eq. (17.24):

$$f = \frac{St^{-1/2}}{2} + K_0$$

where S is the sorptivity and K_0 is the hydraulic conductivity of the soil above the wetting front. Let us assume that the soil above the wetting front is completely saturated such that $K_0 = K_s$.

The infiltration capacity for each 15 min interval can be determined by integrating between two times t_1 and t_2 :

$$\delta F = \int_{t_1}^{t_2} \left(\frac{St^{-1/2}}{2} + K_0 \right) dt = S \cdot (t_2^{1/2} - t_1^{1/2}) + K_0 \cdot (t_2 - t_1)$$

Because of the sharp wetting front assumption, the sorptivity can be found from Eq. (17.23):

$$S = \sqrt{2K_0\delta\psi\delta\theta}$$

Note that $\delta\theta = \theta_0 - \theta_i$ and $\delta\psi = \psi_0 - \psi_i$ where θ_0 and ψ_0 are the moisture content and pressure head at the land surface, respectively. Given that soil above the wetting front is completely saturated, $\psi_0 = 0$ and $\theta_0 = \theta_s$. It follows that

$$S = \sqrt{-2K_s\psi_i(\theta_s - \theta_i)} = 15.04 \text{ cm day}^{-1/2}$$

Converting everything to mm and minutes then leads to $K_0 = 0.03444$ mm min⁻¹ and $S = 3.963$ mm min^{-1/2}. The infiltration capacity, infiltration and surface runoff can now be calculated as follows:

t (min)	Rain (mm)	δF (mm)	Infiltration (mm)	Runoff (mm)
15	25	15.86	15.86	9.140
30	21	6.873	6.873	14.13
45	4	5.394	4	0
60	2	4.628	2	0

Worked Solution 17.2 (see Problem 17.2)

(a) The total water stored in the profile is first obtained by approximately integrating the moisture content data with respect to depth using the rectangle rule. The field capacity is estimated as being the largest value of total water stored observed in the year of observation. The soil moisture deficit is obtained by subtracting the storage level from the field capacity.

The following MATLAB code can be used to determine the soil moisture deficit for each month.

```
%Extract moisture contents from array
theta=data(:,2:5);
%Specify depth of measurements (mm)
depth=[100 300 1000 2900];
%Determine mid-point depths (mm)
MidPoints=(depth(1:end-1)+depth(2:end))/2;
%Determine depth intervals (mm)
dz=diff([0 MidPoints depth(end)]);
%Determine water stored in soil (mm)
STORED=sum(theta.*dz,2);
%Estimate field capacity (mm)
FC=max(STORED);
%Determine soil moisture deficit (mm)
SMD=FC-STORED;
```

(b) To determine the depth to the zero flux plane we need to first determine the hydraulic heads, then determine the hydraulic gradient and then estimate where the hydraulic gradient is zero.

The hydraulic heads, h , are obtained from $h = \psi + z$ where ψ is the pressure head and z is the elevation head. To determine the elevation head we need to first specify a datum. We will take our datum at the land surface. Elevation head can now be determined by multiplying the measurement depths by minus one.

Let the elevation of each measurement point be defined by z_i where $i = 1, 2, 3, 4$. Let $z_{i+1/2} = (z_i + z_{i+1})/2$. An approximation of the hydraulic gradient at $z_{i+1/2}$, $J_{i+1/2}$, can be obtained from

$$J_{i+1/2} \equiv \left. \frac{\partial h}{\partial z} \right|_{i+1/2} = \frac{h_{i+1} - h_i}{z_{i+1} - z_i}$$

An estimate of the elevation of a zero flux plane, c , can be obtained by linear interpolation of two neighbouring hydraulic gradients. Consider the following linear equation

$$z = mJ + c$$

and assume it is satisfied at two neighbouring points such that

$$z_{i+1/2} = mJ_{i+1/2} + c \quad \text{and} \quad z_{i-1/2} = mJ_{i-1/2} + c$$

where m is an undefined slope.

The above equations can be solved simultaneously to get

$$m = \frac{z_{i+1/2} - z_{i-1/2}}{J_{i+1/2} - J_{i-1/2}}$$

and

$$c = \frac{z_{i-1/2}J_{i+1/2} - z_{i+1/2}J_{i-1/2}}{J_{i+1/2} - J_{i-1/2}}$$

Values of $c \notin [z_{i-1/2}, z_{i+1/2}]$ should be considered invalid because these represent an extrapolation.

The depth to the zero flux plane is obtained by multiplying c by minus one because c represents an elevation above the land surface. In this way, depths to zero flux plane can be obtained from the following MATLAB script:

```
%Extract pressure heads (m) from array
psi=data(:,2:5);
%Specify depth of measurements (m)
depth=[1 2 3 4];
%Determine elevation of measurements
%assuming datum at ground surface
z=-depth;
%Determine hydraulic head
h=psi+z;
%Determine hydraulic gradient, J=dh/dz
J=diff(h,1,2)./diff(z,1,2);
%Determine elevation of gradient
z=(z(1:end-1)+z(2:end))/2;
%Determine elevation of ZFP, c (m)
%Use loop for two possible answers
%The first is z(2) < c < z(1)
%and second is z(3) < c < z(2)
for i=1:2
dJ=(J(:,i+1)-J(:,i));
c(:,i)=(z(i)*J(:,i+1)-z(i+1)*J(:,i))./dJ;
%Eliminate extrapolations
c(c(:,i)<z(i+1)|c(:,i)>z(i),i)=NaN;
end
%Determine the depth to ZFP
ZFP=-c;
```

(c) The graphs for all of the results are shown in Fig. 17.13.

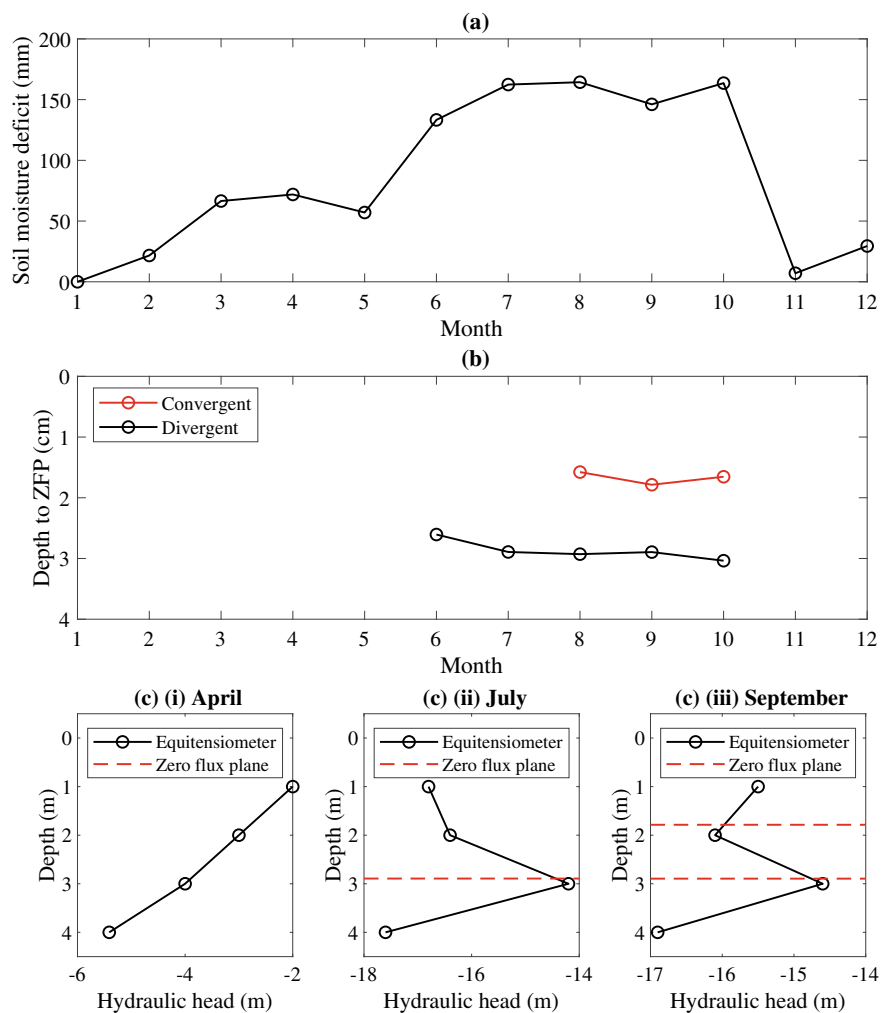


Fig. 17.13 Results from Problem 17.2. **a** Plot of soil moisture deficit against time. **b** Plots of depth to both the convergent and divergent zero-flux-planes (ZFP). **c** Plots of hydraulic head against depth for (i) April, (ii) July and (iii) September with the location of ZFPs shown as dashed red lines

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Abstract

This chapter focuses on the meaning and measurement of humidity. Mathematical equations for ideal gas mixtures are used to derive relationships between absolute, specific and relative humidity. Latent heat of evaporation is calculated using the Clapeyron equation in conjunction with Teten's empirical equation for saturated vapour pressure. Monin-Obhukov similarity theory is used to derive equations for determining vapour pressure measurements from dry bulb and wet bulb temperature measurements. It is also explained how to estimate daily mean humidity from daily minimum and daily maximum air temperature data. Practical applications are presented through a problem sheet with worked solutions.

Notation

c_p	Specific heat capacity of air [$L^2T^{-2}\Theta^{-1}$].
C	Sensible heat flux [MT^{-3}].
C_d	Mass concentration of dry components [ML^{-3}].
C_i	Mass concentration of i th component [ML^{-3}].
C_v	Mass concentration of water vapour (i.e., absolute humidity) [ML^{-3}].
D_0	Diffusion coefficient of water vapour in air [L^2T^{-1}].
E_0	Potential evaporation from an open water surface [LT^{-1}].
h	Enthalpy per unit mass of gas mixture [L^2T^{-2}].
L	Latent heat of evaporation [L^2T^{-2}].
m	Mass of gas [M].
m_d	Mass of dry-air components [M].
m_i	Mass of component i [M].
m_v	Mass of water vapour [M].
M_d	Molecular mass of dry-air components [M].
M_i	Molecular mass of i th component [M].
M_v	Molecular mass of water vapour [M].

N	Number of moles [-].
N_d	Number of moles of dry-air components [-].
N_i	Number of moles of i th component [-].
N_m	Total number of moles in gas mixture [-].
N_v	Number of moles of water vapour [-].
Nu	Nusselt number [-].
p	Pressure [$ML^{-1}T^{-2}$].
p_d	Partial pressure of dry components [$ML^{-1}T^{-2}$].
p_i	Partial pressure of i th component [$ML^{-1}T^{-2}$].
p_m	Gas mixture pressure (i.e., air pressure) [$ML^{-1}T^{-2}$].
p_v	Partial pressure for water vapour (i.e., vapour pressure) [$ML^{-1}T^{-2}$].
p_{vs}	Saturated vapour pressure [$ML^{-1}T^{-2}$].
r_a	Aerodynamic resistance [$L^{-1}T$].
R	Universal ideal gas constant [$ML^2T^{-2}\Theta^{-1}$].
s	Distance normal to the water surface [L].
s_0	Distance of the water surface from an arbitrary datum [L].
Sh	Sherwood number [-].
T	Temperature [Θ].
T_{dew}	Dew-point temperature [Θ].
T_{dry}	Dry-bulb temperature [Θ].
T_{max}	Daily maximum temperature [Θ].
T_{min}	Daily minimum temperature [Θ].
T_{wet}	Wet-bulb temperature [Θ].
u	Wind speed [LT^{-1}].
u_τ	Friction velocity [LT^{-1}].
V	Volume of gas [L^3].
V_d	Partial volume of dry components [L^3].
V_i	Partial volume of i th component [L^3].
V_m	Volume of gas mixture [L^3].
V_v	Partial volume of water vapour [L^3].
X_v	Specific humidity [-].
α	Saturated vapour pressure slope [$ML^{-1}T^{-2}\Theta^{-1}$].
γ	Psychrometric constant [$ML^{-1}T^{-2}\Theta^{-1}$].
ε	Ratio of the molecular mass of water vapour to that of dry air [-].
κ	Thermal diffusivity [L^2T^{-1}].
ν	Kinematic viscosity of air [L^2T^{-1}].
ν_E	Kinematic Eddy viscosity [L^2T^{-1}].
ρ_d	Density of dry air [ML^{-3}].
ρ_m	Density of gas mixture [ML^{-3}].
ρ_v	Density of water vapour [ML^{-3}].
ρ_{vs}	Density of water vapour at saturation [ML^{-3}].
ρ_w	Density of liquid water [ML^{-3}].
τ_0	Boundary shear stress [$ML^{-1}T^{-2}$].
ϕ_v	Relative humidity [-].

18.1 Introduction

Evaporation is an important driving force in most hydrological systems. Evaporation involves the transformation of liquid water to water vapour in the atmosphere. Evaporation is an endothermic process, which means it consumes heat energy known as latent heat. In the context of hydrology, this heat is mostly derived from solar radiation. However, evaporative fluxes themselves are driven by humidity gradients. Humidity is a term used to describe how much moisture is in the air. Before we can learn more about evaporation it is important to lay down some basic thermodynamic principles concerning the description and measurement of humidity.

This chapter is structured as follows: First we will look at how ideal gas mixtures can be used to represent water-air systems. We will introduce three different representations of humidity: absolute humidity, specific humidity and relative humidity. We will derive two important rules for ideal gas mixtures, Dalton's law of additive pressures and Amagat's law of additive volumes. These will enable us to derive relationships between absolute humidity, specific humidity and vapour pressure. We will also derive an expression to determine the Latent heat capacity of water using the Clapeyron equation. We will then look at how humidity can be measured using dry-bulb and wet-bulb temperatures. This will involve developing an understanding about latent heat and sensible heat fluxes, which in turn requires an understanding about how to determine mass fluxes and heat fluxes in turbulent air streams using Monin-Obhukov similarity theory. Finally, we will look at how to estimate humidity by comparing day-time and night-time air temperatures.

18.2 Absolute, Specific and Relative Humidity

Moistened air is often described as a two component gas mixture, comprising water vapour and dry air. Three important properties used to describe the quantity of moisture in the air are absolute humidity, specific humidity and relative humidity.

Absolute humidity, C_v [ML^{-3}], represents the mass concentration of water in the air, defined by

$$C_v = \frac{m_v}{V_m} \quad (18.1)$$

where m_v [M] is the mass of water vapour contained in a gas mixture of volume, V_m [L^3].

Specific humidity, X_v [-], represents the mass fraction of water in the air, defined by

$$X_v = \frac{C_v}{\rho_m} \quad (18.2)$$

where ρ_m [ML^{-3}] is the mass density of the moistened air mixture.

Absolute and specific humidity have an upper limit. When this limit is reached, the air is said to be saturated. Relative humidity, ϕ_v [-], is a fractional term, ranging

from 0 to 1, used to describe how close the air is to vapour saturation and is defined by [1, p.719]

$$\phi_v = \frac{p_v}{p_{vs}} \quad (18.3)$$

where p_v [$\text{ML}^{-1}\text{T}^{-2}$] and p_{vs} [$\text{ML}^{-1}\text{T}^{-2}$] are referred to as the vapour pressure and saturated vapour pressure, respectively.

Vapour pressure is the partial pressure of water in air (we will learn more about partial pressure below). The higher the vapour pressure the more moisture is held in the air. The saturated vapour pressure is an upper limit on vapour pressure. Saturated vapour pressure is controlled by temperature and can be determined from Tetens' empirical equation [2]

$$p_{vs} = 610.8 \exp \left[\frac{17.27(T - 273.2)}{T - 35.86} \right] \quad (18.4)$$

where p_{vs} is calculated in Pa and T [$^{\circ}\text{C}$] is temperature specified in Kelvin (degrees Kelvin equals degrees Centigrade + 273.2).

18.3 Ideal Gas Model for Water and Air

The transformation of liquid water to vapour is referred to as evaporation. The transformation of vapour to liquid water is referred to as condensation. The process of evaporation consumes heat. The process of condensation produces heat. The quantity of heat consumed or produced by evaporation or condensation is referred to as the latent heat of evaporation. A sound understanding of how these processes take place is significantly enhanced by some basic knowledge concerning the thermodynamics of gas mixtures and liquid-gas phase equilibrium. Here we will develop and study some critical concepts including:

- The ideal gas law;
- Ideal gas mixtures and partial pressures;
- Dalton's law of additive pressures;
- Amagat's law of additive volumes;
- The relationship between absolute humidity, specific humidity and vapour pressure;
- Latent heat capacity and the Clapeyron equation.

18.3.1 The Ideal Gas Law

The ideal gas law underpins many important thermodynamic relationships. The ideal gas law is often assumed to apply to moist air, dry air and water vapour.

The ideal gas law simply states that [1, p. 137]

$$pV = NRT$$

where p [$\text{ML}^{-1}\text{T}^{-2}$] is pressure, V [L^3] is the volume of a gas, N [–] is the number of moles of that gas in its volume, R [$\text{ML}^2\text{T}^{-2}\Theta^{-1}$] is the universal ideal gas constant and T [Θ] is temperature, normally specified in degrees Kelvin. The universal ideal gas constant, $R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$.

The number of moles is defined by [1, p. 138]

$$N = \frac{m}{M} \quad (18.5)$$

where m [M] is the mass of the gas contained within the volume, V , and M [M] is the molecular mass of the gas of concern.

18.3.2 Ideal Gas Mixtures and Partial Pressures

Consider a mixture of k [–] different components where each component can be treated as an ideal gas. The volume of this mixture, V_m [L^3], is found from

$$p_m V_m = N_m R T \quad (18.6)$$

where p_m [$\text{ML}^{-1}\text{T}^{-2}$] is the pressure experienced by the gas mixture and N_m [–] is the total number of moles in the gas mixture, which, in turn, is found from [1, p. 682]

$$N_m = \sum_{i=1}^k N_i \quad (18.7)$$

where N_i [–] is the number of moles of the i th component present in the volume of gas mixture, V_m .

Each of the individual components exert a partial pressure on the mixture, p_i , which can be found from

$$p_i V_m = N_i R T. \quad (18.8)$$

18.3.3 Dalton's Law of Additive Pressures

Challenge 18.1 Use Eqs. (18.6)–(18.8) to derive an expression for the mixture pressure, p_m , in terms of the partial pressures of the individual components, p_i .

Rearranging Eqs. (18.6) and (18.8) gives us

$$N_m = \frac{p_m V_m}{RT} \quad (18.9)$$

and

$$N_i = \frac{p_i V_m}{RT} \quad (18.10)$$

Substituting Eqs. (18.9) and (18.10) into Eq. (18.7) then leads to [1, p. 685]

$$p_m = \sum_{i=1}^k p_i \quad (18.11)$$

Equation (18.11) is often referred to as Dalton's law of additive pressures. Dalton's law states that, for an ideal gas mixture, the total pressure exerted by a gas mixture equals the sum of the partial pressures of the individual components.

18.3.4 Amagat's Law of Additive Volumes

Although the individual components in the aforementioned gas mixture exert a partial pressure, p_i , on the mixture, they collectively experience the same mixture pressure, p_m . Consequently, the volumes of the individual components, V_i [L^3], are defined by

$$p_m V_i = N_i R T \quad (18.12)$$

These individual volumes, V_i , are generally referred to as partial volumes. The partial volume of a given component represents the volume of that component if it was separated out from the mixture.

Challenge 18.2 Use Eqs. (18.7), (18.9) and (18.12) to derive an expression for the mixture volume, V_m , in terms of the partial volumes of the individual components, V_i .

Rearranging Eq. (18.12) gives us

$$N_i = \frac{p_m V_i}{R T} \quad (18.13)$$

Substituting Eqs. (18.9) and (18.13) into Eq. (18.7) leads to [1, p. 685]

$$V_m = \sum_{i=1}^k V_i \quad (18.14)$$

Equation (18.14) is often referred to as Amagat's law of additive volumes. Amagat's law states that, for an ideal gas mixture, the total volume of a gas mixture equals the sum of the partial volumes of the individual components.

18.3.5 The Relationship Between Absolute Humidity, Specific Humidity and Vapour Pressure

Given mass conservation, Amagat's law and Dalton's law, it can be understood that the number of moles, N_m , mass, m_m , volume, V_m , and pressure, p_m , of a two-component ideal gas mixture of water vapour and dry air are found from:

$$N_m = N_v + N_d \quad (18.15)$$

$$m_m = m_v + m_d \quad (18.16)$$

$$V_m = V_v + V_d \quad (18.17)$$

$$p_m = p_v + p_d \quad (18.18)$$

where N_v , N_d , m_v , m_d , V_v , V_d , p_v and p_d are the number of moles, masses, partial volumes and partial pressures of the water vapour and dry-air components, respectively.

The mass concentration, C_i [ML^{-3}], and mass density, ρ_i [ML^{-3}], of a given component, i , are found from

$$C_i = \frac{m_i}{V_m} \quad (18.19)$$

and

$$\rho_i = \frac{m_i}{V_i} \quad (18.20)$$

where $i = v$ for water vapour and d for dry air. Recall that C_v and p_v were previously referred to as the absolute humidity and vapour pressure, respectively.

Considering Eq. (18.5), it can also be said that

$$N_i = \frac{m_i}{M_i} \quad (18.21)$$

where M_i [M] is the molecular mass of component i . The molecular mass of water is, $M_v = 18.02 \text{ g mol}^{-1}$. The molecular mass of dry air is, $M_d = 28.96 \text{ g mol}^{-1}$ [3, p. 6].

From Eqs. (18.19) and (18.21) we have $V_m = \frac{N_i M_i}{C_i}$, which on substitution into Eq. (18.8) leads to

$$p_i M_i = C_i R T \quad (18.22)$$

From Eqs. (18.20) and (18.21) we have $V_i = \frac{N_i M_i}{\rho_i}$, which on substitution into Eq. (18.12) leads to

$$p_m M_i = \rho_i R T \quad (18.23)$$

Challenge 18.3 Use Eqs. (18.22) and (18.23) to derive an expression for absolute humidity, C_v , in terms of the molecular masses of water vapour and dry air, M_v and M_d , respectively, the vapour pressure, p_v , the mass-density of dry air, ρ_d , and the gas mixture pressure, p_m .

Dividing Eq. (18.22) by Eq. (18.23) and solving for C_i leads to

$$C_i = \frac{\rho_i p_i}{p_m} \quad (18.24)$$

from which it follows that

$$C_v = \frac{\rho_v p_v}{p_m} \quad (18.25)$$

Equation (18.23) also tells us that

$$\frac{M_v}{M_d} = \frac{\rho_v}{\rho_d}$$

Letting $\varepsilon = \frac{M_v}{M_d}$, it can be further stated that $\rho_v = \varepsilon \rho_d$, which on substitution into Eq. (18.25) gives us

$$C_v = \frac{\varepsilon \rho_d p_v}{p_m} \quad (18.26)$$

Substituting the values for M_v and M_d gives that $\varepsilon = 0.6222$. Also note that from Eq. (18.23)

$$\rho_d = \frac{p_m M_d}{RT} \quad (18.27)$$

Challenge 18.4 Determine an expression for the gas mixture density, ρ_m , for moist air in terms of the molecular masses of water vapour and dry air, M_v and M_d , respectively, the vapour pressure, p_v , the mass-density of dry air, ρ_d , and the gas mixture pressure, p_m .

From Eqs. (18.16), (18.19) and (18.20) we have

$$\rho_m = \frac{m_m}{V_m} = \frac{m_v + m_d}{V_m} = C_v + C_d \quad (18.28)$$

From Eqs. (18.18) and (18.24) we have

$$C_d = \frac{\rho_d p_d}{p_m} = \rho_d \left(1 - \frac{p_v}{p_m} \right) \quad (18.29)$$

Substituting Eqs. (18.26) and (18.29) into Eq. (18.28) leads to

$$\rho_m = \rho_d \left[1 - (1 - \varepsilon) \frac{p_v}{p_m} \right] \quad (18.30)$$

Substituting Eqs. (18.26) and (18.30) into Eq. (18.2) leads to the following expression for the specific humidity [3, p.15]

$$X_v = \frac{\varepsilon p_v}{p_m - (1 - \varepsilon) p_v} \quad (18.31)$$

18.3.6 Latent Heat of Evaporation

When liquids transform to a gaseous form the phase change consumes thermal energy. This associated heat energy is referred to as the latent heat of evaporation and is equivalent to the energy that would be released if that same gas were transformed back to a liquid. Latent heat is the reason why we feel cold when we wear wet clothes. As water evaporates from wet clothing it consumes heat energy supplied by our warm bodies.

The specific Latent heat capacity, L [L^2T^{-2}], is the enthalpy consumed by evaporating a unit mass of a substance. Mathematically we can say that

$$L = -\rho_m \frac{\partial h}{\partial C_v} \quad (18.32)$$

where h [L^2T^{-2}] is the enthalpy per unit mass of air (the gas mixture). Enthalpy is another word for heat energy.

The specific Latent heat capacity of a substance can be obtained from the Clapeyron equation [1, p. 659], which for a pure water vapour system, takes the form

$$\alpha \equiv \frac{dp_{vs}}{dT} = \frac{L}{T(\rho_{vs}^{-1} - \rho_w^{-1})} \quad (18.33)$$

where α [$ML^{-1}T^{-2}\Theta^{-1}$] is the slope of the saturated vapour pressure function (i.e., the derivative of Eq. (18.4) with respect to temperature), $\rho_{vs} \equiv \rho_v(p_m = p_{vs})$ [ML^{-3}] is the density of water vapour at saturation and ρ_w [ML^{-3}] is the density of liquid water. Note that for a pure water vapour system (i.e., no dry air component), Dalton's law gives that $p_m = p_v$.

Equation (18.33) can be rearranged to get

$$L = \alpha T(\rho_{vs}^{-1} - \rho_w^{-1})$$

and from the ideal gas law (Eq. (18.12)), $p_m V_v = N_v RT$ where $N_v = m_v/M_v$ (recall Eq. (18.21)). It follows that

$$\rho_v = \frac{p_m M_v}{RT} \quad \text{and} \quad \rho_{vs} = \frac{p_{vs} M_v}{RT}$$

and therefore

$$L = \alpha T \left(\frac{RT}{p_{vs} M_v} - \frac{1}{\rho_w} \right). \quad (18.34)$$

18.4 Measurement of Humidity

Humidity is traditionally measured using a psychrometer, which contains two thermometers. The bulb of one of the thermometers is enclosed within a water moistened wick. Temperature measured from the dry thermometer is referred to as the dry-bulb temperature, T_{dry} [Θ]. Temperature measured from the moistened thermometer is referred to as the wet-bulb temperature, T_{wet} [Θ]. The psychrometer also includes

a fan which continuously moves air from the surrounding atmosphere across both the wet and dry thermometer bulbs. Water evaporates from the wet-bulb into the surrounding air leading to a latent heat induced decline in the wet-bulb temperature. The humidity of the psychrometer is determined using the two temperature measurements in conjunction with an energy balance equation.

18.4.1 Energy Balance in a Psychrometer

The energy balance equation for the psychrometer takes the form

$$\rho_w L E_0 + C = 0 \quad (18.35)$$

where ρ_w [ML^{-3}] is the density of liquid water, L [L^2T^{-2}] is the specific latent heat capacity of water, E_0 [LT^{-1}] is the evaporative flux from the moistened wick, the term $\rho_w L E_0$ [MT^{-3}] is referred to as the latent heat flux and C [MT^{-3}] is the convective heat flux out of the moistened wick. This convective heat flux is often referred to as a sensible heat flux in this context, meaning the heat flux that we can sense. Note that C will be a negative quantity because heat will be entering the moistened wick from the warmer air.

18.4.2 Diffusive Approach to Defining Fluxes

The evaporative flux, E_0 , immediately above a water surface bounded by a static body of air will satisfy Fick's first law of diffusion [3, p. 29]

$$E_0 = -\frac{D_0}{\rho_w} \frac{\partial C_v}{\partial s} \bigg|_{s=s_0} \quad (18.36)$$

where D_0 [L^2T^{-1}] is the diffusion coefficient of water vapour in air, C_v [ML^{-3}] is the mass concentration of water vapour in air (i.e., the absolute humidity), s [L] is a distance normal to the water surface and s_0 [L] is the distance of the water surface from an arbitrary datum.

In practice, air is rarely static and there is turbulent mixing due to Eddy currents. In this case [3, p. 180]

$$E_0 = -\frac{\text{Sh} D_0}{\rho_w} \frac{\partial C_v}{\partial s} \bigg|_{s=s_0} \quad (18.37)$$

where Sh [–] is the dimensionless Sherwood number.

The sensible heat flux, C , immediately above a water surface bounded by a static body of air will satisfy Fourier's law of heat conduction [3, p. 28]

$$C = -\rho_m c_p \kappa \frac{\partial T}{\partial s} \bigg|_{s=s_0} \quad (18.38)$$

where ρ_m [ML^{-3}] is the density of air, c_p [$\text{L}^2\text{T}^{-2}\Theta^{-1}$] is the constant pressure specific heat capacity of air and κ [L^2T^{-1}] is the thermal diffusivity. The specific heat capacity of air, $c_p = 1005 \text{ J kg}^{-1} \text{ K}^{-1}$.

To take into account turbulent mixing, the sensible heat flux can be modified accordingly [3, p.152]

$$C = -\rho_m c_p \text{Nuk} \left. \frac{\partial T}{\partial s} \right|_{s=s_0} \quad (18.39)$$

where Nu [–] is the dimensionless Nusselt number.

18.4.3 Monin-Obhukov Similarity Theory

Moving air will lead to a shear stress on the water surface, τ_0 [$\text{ML}^{-1}\text{T}^{-2}$]. Under laminar flow conditions, the shear stress is defined by

$$\tau_0 = \rho_m \nu \left. \frac{\partial u}{\partial s} \right|_{s=s_0} \quad (18.40)$$

where ν [L^2T^{-1}] is the kinematic viscosity and u [LT^{-1}] is the air velocity normal to the s -direction. Under turbulent flow conditions this takes the form

$$\tau_0 = \rho_m \nu_E \left. \frac{\partial u}{\partial s} \right|_{s=s_0} \quad (18.41)$$

where ν_E [L^2T^{-1}] is the kinematic Eddy viscosity.

Just as Eqs. (18.37) and (18.39) are referred to as the evaporative and sensible heat fluxes, respectively, Eq. (18.41) can be referred to as a momentum flux. Monin-Obhukov similarity theory involves assuming that mass, heat and momentum are all transported in the same way within the turbulent air stream. This theory leads to the conjecture that [3, p. 306]

$$\text{Sh}D_0 = \text{Nuk} = \nu_E \quad (18.42)$$

and therefore

$$E_0 = -\frac{\nu_E}{\rho_w} \left. \frac{\partial C_v}{\partial s} \right|_{s=s_0} \quad (18.43)$$

and

$$C = -\rho_m c_p \nu_E \left. \frac{\partial T}{\partial s} \right|_{s=s_0} \quad (18.44)$$

18.4.4 Resistance Formulation

The evaporative flux and sensible heat flux within a psychrometer are determined by studying the temperature difference between the dry-bulb and wet-bulb thermometers. The wet-bulb temperature corresponds to a measurement made directly at the water surface; the water surface is represented by the moistened wick in this context. The dry-bulb thermometer provides another measurement of temperature located a small distance away from the water surface.

An important assumption often made is that E , C , ρ and c_p are constant within a small interval, $s \in [s_0, s_1]$. Separating the variables on both sides of Eqs. (18.41) (18.43) and (18.44) and integrating with respect to s then leads to

$$\tau_0 = \frac{\rho_m \cdot (u_1 - u_0)}{r_a} \quad (18.45)$$

$$E_0 = \frac{C_{v0} - C_{v1}}{r_a \rho_w} \quad (18.46)$$

$$C = \frac{\rho_m c_p \cdot (T_0 - T_1)}{r_a} \quad (18.47)$$

where u_0, u_1 , C_{v0} , C_{v1} , T_0 and T_1 are the air speed normal to the s -direction, absolute humidity and temperature at $s = s_0$ and $s = s_1$, respectively, and r_a [L^{-1}T] is referred to as the aerodynamic resistance and is found from

$$r_a = \int_{s_0}^{s_1} \frac{1}{v_E} ds \quad (18.48)$$

18.4.5 Vapour Pressure as a Function of Dry-Bulb and Wet-Bulb Temperatures

Challenge 18.5 Use the energy balance, Eq. (18.35), and the resistance formulae, Eqs. (18.46) and (18.47), to derive an expression for vapour pressure at the location of a dry-bulb thermometer in a psychrometer as a function of dry-bulb and wet-bulb temperatures.

Substituting Eqs. (18.46) and (18.47) into Eq. (18.35) leads to

$$L \cdot \left(\frac{C_{v0} - C_{v1}}{r_a} \right) + \frac{\rho_m c_p \cdot (T_0 - T_1)}{r_a} = 0$$

and so

$$C_{v1} = C_{v0} + \frac{\rho_m c_p \cdot (T_0 - T_1)}{L}$$

Applying the identity in Eq. (18.26) then leads to

$$p_{v1} = p_{v0} + \frac{\rho_m c_p p_m}{L \varepsilon \rho_d} (T_0 - T_1) \quad (18.49)$$

where p_{v0} and p_{v1} are the vapour pressure values at $s = s_0$ and s_1 , respectively.

Let s_0 and s_1 correspond to the locations of the wet-bulb and dry-bulb thermometers, respectively. It follows that $T_0 = T_{\text{wet}}$ and $T_1 = T_{\text{dry}}$.

Let p_{v1} represent the vapour pressure within the psychrometer, p_v . The p_{v0} value corresponds to the vapour pressure at the wet-bulb thermometer. The vapour pressure immediately around the wet-bulb thermometer will be at saturation due to the presence of the moistened wick. It follows that $p_{v0} = p_{vs}(T_{\text{wet}})$ where p_{vs} is the saturated vapour pressure (calculated from Tetens equation Eq. (18.4)) and

$$p_v = p_{vs}(T_{\text{wet}}) - \frac{\rho_m c_p p_m}{L \varepsilon \rho_d} (T_{\text{dry}} - T_{\text{wet}}) \quad (18.50)$$

18.4.6 The Psychrometric Constant

The coefficients in Eq. (18.50) are often lumped together into the so-called psychrometric constant, γ [$\text{ML}^{-1}\text{T}^{-2}\Theta^{-1}$]:

$$\gamma = \frac{\rho_m c_p p_m}{L \varepsilon \rho_d} \quad (18.51)$$

such that Eq. (18.50) reduces to

$$p_v = p_{vs}(T_{\text{wet}}) - \gamma \cdot (T_{\text{dry}} - T_{\text{wet}}) \quad (18.52)$$

Substituting Eq. (18.30) into Eq. (18.51) leads to

$$\gamma = \frac{c_p p_m}{L \varepsilon} \left[1 - (1 - \varepsilon) \frac{p_v}{p_m} \right]$$

from which it can be seen that the psychrometric constant requires prior knowledge about the value of vapour pressure. However, in practice it is assumed that $p_v \ll p_m$ such that

$$\gamma = \frac{c_p p_m}{L \varepsilon} \quad (18.53)$$

The psychrometric constant, γ , represents the cooling effect of evaporating a unit vapor pressure worth of water. The word “psychrometric” comes from the Greek word for “cold means of measurement”. Looking back at Eq. (18.49) it can be seen that

$$\gamma = \frac{p_{v1} - p_{v0}}{T_1 - T_0}.$$

18.4.7 Estimating Humidity from Dry-Bulb Temperature

In many cases, a psychrometer is not present although good dry-bulb temperature data are available. Dry-bulb thermometers provide an estimate of air temperature. Temperature data exhibit diurnal cycles with highest temperatures in the afternoon and lowest temperatures in the early morning. This is driven by a net-import of radiation from the sun during the day and a net-export of radiation to space during the night.

Once the air temperature declines to a certain point, water vapour in the air condenses on the ground surface to form dew. The temperature is thought to stay constant from this point until the incoming morning solar radiation is sufficient to increase the air temperature again. The reason the temperature reaches this minimum point, is that once water starts to condense, latent heat is released and counterbalances the loss of heat by radiation to space. Just as evaporation consumes heat, condensation produces heat. It follows that a record of the daily minimum temperature can be used as an estimate of the so-called dew-point temperature.

The dew-point temperature, T_{dew} [Θ], represents the temperature at which moist air must be cooled to become water saturated for a given vapour pressure, p_v , and gas mixture pressure, p_m . It follows that vapour pressure can be determined from

$$p_v = p_{vs}(T_{\text{dew}})$$

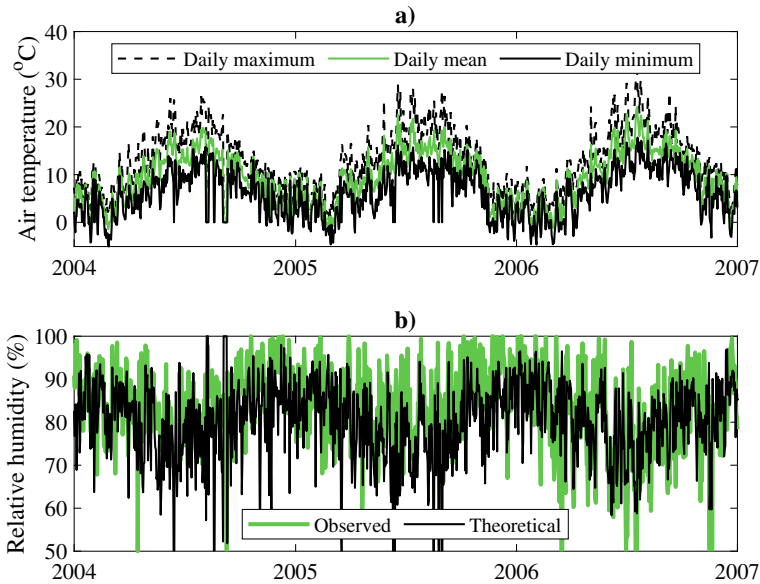


Fig. 18.1 Seasonal variations in temperature and humidity in Berkshire, UK. Observed humidity values were measured using a psychrometer. Theoretical humidity values were determined by calculating saturated vapour pressures using daily mean temperature and actual vapour pressures assuming daily minimum temperatures represent the dew-point temperature. Weather station data used to develop these plots was acquired from [4]

where $p_{vs}(T)$ can be determined from Tetens' equation (Eq. (18.4)). Furthermore, an estimate of the daily mean vapour pressure can be obtained from

$$p_v = p_{vs}(T_{\min})$$

where $T_{\min} [^\circ\text{C}]$ is the daily minimum temperature.

Figure 18.1 shows temperature and humidity data obtained from an automatic weather station in Berkshire, UK. The theoretical humidity values were calculated assuming the daily minimum temperature represents the dew-point temperature. This theoretical approach is far from perfect. However, it leads to the right order of magnitude and provides a good representation of the seasonal dynamics.

18.5 Problem Sheet

Problem 18.1 (see Worked Solution 18.1)

Determine values of saturated vapour pressure at temperatures of 5, 10, 20, 40, 80 and 100 degrees Centigrade. How do these compare to atmospheric pressure at sea level (101.3 kPa)?

Problem 18.2 (see Worked Solution 18.2)

Determine values of absolute humidity and specific humidity assuming a relative humidity of 98%, atmospheric conditions at sea level (i.e., $p_m = 101.3$ kPa) and air temperatures of 5, 10, 20, 40, 80 and 100 degrees Centigrade.

Problem 18.3 (see Worked Solution 18.3)

Determine the latent heat capacity of water for air temperatures of 5, 10, 20, 40, 80 and 100 degrees Centigrade, assuming the density of liquid water is 1000 kg m^{-3} .

Problem 18.4 (see Worked Solution 18.4)

A psychrometer is used to measure wet-bulb temperatures. The dry-bulb temperature is 20°C and the air pressure is 101.3 kPa. Determine relative humidities when the psychrometer measures wet-bulb temperatures of 7, 10, 15, 20 degrees Centigrade.

Problem 18.5 (see Worked Solution 18.5)

Determine the night-time minimum temperatures that would be expected for relative humidities of 10, 20, 50 and 90%. Assume a mean daily temperature of 35°C .

18.6 Worked Solutions

Worked Solution 18.1 (see Problem 18.1)

Convert the temperatures, T , to degrees Kelvin and then calculate the saturated vapour pressure, p_{vs} , from Eq. (18.4). The pressures will need to be divided by 1000 to convert them from Pa to kPa. It follows that: Air temperatures are rarely

T ($^\circ\text{C}$)	T (K)	p_{vs} (kPa)
5	278	0.872
10	283	1.23
20	293	2.34
40	313	7.37
80	353	47.5
100	373	102

far above 40°C and the saturated vapour pressure is normally at least an order of magnitude less than atmospheric pressure. However, the saturated vapour pressure is close to atmospheric pressure at 100°C because 100°C is the boiling point of water at atmospheric pressure.

Worked Solution 18.2 (see Problem 18.2)

Absolute and specific humidity, C_v and X_v , can be determined from Eqs. (18.25) and (18.31), respectively. These require estimates of vapour pressure, p_v , which can be found from Eq. (18.3) using the values of p_{vs} obtained when solving Problem 18.1. Recall that the universal ideal gas constant is $R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$, the gas mixture pressure, $p_m = 101.3 \text{ kPa}$, and the molecular masses of water and dry air, M_v and M_d , are 18.02 and 28.96 g mol⁻¹, respectively. It follows that:

T (°C)	p_v (kPa)	C_v (kg m ⁻³)	X_v (-)
5	0.855	0.00666	0.00527
10	1.20	0.00921	0.00742
20	2.29	0.0169	0.0142
40	7.23	0.0500	0.0456
80	46.6	0.286	0.346
100	100	0.581	0.981

For temperatures less than 40°C the specific humidity is less than 5% despite the relative humidity being 98%. This is why we are able to comfortably breathe oxygen at relative humidities of 100%. However, when the air-temperature is the same as the boiling point of water (100°C) the relative humidities and specific humidities are pretty much the same, the air is almost completely comprised of water and the absolute humidity is close to the value of steam density at atmospheric conditions (0.6 kg m⁻³).

Worked Solution 18.3 (see Problem 18.3)

The Latent heat capacity, L , can be determined from Eq. (18.34). But before we can use this we need an expression for the slope of the saturated vapour pressure, $\alpha = \partial p_{vs} / \partial T$. From Eq. (18.4)

$$p_{vs} = 610.8 \exp \left[\frac{17.27(T - 273.2)}{T - 35.86} \right]$$

Making the substitution $b = (T - 273.2)/(T - 35.86)$ leads to $p_{vs} = 610.8 \exp(17.27b)$ from which we have

$$\alpha = \frac{\partial p_{vs}}{\partial T} = \frac{\partial b}{\partial T} \frac{\partial p_{vs}}{\partial b} = 17.27 p_{vs} \frac{\partial b}{\partial T}$$

where

$$\frac{\partial b}{\partial T} = \frac{(T - 35.86) - (T - 273.2)}{(T - 35.86)^2} = \frac{237.34}{(T - 35.86)^2}$$

It follows that

$$\alpha = \frac{4099 p_{vs}}{(T - 35.86)^2} \quad (18.54)$$

Substituting Eq. (18.54) into Eq. (18.34) then leads to

$$L = \frac{4099T}{(T - 35.86)^2} \left(\frac{RT}{M_v} - \frac{p_{vs}}{\rho_w} \right) \quad (18.55)$$

Recall that $R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$, $M_v = 18.02 \times 10^{-3} \text{ kg mol}^{-1}$ and $\rho_w = 1000 \text{ kg m}^{-3}$ (note that we need to make the units for M_v consistent with those of ρ_w). Therefore:

T (°C)	T (K)	p_{vs} (kPa)	α (kPa K ⁻¹)	L (kJ kg ⁻¹)
5	278.2	0.8723	0.06088	2492
10	283.2	1.228	0.08227	2479
20	293.2	2.338	0.1447	2455
40	313.2	7.373	0.3929	2412
80	353.2	47.5	1.933	2342
100	373.2	102.2	3.68	2313

Worked Solution 18.4 (see Problem 18.4)

In this case the relative humidity, $\phi_v = p_v / p_{vs}(T_{\text{dry}})$, where p_v is the vapour pressure and $p_{vs}(T_{\text{dry}})$ is the saturated vapour pressure when $T = T_{\text{dry}}$ where T_{dry} is the dry-bulb temperature.

For a psychrometer, Eq. (18.52) gives that

$$p_v = p_{vs}(T_{\text{wet}}) - \gamma \cdot (T_{\text{dry}} - T_{\text{wet}})$$

where γ is the psychrometric constant.

Recall that $c_p = 1005 \text{ J kg}^{-1} \text{ K}^{-1}$ and $\varepsilon = 0.6222$. From the information given we have that $p_m = 101.3 \text{ kPa}$ and $T_{\text{dry}} = 20^\circ\text{C}$. From Problem 18.3, we established that at 20°C , $L = 2455 \text{ kJ kg}^{-1}$. From Eq. (18.53)

$$\gamma = \frac{c_p p_m}{L \varepsilon} = \frac{1005 \times 101.3 \times 10^3}{2455 \times 10^3 \times 0.6222} = 66.65 \text{ Pa K}^{-1}$$

and from Eq. (18.4) we have that $p_{vs}(T_{\text{dry}}) = 2.338 \text{ kPa}$. It follows that:

$T_{\text{wet}} (^{\circ}\text{C})$	$T_{\text{wet}} (\text{K})$	$p_{vs}(T_{\text{wet}}) (\text{kPa})$	$p_v (\text{kPa})$	$\phi_v (\%)$
7	280.2	1.002	0.1354	5.79
10	283.2	1.228	0.5614	24.0
15	288.2	1.705	1.372	58.7
20	293.2	2.338	2.338	100

Worked Solution 18.5 (see Problem 18.5)

Recall that an estimate of vapour pressure, p_v , can be obtained from the saturated vapour pressure, p_{vs} , at night-time minimum temperature, $T_{\min}$, i.e., $p_v = p_{vs}(T_{\min})$. In this case, the relative humidity, ϕ_v , should satisfy

$$p_{vs}(T_{\min}) = p_{vs}(T)\phi_v$$

where T is the daily mean temperature.

The night-time minimum temperature can then be obtained from an inversion of Tetens' equation (Eq. (18.4)):

$$T_{\min} = \frac{35.86 \ln \left[\frac{p_{vs}(T_{\min})}{610.8} \right] - 4718}{\ln \left[\frac{p_{vs}(T_{\min})}{610.8} \right] - 17.27}$$

From Tetens' equation we have that $p_{vs}(T = 35^{\circ}\text{C}) = 5.621 \text{ kPa}$. It follows that:

$\phi_v (\%)$	$p_{vs}(T_{\min}) (\text{kPa})$	$T_{\min} (\text{K})$	$T_{\min} (^{\circ}\text{C})$
10	0.5621	272.1	-1.15
20	1.124	282.9	8.68
50	2.810	296.2	23.0
90	5.059	306.3	33.1

The results predict cold nights in dry regions and warm nights in humid regions.

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Abstract

This chapter develops mathematical equations for calculating potential evaporation from an open water surface, potential evapotranspiration and net incoming radiant flux density (RFD). The Penman-Monteith equation for potential evapotranspiration is derived by assuming a constant saturated vapour pressure gradient. An aerodynamic resistance function is derived by invoking a logarithmic wind speed profile. A value for the solar constant is derived from Planck's law. A semi-empirical equation is derived to estimate net incoming shortwave RFD in terms of time, date, latitude, air temperature and albedo. An empirical equation is presented for estimating net outgoing longwave RFD. Practical applications are presented through a problem sheet with worked solutions.

Notation

A	Albedo constant [-].
b	Spectral radiant flux density of a black-body [$\text{ML}^{-1}\text{T}^{-3}$].
b_{SE}	Spectral radiant flux density of the Sun on Earth [$\text{ML}^{-1}\text{T}^{-3}$].
B	Total radiant flux density of a black-body [MT^{-3}].
c	Speed of light [LT^{-1}].
c_p	Specific heat capacity of air [$\text{L}^2\text{T}^{-2}\Theta^{-1}$].
C	Sensible heat flux [MT^{-3}].
C_v	Absolute humidity [ML^{-3}].
E_0	Potential evaporation from an open water surface [LT^{-1}].
E_p	Potential evapotranspiration [LT^{-1}].
G	Rate at which heat is lost to the ground [MT^{-3}].
h	Planck's constant [ML^2T^{-1}].
k	Boltzmann's constant [$\text{ML}^2\text{T}^{-2}\Theta^{-1}$].
k_{Rs}	Atmospheric attenuation factor [-].
k_{Rs0}	Empirical factor for calculating k_{Rs} [Θ^{-1}].

L	Latent heat of evaporation [L^2T^{-2}].
p_m	Air pressure [$ML^{-1}T^{-2}$].
p_{sun}	Spectral power of the Sun [MLT^{-3}].
P_{sun}	Total power of the Sun [ML^2T^{-3}].
p_v	Vapour pressure [$ML^{-1}T^{-2}$].
p_{vs}	Saturated vapour pressure [$ML^{-1}T^{-2}$].
r_a	Aerodynamic resistance [$L^{-1}T$].
r_s	Stomatal resistance [$L^{-1}T$].
r_{sun}	Radius of the Sun [L].
r_{SE}	Distance from the Sun to the Earth [L].
R_0	Solar constant [MT^{-3}].
R_{dl}	Downward LW RFD [MT^{-3}].
R_{ds}	Downward SW RFD [MT^{-3}].
R_n	Net incoming RFD [MT^{-3}].
R_{nl}	Net outgoing LW RFD [MT^{-3}].
R_{ns}	Net incoming SW RFD [MT^{-3}].
R_{ul}	Upward LW RFD [MT^{-3}].
R_{us}	Upward SW RFD [MT^{-3}].
T	Temperature [Θ].
T_{max}	Daily maximum temperature [Θ].
T_{min}	Daily minimum temperature [Θ].
t_d	Time in decimalised days since 1st January of current year [T].
t_h	24-hour time in hours [T].
t_l	Total number of daylight hours [T].
u	Wind speed [LT^{-1}].
u_τ	Friction velocity [LT^{-1}].
z	Elevation [L].
α	Saturated vapour pressure gradient [$ML^{-1}T^{-2}\Theta^{-1}$].
β	Factor accounting for dynamic changes in the distance from the Sun to the Earth [-].
γ	Psychrometric constant [$ML^{-1}T^{-2}\Theta^{-1}$].
δ	Solar declination angle [-].
ε	Ratio of the molecular mass of water vapour to that of dry air [-].
λ	Wavelength [L].
ρ_d	Density of dry air [ML^{-3}].
ρ_m	Density of air [ML^{-3}].
ρ_w	Density of liquid water [ML^{-3}].
σ	Stefan-Boltzmann constant [$MT^{-3}\Theta^{-4}$].
τ_0	Boundary shear stress [$ML^{-1}T^{-2}$].
φ	Latitude [-].
ψ	Solar-zenith-angle [-].
ω	Hour angle [-].
ω_s	Sunset/sunrise angle [-].
Ω	Solar calendar angle [-].
LW	Longwave.

RFD	Radiant flux density.
SDA	Solar declination angle.
SW	Shortwave.
SZA	Solar zenith angle.

19.1 Introduction

Evaporation and transpiration form a significant component of catchment water balances around the world. Evaporation and transpiration are collectively referred to as evapotranspiration. The amount of actual evapotranspiration that takes place is strongly dependent on the amount of locally available liquid water. A related term is potential evapotranspiration, which represents how much evapotranspiration would occur in the presence of an infinite supply of liquid water. Potential evapotranspiration (PE) is calculated from variables referred to collectively as weather station data. Weather station data includes radiation, temperature, humidity and wind-speed.

Solar radiation is the main contributor of the energy required to overcome the latent heat of evaporation. Temperature controls how readily water is evaporated and how much water the air can hold. Humidity tells us how close the air is to vapour saturation. Once the air is vapour saturated, evaporation will cease. Winds replace vapour saturated air with dry air from above. High wind speeds lead to enhanced evaporation rates.

This chapter is split into two parts. Building heavily on theory developed in the preceding chapter concerning humidity, the first part of this chapter involves the development of the Penman-Monteith equation, which enables the prediction of PE from weather station data. The second part concerns the measurement and prediction of net incoming radiation, required for PE calculation.

19.2 Evaporation and Evapotranspiration

19.2.1 Potential Evapotranspiration

Recall from Eq. (18.46) that the potential evaporation rate from an open water surface, E_0 [LT^{-1}], can be determined from the resistance equation

$$E_0 = \frac{C_{v0} - C_{v1}}{r_a \rho_w} \quad (19.1)$$

where C_{v0} [ML^{-3}] is the absolute humidity at the water surface, C_{v1} [ML^{-3}] is the absolute humidity at some elevation above the water surface, r_a [L^{-1}T] is the aerodynamic resistance and ρ_w [ML^{-3}] is the density of liquid water.

The potential evapotranspiration rate from a plant with access to unlimited water supply, E_p [LT^{-1}], can be determined from a similar resistance equation [1]:

$$E_p = \frac{C_{v0} - C_{v1}}{(r_a + r_s)\rho_w} \quad (19.2)$$

where C_{v0} now represents the absolute humidity at a water surface within the plant and r_s [L^{-1}T] is referred to as the stomatal resistance. The idea here is that the plant offers additional resistance to vapour flow. Note that r_s is an empirical parameter and a function of plant physiology. For grass reference crop it is normally assumed that $r_s = 70 \text{ m}^{-1} \text{ s}$ [2].

In practice there is a tendency to monitor vapour pressure, p_v [$\text{ML}^{-1}\text{T}^{-2}$], as opposed to absolute humidity. Equation (19.2) can be written in terms of p_v by substituting Eq. (18.26) to get

$$E_p = \frac{\varepsilon \rho_d}{\rho_w p_m} \left(\frac{p_{v0} - p_{v1}}{r_a + r_s} \right)$$

where ρ_d [ML^{-3}] is the density of dry air, ε [-] is the ratio of the molecular mass of water vapour to that of dry air (recall $\varepsilon = 0.6222$), and p_m [$\text{ML}^{-1}\text{T}^{-2}$] is the air pressure.

Providing the plant of concern has access to sufficient water, the relative humidity within the plant will be 100% and

$$E_p = \frac{\varepsilon \rho_d}{\rho_w p_m} \left(\frac{p_{vs}(T_0) - p_{v1}}{r_a + r_s} \right) \quad (19.3)$$

where T_0 [$^{\circ}\text{C}$] is the temperature within the plant and $p_{vs}(T_0)$ [$\text{ML}^{-1}\text{T}^{-2}$] is the saturated vapour pressure within the plant, which can be calculated using Tetens' equation (Eq. (18.4)).

Unfortunately, it is rarely possible to directly evaluate Eq. (19.3) due to difficulties in accurately measuring T_0 . However, T_0 can be determined from the energy balance equation,

$$\rho_w L E_p = R_n - G - C \quad (19.4)$$

where L [L^2T^{-2}] is the latent heat of evaporation, R_n [MT^{-3}] is net incoming radiant flux density (RFD) (see Sect. 19.3.1), G [MT^{-3}] is the rate at which heat is lost to the ground and C [MT^{-3}] is the sensible heat flux (loss of heat by convection into the atmosphere).

From Eq. (18.47) we have that

$$C = \frac{\rho_m c_p \cdot (T_0 - T_1)}{r_a} \quad (19.5)$$

where ρ_m [ML^{-3}] is the air density, c_p [$\text{L}^2\text{T}^{-2}\Theta^{-1}$] is the constant pressure specific heat capacity of air ($= 1005 \text{ J kg}^{-1} \text{ K}^{-1}$) and T_1 [$^{\circ}\text{C}$] is the air-temperature at some elevation above the plant.

The T_0 term can be eliminated by assuming that the saturated vapour pressure gradient, α [$\text{ML}^{-1}\text{T}^{-2}\Theta^{-1}$], can be treated as a constant, which enables us to say

$$\alpha = \frac{\partial p_{vs}}{\partial T} \approx \frac{p_{vs}(T_0) - p_{vs}(T_1)}{T_0 - T_1} \quad (19.6)$$

Challenge 19.1 Substitute Eqs. (19.3), (19.5) and (19.6) into Eq. (19.4) and derive an expression for T_0 in terms of T_1 , R_n , G , ρ_m , c_p , $p_{vs}(T_1)$, α , r_a , r_s and the psychrometric constant, γ , given by Eq. (18.51).

Substituting Eqs. (19.3) and (19.5) into Eq. (19.4) leads to

$$\frac{L\varepsilon\rho_d}{p_m} \left(\frac{p_{vs}(T_0) - p_{v1}}{r_a + r_s} \right) = R_n - G - \frac{\rho_m c_p \cdot (T_0 - T_1)}{r_a} \quad (19.7)$$

From Eq. (19.6) we have

$$p_{vs}(T_0) = \alpha \cdot (T_0 - T_1) + p_{vs}(T_1) \quad (19.8)$$

Substituting Eq. (19.8) into Eq. (19.7) leads to

$$\frac{L\varepsilon\rho_d}{p_m} \left(\frac{\alpha \cdot (T_0 - T_1) + p_{vs}(T_1) - p_{v1}}{r_a + r_s} \right) = R_n - G - \frac{\rho_m c_p \cdot (T_0 - T_1)}{r_a} \quad (19.9)$$

Solving Eq. (19.9) for T_0 gives us

$$T_0 = T_1 + \frac{R_n - G - \frac{L\varepsilon\rho_d}{p_m} \left(\frac{p_{vs}(T_1) - p_{v1}}{r_a + r_s} \right)}{\frac{L\varepsilon\rho_d\alpha}{p_m \cdot (r_a + r_s)} + \frac{\rho_m c_p}{r_a}} \quad (19.10)$$

Substituting the expression for the psychrometric constant, γ [$\text{ML}^{-1}\text{T}^{-2}\Theta^{-1}$], given by Eq. (18.51), into Eq. (19.10) leads to [3]

$$T_0 = T_1 + \frac{\frac{\gamma \cdot (R_n - G)}{\rho_m c_p} - \left(\frac{p_{vs}(T_1) - p_{v1}}{r_a + r_s} \right)}{\frac{\alpha}{(r_a + r_s)} + \frac{\gamma}{r_a}} \quad (19.11)$$

Note that $\alpha \equiv \alpha(T_1)$ can be determined from Eq. (18.54).

Challenge 19.2 Substitute Eq. (19.11) into Eq. (19.5) and then substitute the result into Eq. (19.4).

Substituting Eq. (19.11) into Eq. (19.5) Gives us

$$\begin{aligned} C &= \frac{1}{r_a} \left[\frac{\gamma \cdot (R_n - G) - \rho_m c_p \cdot \left(\frac{p_{vs}(T_1) - p_{v1}}{r_a + r_s} \right)}{\frac{\alpha}{(r_a + r_s)} + \frac{\gamma}{r_a}} \right] \\ &= \frac{\gamma \cdot (r_a + r_s)(R_n - G) - \rho_m c_p [p_{vs}(T_1) - p_{v1}]}{\alpha r_a + \gamma \cdot (r_a + r_s)} \end{aligned} \quad (19.12)$$

Substituting Eq. (19.12) into Eq. (19.4) then leads to [1]

$$\rho_w L E_p = \frac{\alpha r_a \cdot (R_n - G) + \rho_m c_p [p_{vs}(T_1) - p_{v1}]}{\alpha r_a + \gamma \cdot (r_a + r_s)} \quad (19.13)$$

which is widely referred to as the Penman-Monteith equation for potential evapotranspiration.

19.2.2 Open-Water Evaporation

Comparing Eqs. (19.1) and (19.2) it can be understood that Eq. (19.13) reduces to an equation for potential evaporation from an open water surface, E_0 , by setting the stomatal resistance, $r_s = 0$, to get [3]

$$\rho_w L E_0 = \frac{\alpha \cdot (R_n - G) + \rho_m c_p \left[\frac{p_{vs}(T_1) - p_{v1}}{r_a} \right]}{\alpha + \gamma} \quad (19.14)$$

which is commonly referred to as the original Penman equation.

19.2.3 Note About Penman

The Penman-Monteith equation is the most commonly used method of determining potential evapotranspiration and is a cornerstone of the Food and Agriculture Organisation's (FAO) recommended method for determining crop-water requirements, referred to as FAO56 [2]. Howard Penman (1909–1984) grew up in Dunston on Tyne and studied mathematics and physics at Durham University [4]. The particular genius of [3] is the development of Eq. (19.11) which eliminated the requirement to directly measure the temperature at the water surface, T_0 .

19.2.4 Aerodynamic Resistance

The aerodynamic resistance can be obtained by rearranging Eq. (18.45) to get

$$r_a = \frac{\rho_m \cdot (u_1 - u_0)}{\tau_0} \quad (19.15)$$

and thinking of u_0 and u_1 as being the wind speed at elevations, z_0 and z_1 , respectively, and τ_0 as being the boundary shear stress caused by the overlying moving air body.

Air flow in natural systems is turbulent. An important empirical law in this context is [5, p.348]

$$\frac{u}{u_\tau} = 2.5 \ln \left(\frac{z u_\tau}{\nu} \right) + 5.5 \quad (19.16)$$

where u_τ [LT^{-1}] is known as the friction velocity, found from [5, p.344]

$$u_\tau = \left(\frac{\tau_0}{\rho_m} \right)^{1/2} \quad (19.17)$$

Challenge 19.3 Given Eqs. (19.15), (19.16) and (19.17), derive an expression for r_a purely in terms of z_0 , z_1 , u_0 and u_1 .

From Eq. (19.16) we have that

$$\frac{u_0}{u_\tau} = 2.5 \ln \left(\frac{z_0 u_\tau}{\nu} \right) + 5.5$$

and

$$\frac{u_1}{u_\tau} = 2.5 \ln \left(\frac{z_1 u_\tau}{\nu} \right) + 5.5$$

from which it follows that

$$u_1 - u_0 = 2.5 u_\tau \ln \left(\frac{z_1}{z_0} \right) \quad (19.18)$$

From Eq. (19.17) we have that

$$\tau_0 = \rho_m u_\tau^2 \quad (19.19)$$

Substituting Eqs. (19.18) and (19.19) into Eq. (19.15) leads to

$$r_a = \frac{2.5}{u_\tau} \ln \left(\frac{z_1}{z_0} \right) \quad (19.20)$$

The u_τ term is obtained by rearranging Eq. (19.18) to get

$$u_\tau = \frac{u_1 - u_0}{2.5 \ln \left(\frac{z_1}{z_0} \right)} \quad (19.21)$$

Substituting Eq. (19.21) into Eq. (19.20) then gives us

$$r_a = \frac{6.25}{(u_1 - u_0)} \left[\ln \left(\frac{z_1}{z_0} \right) \right]^2 \quad (19.22)$$

Most weather stations measure wind speed using an anemometer held at 2 m above the land surface. Equation (19.22) can be used to determine r_a for a given set of wind speed observations by setting u_1 equal to the measured wind speed and setting z_1 to the elevation of the anemometer above the land surface (i.e. $z_1 = 2$ m). The elevation z_0 , is thought to represent a roughness length where the wind-speed can be treated as zero (i.e., $u_0 = 0$). [2] use a slightly different equation for r_a for determining reference crop evapotranspiration, which becomes equivalent to Eq. (19.22) when $z_0 = 0.006247$ m.

19.3 Radiation

Net incoming radiation is one of the most important drivers for evaporation and evapotranspiration because it provides the energy required to overcome the latent heat of evaporation.

Objects containing heat emit electromagnetic waves with a distribution of different wavelengths, λ [L]. The higher the temperature of an object the shorter the modal wavelength within the distribution. It is useful to distinguish between shortwave (SW) and longwave (LW) radiation. SW radiation includes wavelengths $< 3 \mu\text{m}$. LW radiation includes wavelengths $> 3 \mu\text{m}$. The Sun emits mostly SW radiation. Because the Earth is cooler, it emits mostly LW radiation.

In what follows, Planck's law of black-body radiation is used to explain why SW and LW radiation observed on the Earth mostly relate to radiation emitted from the Sun and the Earth, respectively. It is then explained how net incoming radiation can be measured using a net radiometer. Semi-empirical equations are derived for predicting SW and LW radiation using air temperature along with knowledge about latitude, time of day and time in year. A case study is then presented from the UK.

19.3.1 Black-Body Radiation

The rate at which energy radiates from a unit of surface area is referred to as the radiant flux density (RFD) (SI units: W m^{-2}). Spectral RFD is a quantity used to describe the RFD emitted per unit wavelength. The spectral RFD from a black-body, b [$\text{ML}^{-1}\text{T}^{-3}$], is described by Planck's law [6, p.40]

$$b(\lambda, T) = \frac{2\pi hc^2 \lambda^{-5}}{\exp\left(\frac{hc}{k\lambda T}\right) - 1} \quad (19.23)$$

where h [ML^2T^{-1}] is Planck's constant ($= 6.626 \times 10^{-34} \text{ J s}$), c [LT^{-1}] is the speed of light ($= 2.998 \times 10^8 \text{ m s}^{-1}$), k [$\text{ML}^2\text{T}^{-2}\Theta^{-1}$] is Boltzmann's constant ($= 1.381 \times 10^{-23} \text{ J K}^{-1}$) and T [Θ] is temperature in Kelvin.

Figure 19.1 shows plots of spectral RFD against wavelength according to Planck's law. The green line shows the spectral RFD distribution for 5771 K, which is the

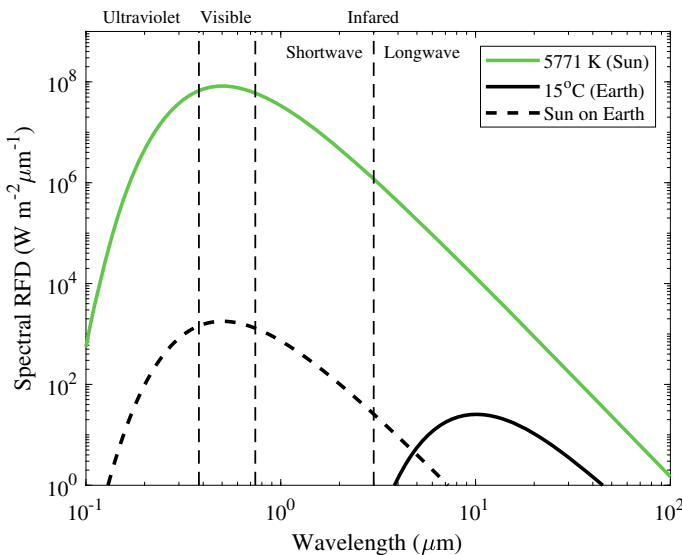


Fig. 19.1 Plot of spectral radiance flux density (RFD) according to Planck's law (Eq. (19.23)) using temperatures representative of the Earth and the Sun. The "Sun on Earth" curve is obtained by scaling the spectral RFD to account for the distance of the Earth from the Sun

temperature of the Sun. The black solid line shows the spectral RFD distribution for 15°C (288.15 K), which is the mean temperature on Earth. It can be understood that the higher the temperature of an object, the higher the peak spectral RFD and the lower the modal wavelength. The Sun predominantly emits radiation in the visible light range whereas the Earth emits almost exclusively within the infrared range.

The Sun emits mostly SW radiation. In contrast, the Earth almost exclusively emits LW radiation. However, LW radiation from the Earth is small compared to that from the Sun (see Fig. 19.1). But an important consideration is that Planck's law gives the RFD of an object at its location. The RFD of the Sun, as experienced on Earth, is significantly reduced from that predicted by Planck's law because the Earth is located 1.496×10^{11} m away. The spectral RFD of the Sun as experienced on Earth can be determined as follows.

Note that spectral RFD represents the radiation power per unit area per unit wavelength. The spectral power of a source can be determined by multiplying its spectral RFD by its surface area. Assuming the Sun to be of spherical geometry, the spectral power of the Sun, p_{sun} [MLT^{-3}], is found from

$$p_{\text{sun}}(\lambda) = 4\pi r_{\text{sun}}^2 b(\lambda, T_{\text{sun}})$$

where r_{sun} [L] is the radius of the Sun ($= 6.963 \times 10^8$ m) and T_{sun} [$^{\circ}\text{K}$] ($= 5771$ K) is the temperature of the Sun.

Let $\hat{r}_{SE}$ [L] be the mean distance from the Sun to the Earth, otherwise known as the astronomical unit ($= 1.496 \times 10^{11}$ m). We will assume that radiation from the Sun is isotropic. Therefore the RFD of the Sun will vary only with radial distance from the Sun and should be uniform over a spherical surface about the Sun. It follows that the spectral RFD of the Sun at the location of the Earth, denoted b_{SE} [$\text{ML}^{-1}\text{T}^{-3}$], can be found from

$$b_{SE}(\lambda) = \frac{p_{\text{sun}}(\lambda)}{4\pi \hat{r}_{SE}^2} = \left(\frac{r_{\text{sun}}}{\hat{r}_{SE}} \right)^2 b(\lambda, T_{\text{sun}})$$

The factor, $(r_{\text{sun}}/\hat{r}_{SE})^2 = 2.17 \times 10^{-5}$. A plot for spectral RFD of the Sun at the location of Earth is shown in Fig. 19.1 as a black dashed line, labelled “Sun on Earth”. Total LW RFD can be found by integrating spectral RFD with respect to λ from $3 \mu\text{m}$ to infinity. Noting that the x -axis in Fig. 19.1 uses a logarithmic scale, it can be understood that total LW RFD from the Sun, as experienced on Earth, is substantially less than that emitted directly from Earth. For this reason, observed ambient LW radiation is assumed to be exclusively emitted from the Earth.

19.3.2 Net Incoming RFD

The net incoming RFD normal to the land surface, R_n [MT^{-3}], is determined from

$$R_n = R_{ns} - R_{nl} \quad (19.24)$$

where R_{ns} [MT^{-3}] and R_{nl} [MT^{-3}] are the net incoming SW RFD and net outgoing LW RFD, respectively, found from

$$R_{ns} = R_{ds} - R_{us}$$

and

$$R_{nl} = R_{ul} - R_{dl}$$

where R_{ds} [MT^{-3}] and R_{us} [MT^{-3}] are the downward and upward SW RFD, respectively, and R_{dl} [MT^{-3}] and R_{ul} [MT^{-3}] are the downward and upward LW RFD, respectively.

R_{ds} is due to incoming solar radiation. R_{us} is due to solar radiation that is reflected from the land surface. The land surface emits LW radiation, which is the R_{ul} term. The Earth's atmosphere emits LW radiation back to the land surface, which is the R_{dl} term.

19.3.3 Measuring RFD with a Net Radiometer

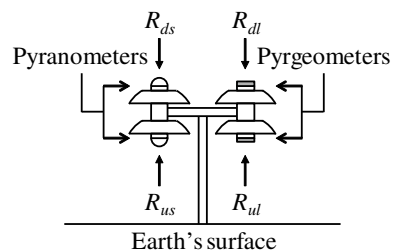
Net incoming RFD can be directly observed using a net radiometer (Fig. 19.2). A net radiometer typically comprises four radiation sensors: downward and upward facing pyranometers to measure R_{ds} and R_{us} , respectively, and downward and upward facing pyrgeometers to measure R_{dl} and R_{ul} , respectively. Pyranometers and pyrgeometers are similar instruments except pyranometers measure SW radiation whereas pyrgeometers measure LW radiation. By distinguishing between SW and LW radiation, it is possible to separate out Earth-based radiation from solar radiation.

Both pyranometers and pyrgeometers contain a thermopile and thermometer. A thermopile is a thermoelectric device that transforms heat energy to a voltage. An empirical equation is used to relate the measured voltage to a radiant flux density (RFD). The thermopile measures the net RFD coming into the radiation sensor. The thermometer is used to estimate outgoing RFD emitted from the radiation sensor. Both flux densities are added together to determine the total incoming RFD.

The pyranometer is limited to measure SW radiation by emplacing the thermopile within a glass hemispherical dome. The glass filters out LW frequencies. The hemispherical dome enables the sensor to collect solar radiation from sunrise to sunset.

The pyrgeometer is limited to measure LW radiation by placing the thermopile beneath a silicon filter, which filters out SW frequencies.

Fig. 19.2 Schematic diagram of a net radiometer



19.3.4 Estimating SW RFD

An estimate of net incoming SW RFD, R_{ns} , can be determined by considering the rate of energy emitted from the Sun along with the latitude of the observation point, the time of the day, the time in the year and the reflectance of the land surface.

Below we will derive a semi-empirical equation to estimate R_{ns} from these factors. First we will look at the solar constant, which represents the mean solar RFD experienced at the edge of the Earth's atmosphere. We account for the way in which the distance between Earth and the Sun changes throughout the year. An empirical expression is introduced to account for radiation absorption within the Earth's atmosphere. A trigonometric expression is derived to account for the way in which the angle of the Sun's rays changes from sunrise to sunset. This is then integrated with respect to time to derive a daily mean estimate of incoming SW RFD. An empirical reflectance parameter, known as albedo, is introduced to account for upward SW radiation due to reflection.

19.3.4.1 The Solar Constant

Challenge 19.4 Use Planck's law to derive an expression for the total RFD of a black-body, B [MT^{-3}]. You will need to exploit the identity

$$\int_0^\infty \frac{u^3}{e^u - 1} du = \frac{\pi^4}{15}$$

The total RFD of a black-body, B [MT^{-3}], can be obtained from

$$B(T) = \int_0^\infty b(\lambda, T) d\lambda \quad (19.25)$$

where b is found from Planck's law (Eq. (19.23)).

Evaluation of this integral is made easier by introducing the substitution, $u = \frac{hc}{k\lambda T}$, such that

$$b(u, T) = \frac{2\pi(kTu)^5}{h^4 c^3 (e^u - 1)} \quad \text{and} \quad \frac{d\lambda}{du} = -\frac{hc}{kTu^2}$$

and Eq. (19.25) reduces to

$$B(T) = \int_\infty^0 b(u, T) \frac{d\lambda}{du} du = \frac{2\pi k^4 T^4}{h^3 c^2} \int_0^\infty \frac{u^3}{e^u - 1} du \quad (19.26)$$

It turns out that

$$\int_0^\infty \frac{u^3}{e^u - 1} du = \frac{\pi^4}{15}$$

which on substitution into Eq. (19.26) leads to Stefan's law [6, p.40]:

$$B(T) = \sigma T^4 \quad (19.27)$$

where σ [$\text{MT}^{-3}\Theta^{-4}$] is the Stefan-Boltzmann constant found from

$$\begin{aligned}\sigma &= \frac{2\pi^5 k^4}{15h^3 c^2} \\ &= \frac{2\pi^5 \times (1.381 \times 10^{-23})^4}{15 \times (6.626 \times 10^{-34})^3 \times (2.998 \times 10^8)^2} \\ &= 5.670 \times 10^{-8} \text{ W m}^{-2}\text{K}^{-4}\end{aligned}$$

Challenge 19.5 Calculate the mean total RFD of the Sun as experienced on the Earth.

The mean total RFD of the Sun, as experienced at the edge of the Sun, is found from $B(T_{\text{sun}})$ where T_{sun} [Θ] is the temperature of the Sun.

The total RFD of the Sun as experienced on the Earth, R_0 [MT^{-3}], is found from

$$R_0 = \frac{P_{\text{sun}}}{4\pi \hat{r}_{SE}^2} \quad (19.28)$$

where P_{sun} [ML^2T^{-3}] is the total power of the Sun and $\hat{r}_{SE}$ [L] is the mean distance between the Earth and the Sun.

The total power of the Sun is found from

$$P_{\text{sun}} = 4\pi r_{\text{sun}}^2 B(T_{\text{sun}}) \quad (19.29)$$

where r_{sun} [L] is the radius of the Sun.

Substituting Eq. (19.27) into Eq. (19.29) and then substituting the result into Eq. (19.28) leads to

$$R_0 = \left(\frac{r_{\text{sun}}}{\hat{r}_{SE}} \right)^2 \sigma T_{\text{sun}}^4 \quad (19.30)$$

Substituting the values for r_{sun} , $\hat{r}_{SE}$, σ and T_{sun} , listed above, into Eq. (19.30) gives us

$$\begin{aligned}R_0 &= \left(\frac{6.963 \times 10^8}{1.496 \times 10^{11}} \right)^2 \times 5.670 \times 10^{-8} \times 5771^4 \\ &= 1362 \text{ W m}^{-2}\end{aligned} \quad (19.31)$$

which is commonly referred to as the solar constant. It represents the mean solar RFD experienced at the edge of the Earth's atmosphere.

19.3.4.2 Distance Between the Earth and the Sun

The Earth's orbit about the Sun is elliptical. Consequently the distance between the Earth and the Sun, r_{SE} , is not constant. Reference [7] derived an empirical expression for r_{SE} by fitting a Fourier series to tabulated astronomical data. The first three terms of this Fourier series provide sufficient accuracy for our purpose and are provided below [7]:

$$\beta \equiv \left(\frac{\hat{r}_{SE}}{r_{SE}} \right)^2 = 1.000 + 0.03422 \cos \Omega + 0.001280 \sin \Omega \quad (19.32)$$

where

$$\Omega = \frac{2\pi t_d}{365} \quad (19.33)$$

and t_d (days) is time in decimalised days since the beginning of 1st January for the year in question. Given Eq. (19.31), it follows that the solar RFD experienced at the edge of the Earth's atmosphere, for a given time, t_d , is found from βR_0 .

19.3.4.3 Radiation Attenuation in the Atmosphere

Solar radiation is partially absorbed by the chemical constituents of the Earth's atmosphere. On a clear day around 25% of solar radiation is absorbed [2]. On a cloudy day up to 75% of solar radiation is absorbed [2]. The attenuation factor due to atmospheric absorption, k_{Rs} [–], is often estimated using the following empirical function [8]

$$k_{Rs} = k_{Rs0} \cdot (T_{\max} - T_{\min})^{1/2} \quad (19.34)$$

where $T_{\max}$ (K) and $T_{\min}$ (K) are the daily maximum and minimum air temperatures, respectively, and k_{Rs0} is an empirical factor taken to be $0.16 \text{ K}^{-1/2}$ and $0.19 \text{ K}^{-1/2}$ for inland and coastal regions, respectively.

The link between k_{Rs} , $T_{\max}$ and $T_{\min}$ is due to the link between $T_{\max}$, $T_{\min}$ and humidity, which in turn has a strong control on cloud cover.

It follows that the solar RFD (normal to the Sun's surface) at the Earth's land surface (i.e., beneath the Earth's atmosphere), for a given time, t_d , is found from $k_{Rs} \beta R_0$.

19.3.4.4 Solar-Zenith-Angle (SZA)

The angle of the Sun's rays intersecting the land surface (see Fig. 19.3) are dependent on the latitude of the observation point, the time of the day and the time in the year. The angle between the Sun's rays and the vertical (i.e., a line normal to the land surface) is referred to as the solar-zenith-angle (SZA), ψ [–]. Only the vertical component of the Sun's rays (i.e., the component normal to the land surface) are relevant to the downward SW RFD. It follows that, providing there is daylight, the downward SW RFD at the land surface, R_{ds} , is found from

$$R_{ds} = \begin{cases} k_{Rs} \beta R_0 \cos \psi, & \psi \in \left[-\frac{\pi}{2}, \frac{\pi}{2} \right] \\ 0, & \psi \notin \left[-\frac{\pi}{2}, \frac{\pi}{2} \right] \end{cases} \quad (19.35)$$

Fig. 19.3 Diagram illustrating the meaning of the solar zenith angle (SZA), ψ , and albedo, A

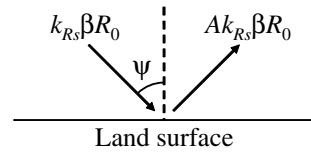
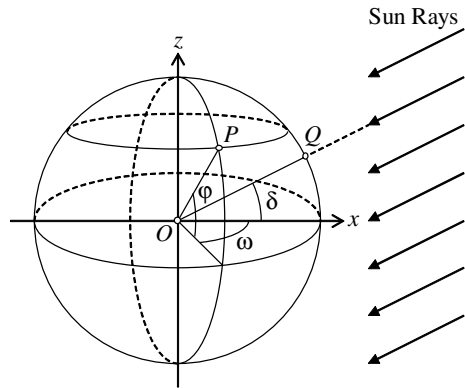


Fig. 19.4 Schematic showing hour angle, ω , latitude, φ , and angle of declination, δ . Note that the y -axis cannot be seen because it is normal to the page



It is possible to derive a theoretical relationship between $\cos \psi$, the latitude of a location of concern, φ , the hour angle, ω , and the so-called solar declination angle (SDA), δ (see Fig. 19.4).

The hour angle, ω , is the clockwise angle, on a plane of constant latitude, from the location of current noon to the location of the observer. If t_h is 24-hour time in hours

$$\omega = \frac{2\pi(t_h - 12)}{24} \quad (19.36)$$

The SDA represents the latitude at which the SZA is zero at noon. The SDA varies throughout the year due to the eccentricity of Earth's orbit about the Sun. A commonly used empirical equation to determine δ is another Fourier series derived by [7]. Again, the first three terms are sufficient for our purpose [7]:

$$\delta = 0.006918 - 0.3999 \cos \Omega + 0.07026 \sin \Omega \quad (19.37)$$

where Ω is as previously defined in Eq. (19.33).

Consider Fig. 19.4. The vector $\vec{OP}$ is a line from the centre of the Earth to an observer at latitude, φ , and hour angle, ω . The vector $\vec{OQ}$ represents the direction of sun rays, and is controlled by the SDA, δ . The SZA, ψ , represents the angle between the two vectors $\vec{OP}$ and $\vec{OQ}$.

Challenge 19.6 Use the rule $\vec{OP} \cdot \vec{OQ} = \|\vec{OP}\| \|\vec{OQ}\| \cos \psi$ to determine an expression for $\cos \psi$ in terms of φ , δ and ω .

Let r [L] be the radius of the sphere. It can then be said that:

$$\begin{aligned}\overrightarrow{OP} &= r \cos \varphi \cos \omega \hat{\mathbf{i}} + r \cos \varphi \sin \omega \hat{\mathbf{j}} + r \sin \varphi \hat{\mathbf{k}} \\ \overrightarrow{OQ} &= r \cos \delta \hat{\mathbf{i}} + r \sin \delta \hat{\mathbf{k}}\end{aligned}$$

The Euclidean norms:

$$\|\overrightarrow{OP}\| = \|\overrightarrow{OQ}\| = r$$

The dot-product is

$$\overrightarrow{OP} \cdot \overrightarrow{OQ} = r^2 \cos \varphi \cos \omega \cos \delta + r^2 \sin \varphi \sin \delta$$

Given $\overrightarrow{OP} \cdot \overrightarrow{OQ} = \|\overrightarrow{OP}\| \|\overrightarrow{OQ}\| \cos \psi$ it follows that

$$\cos \psi = \sin \varphi \sin \delta + \cos \varphi \cos \delta \cos \omega \quad (19.38)$$

19.3.4.5 Total Duration of Daylight

Challenge 19.7 Use Eqs. (19.36) and (19.38) to determine when the Sun is up and the total duration of daylight, t_t , for a given day and given latitude.

Let $\pm\omega_s$ be the value of ω at sunset and sunrise, respectively. Given the relationship in Eq. (19.36) it follows that the sun is up when

$$t_h \in \left[12 - \frac{24\omega_s}{2\pi}, 12 + \frac{24\omega_s}{2\pi} \right]$$

and the total duration of daylight, t_t (in hours), is found from

$$t_t = \frac{24|\omega_s|}{\pi} \quad (19.39)$$

Given Eq. (19.35), it can also be understood that

$$R_{ds} = \begin{cases} k_{Rs} \beta R_0 \cos \psi, & \omega \in [-\omega_s, \omega_s] \\ 0, & \omega \notin [-\omega_s, \omega_s] \end{cases} \quad (19.40)$$

At sunrise, $\psi = -\pi/2$. At sunset, $\psi = \pi/2$. For both scenarios $\cos \psi = 0$. From Eq. (19.38), it follows that

$$0 = \sin \varphi \sin \delta + \cos \varphi \cos \delta \cos(\pm\omega_s)$$

and therefore the sunset/sunrise angle, ω_s , is found from

$$\omega_s = \arccos(-\tan \varphi \tan \delta). \quad (19.41)$$

19.3.4.6 Daily Mean Downward SW RFD

Challenge 19.8 Assume that all quantities are constant over a day with the exception of the SZA and integrate Eq. (19.40) with respect to t_h over a 24-hour period to obtain an expression for daily mean downward SW RFD, $\hat{R}_{ds}$.

From Eq. (19.40) it can be said that

$$\hat{R}_{ds} \equiv \frac{1}{24} \int_0^{24} R_{ds} dt_h = \frac{k_{Rs} \beta R_0}{24} \int_0^{24} \cos \psi dt_h$$

Rather than writing $\cos \psi$ in terms of t_h it makes sense to write the integral in terms of the hour-angle, ω . From Eq. (19.36)

$$\frac{d\omega}{dt_h} = \frac{2\pi}{24}$$

so

$$\hat{R}_{ds} = \frac{k_{Rs} \beta R_0}{2\pi} \int_{-\pi}^{\pi} \cos \psi d\omega$$

However, we established previously that we will only receive solar energy during the period $\omega \in [-\omega_s, \omega_s]$ where ω_s is the sunset/sunrise angle, defined in Eq. (19.41). Therefore

$$\hat{R}_{ds} = \frac{k_{Rs} \beta R_0}{2\pi} \int_{-\omega_s}^{\omega_s} \cos \psi d\omega$$

Considering again Eq. (19.38)

$$\begin{aligned} \int_{-\omega_s}^{\omega_s} \cos \psi d\omega &= \int_{-\omega_s}^{\omega_s} (\sin \varphi \sin \delta + \cos \varphi \cos \delta \cos \omega) d\omega \\ &= [\omega \sin \varphi \sin \delta + \cos \varphi \cos \delta \sin \omega]_{-\omega_s}^{\omega_s} \\ &= 2\omega_s \sin \varphi \sin \delta + 2 \cos \varphi \cos \delta \sin \omega_s \end{aligned}$$

It follows that similar to [2, p. 46]

$$\hat{R}_{ds} = \frac{k_{Rs} \beta R_0}{\pi} (\omega_s \sin \varphi \sin \delta + \cos \varphi \cos \delta \sin \omega_s) \quad (19.42)$$

19.3.4.7 Albedo

The upward SW RFD, R_{us} , is attributed purely to reflection of the downward SW radiation from the surface of concern. The reflectance of a surface is referred to as the albedo, A [–], defined by $A = R_{us}/R_{ds}$. It follows that the net incoming SW RFD is found from

$$R_{ns} = (1 - A)R_{ds} \quad (19.43)$$

and the daily mean net incoming SW RFD is found from

$$\hat{R}_{ns} = (1 - A)\hat{R}_{ds} \quad (19.44)$$

Table 19.1 Values of albedo for different surfaces. Values are from [6, pp. 82–83] except those for wet bare soil and fresh fallen snow, which are taken from [2, p. 43]

Surface	Albedo, A (–)
Water surface	0.05
Wet bare soil	0.05
Heather	0.14
Coniferous woodland	0.16
Deciduous woodland	0.18
Wheat	0.22
Grass	0.24
Freshly fallen snow	0.95

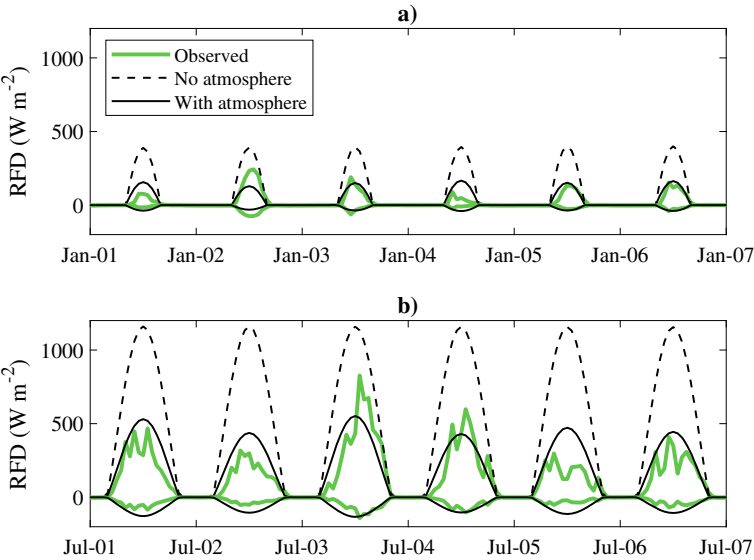


Fig. 19.5 Diurnal fluctuations in SW radiant flux density (RFD) in Berkshire, UK, during January and July of 2005. Positive values are downward fluxes. Negative fluxes are upward fluxes. Observations were made using pyranometers. Weather station data used to develop these plots was acquired from [9]

The word, albedo, is Latin for whiteness. A black-body that absorbs all radiation will have an A of zero. A perfect reflector will have an A of one. Some intermediate values are provided in Table 19.1.

Figures 19.5a and b compare winter and summer SW RFD, respectively, for a grassland site in Berkshire, UK. Both theoretical and observed values are presented. Observed values were obtained using upward and downward facing pyranometers.

Not surprisingly, both the duration and magnitude of SW RFD are smaller in the winter as compared to the summer.

The theoretical downward fluxes, R_{ds} , were calculated using Eq. (19.40). The upward fluxes were calculated using $R_{us} = AR_{ds}$ with $A = 0.24$. The “No atmosphere” fluxes (the dashed lines) were calculated from R_{ds}/k_{Rs} . Astronomical theory can be seen to provide an excellent prediction for the daily fluctuations in SW radiation. A constant albedo provides a reasonable method for predicting upward SW RFD. The empirical atmospheric attenuation factor, based on daily maximum and minimum temperatures, is shown to be effective at predicting how much energy is lost within the atmosphere on a given day.

19.3.5 Estimating Longwave Radiation

In principle, the LW radiation can be determined from Eq. (19.27) using knowledge of temperature at the land surface and within the atmosphere. In practice, we often only have a measurement of the air temperature immediately above the land surface. Furthermore the radiation emitted from the atmosphere will be dependent on cloud cover and humidity. Therefore, the following empirical function is often used to estimate the daily mean net outgoing LW radiation, denoted $\hat{R}_{nl}$ [MT^{-3}], [2, p. 52]:

$$\hat{R}_{nl} = \sigma \cdot \left(\frac{T_{\max}^4 + T_{\min}^4}{2} \right) (0.34 - 0.14\sqrt{p_v})(1.80k_{Rs} - 0.35) \quad (19.45)$$

where σ [$\text{MT}^{-3}\Theta^{-4}$] is the Stefan-Boltzmann constant, $T_{\max}$ (K) is the daily maximum temperature, $T_{\min}$ (K) is the daily minimum temperature, p_v (kPa) is the vapour pressure and k_{Rs} (-) is the atmospheric attenuation factor previously defined in Eq. (19.34). Equation (19.45) was developed by [2] using empirical equations previously presented by [3] and [10].

Figure 19.6 compares simulated (using the above set of equations) net incoming SW and LW RFD with observations made using weather station data from Berkshire. It can be seen that RFD is mostly dominated by SW radiation from the Sun. The semi-empirical models are remarkably good at predicting the main trends in the data.

Figure 19.7 compares forecasts of daily mean and weekly mean reference crop potential evapotranspiration according to Eq. (19.13). The black lines are results determined using only dry-bulb temperature data. The green lines are results determined using a full suit of weather station data (temperature, humidity, wind speed and net incoming radiation). At a daily scale there are some significant differences between the two results. However, at a weekly scale, the forecasts using just temperature data are very close to results using the full data. Indeed for many hydrological applications, daily minimum and maximum temperature data are sufficient for estimating daily mean potential evapotranspiration.

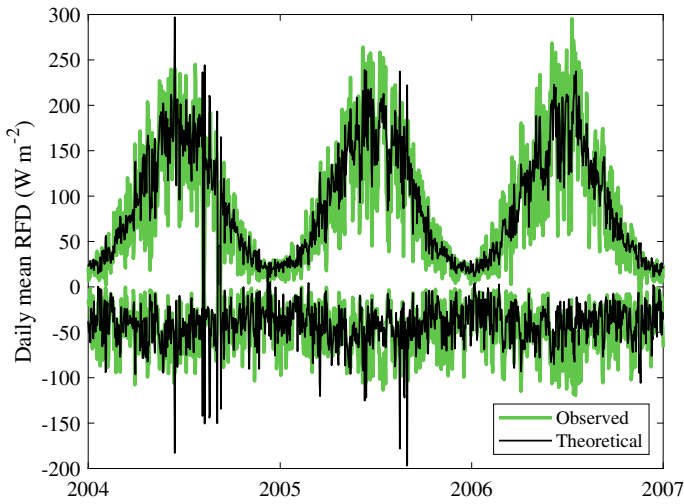


Fig. 19.6 Seasonal variations in net radiant flux density (RFD) in Berkshire, UK. Positive values are daily mean net incoming SW RFD. Negative values are daily mean net outgoing LW RFD. SW and LW observations were made using pyranometers and pyrgeometers, respectively. Weather station data used to develop these plots was acquired from [9]

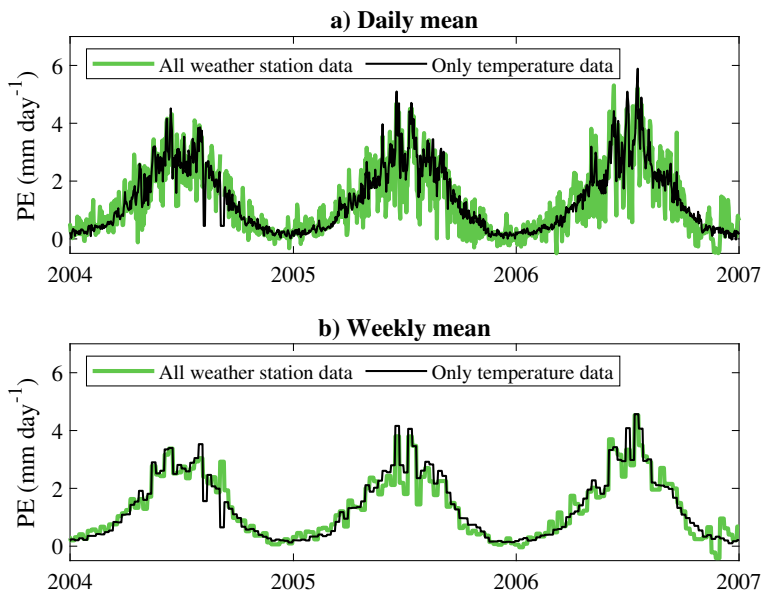


Fig. 19.7 Comparison of grass reference crop potential evapotranspiration (PE), in Berkshire, UK, determined from a full weather station dataset and only temperature data. **a** Shows daily mean data. **b** Shows weekly mean data. Weather station data used to develop these plots was acquired from [9]

19.4 Problem Sheet

Problem 19.1 (see Worked Solution 19.1)

Wind speeds of 1.83 m s^{-1} and 2.08 m s^{-1} are recorded at 1 m and 2 m above the land surface, respectively.

- (a) Use Eq. (19.16) to estimate the elevation at which the wind speed is zero.
- (b) Determine a corresponding value of aerodynamic resistance between the land surface and a measurement probe located 2 m above the land surface.

Problem 19.2 (see Worked Solution 19.2)

The air temperature is 20°C , the relative humidity is 80%, the air pressure is 101.3 kPa, the net incoming RFD is 150 W m^{-2} and heat lost to the ground can be ignored (i.e., $G = 0$).

- (a) Determine expected rates of reference crop potential evapotranspiration (in mm day^{-1}) for wind speeds of 0.5 m s^{-1} , 2 m s^{-1} and 5 m s^{-1} (as measured 2 m above the land surface).
- (b) Determine corresponding rates of open-water potential evaporation (in mm day^{-1}).

Problem 19.3 (see Worked Solution 19.3)

- (a) Determine the duration of daylight for $t_d = 0, 90$ and 180 days in (i) Durham, UK (Latitude 54.73°), (ii) Bandung, Indonesia (Latitude -6.90°) and (iii) Gaborone, Botswana (Latitude -24.68°).
- (b) Determine corresponding values of daily mean downward SW RFD for a clear day.
- (c) Determine net incoming SW RFD in Durham when $t_d = 0$ for (i) wet bare soil, (ii) grass and (iii) freshly fallen snow.

19.5 Worked Solutions

Worked Solution 19.1 (see Problem 19.1)

(a) Let $u_1 = 1.83 \text{ m s}^{-1}$, $u_2 = 2.08 \text{ m s}^{-1}$, $z_1 = 1 \text{ m}$ and $z_2 = 2 \text{ m}$. Furthermore, let $u = 0$ at $z = z_0$.

Recall Eq. (19.16)

$$\frac{u}{u_\tau} = 2.5 \ln \left(\frac{zu_\tau}{\nu} \right) + 5.5$$

It follows that

$$\frac{u_2 - u_1}{u_\tau} = 2.5 \ln \left(\frac{z_2}{z_1} \right)$$

and

$$\frac{u_2}{u_\tau} = 2.5 \ln \left(\frac{z_2}{z_0} \right)$$

and therefore

$$z_0 = z_2 \exp \left[\frac{u_2}{u_1 - u_2} \ln \left(\frac{z_1}{z_2} \right) \right] = 0.006258 \text{ m}$$

so the elevation at which the wind speed is zero is 0.00626 m.

(b) Considering Eq. (19.22)

$$r_a = \frac{6.25}{u_2} \left[\ln \left(\frac{z_2}{z_0} \right) \right]^2 = 99.93 \text{ m}^{-1} \text{ s}$$

So the aerodynamic resistance is $99.9 \text{ m}^{-1} \text{ s}$.

Worked Solution 19.2 (see Problem 19.2)

(a) Reference crop potential evapotranspiration, E_p , can be calculated from Eq. (19.13). From the solution to Problem 18.3 for 20°C : $p_{vs} = 2.338 \text{ kPa}$, $\alpha = 0.1447 \text{ kPa K}^{-1}$ and $L = 2455 \text{ kJ kg}^{-1}$. From the solution to Problem 18.4, $\gamma = 66.65 \text{ Pa K}^{-1}$. Given that the relative humidity is 80%, $p_v = 0.8 \times 2.338 = 1.870 \text{ kPa}$.

The moist air density, ρ_m , can be calculated from Eq. (18.30):

$$\rho_m = \rho_d \left[1 - (1 - \varepsilon) \frac{p_v}{p_m} \right]$$

where the dry air density, ρ_d , can be calculated from Eq. (18.27)

$$\rho_d = \frac{p_m M_d}{RT}$$

where $\varepsilon = 0.6222$, $M_d = 28.96 \text{ g mol}^{-1}$, $R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$, $p_m = 101.3 \text{ kPa}$ and $T = 20 + 273.2 \text{ K}$. It follows that $\rho_d = 1.204 \text{ kg m}^{-3}$ and $\rho_m = 1.195 \text{ kg m}^{-3}$. Recall that the specific heat capacity of air, $c_p = 1005 \text{ J kg}^{-1} \text{ K}^{-1}$.

Given $u_0 = 0$, $z_0 = 0.006247$ m (for reference crop grass) and $z_1 = 2$ m, the aerodynamic resistance, r_a , is calculated from

$$r_a = \frac{6.25}{u_1 - u_0} \left[\ln \left(\frac{z_1}{z_0} \right) \right]^2 = \frac{208.0}{u_1}$$

From the data given in Problem 19.2, the net incoming RFD, $R_n = 150 \text{ W m}^{-2}$. Also note that the stomatal resistance, $r_s = 70 \text{ m}^{-1} \text{ s}$ for reference crop grass. It follows that:

u_1 (m s^{-1})	E_p ($\mu\text{m s}^{-1}$)	E_p (mm day^{-1})
0.5	0.04220	3.65
2	0.04310	3.72
5	0.04434	3.83

(b) Open water potential evaporation, E_0 , can be calculated from Eq. (19.13). It follows that:

u_1 (m s^{-1})	E_0 ($\mu\text{m s}^{-1}$)	E_0 (mm day^{-1})
0.5	0.04443	3.84
2	0.05221	4.51
5	0.06777	5.86

It is interesting to note that the open water evaporation rate is much more responsive to changes in the wind speed as compared to the evapotranspiration rate.

Worked Solution 19.3 (see Problem 19.3)

(a) To calculate the duration of daylight hours, we must determine the solar declination angle, δ , from Eq. (19.37), calculate the corresponding sunset/sunrise angle, ω_s , from Eq. (19.41) and then apply Eq. (19.39). It follows that:

t_d (days)	0	90	180
δ (rad)	-0.3930	0.06856	0.4095
Durham ω_s (rad)	0.9445	1.668	2.232
Bandung ω_s (rad)	1.621	1.562	1.518
Gaborone ω_s (rad)	1.762	1.539	1.370
Durham daylight hours	7.216	12.74	17.05
Bandung daylight hours	12.39	11.94	11.60
Gaborone daylight hours	13.46	11.76	10.47

For Durham, the days are shortest in January and longest in June. For Bandung, the day length is quite uniform through out the year. For Gaborone, the days are longest in January and shortest in June.

(b) Daily mean downward SW RFD, $\hat{R}_{ds}$, on a clear day can be obtained from Eq. (19.42) by setting $k_{Rs} = 0.75$ (on a clear day around 25% of solar radiation is absorbed by the Earth’s atmosphere). We must also determine the correction factor, β , for the radial distance to the sun, found from Eq. (19.32). It follows that:

t_d (days)	0	90	180
β (-)	1.034	1.002	0.9659
Durham $\hat{R}_{ds}$ (W m^{-2})	46.03	217.2	359.1
Bandung $\hat{R}_{ds}$ (W m^{-2})	333.1	318.4	262.6
Gaborone $\hat{R}_{ds}$ (W m^{-2})	371.9	280.9	185.0

Downward SW RFD is significantly reduced for January in Durham. Downward SW RFD is much more steady in Bandung. Downward SW RFD is reduced for June in Gaborone, but remains over four times higher than the January downward SW RFD in Durham.

(c) Net incoming SW RFD can be obtained by multiplying $\hat{R}_{ds}$ by $(1 - A)$, where A is the albedo constant, which can be found from Table 19.1. For $t_d = 0$ in Durham, the net incoming SW RFD is: (i) 43.7 W m^{-2} for wet bare soil, (ii) 35.0 W m^{-2} for grass, and (iii) 2.30 W m^{-2} for freshly fallen snow.

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Abstract

This chapter focuses on river flow modelling with lumped conceptual rainfall runoff models. A water balance model is developed, which implicitly accounts for both canopy interception and soil water storage. The probability distributed model (PDM) for estimating surface runoff is introduced. Mathematical PDM functions are derived using exponential and Pareto statistical distribution functions. A river flow routing function is developed using an empirical non-linear flow equation. Theoretical relationships are derived for the associated empirical parameters using the Poiseuille equation and Manning's equation. A Taylor series expansion is used to derive a numerical stability constraint for an Euler explicit time-stepping scheme. Practical applications are presented through worked examples and a problem sheet with worked solutions.

Notation

a	Empirical coefficient for river flow routing function [$L^{1-b}T^{-1}$].
A	Catchment area [L^2].
A_c	Flowing cross-sectional area of the river channel [L^2].
A_v	Area of vegetative canopy within the catchment area [L^2].
A_w	Area of waterlogged soil and canopy [L^2].
b	Empirical exponent for river flow routing function [-].
c	Storage capacity [L].
$c_{\max}$	Maximum value of c within the catchment [L].
c_0	Laminar flow geometrical factor [-].
c_s	Soil water storage capacity [L].
c_v	Vegetative canopy water storage capacity [L].
C	Maximum value of storage capacity within waterlogged areas [L].
E_a	Actual evapotranspiration from the catchment [LT^{-1}].
E_p	Potential evapotranspiration from the catchment [LT^{-1}].

E_s	Evapotranspiration of water stored within the soil [LT^{-1}].
E_v	Evaporation of water stored within the vegetative canopy [LT^{-1}].
$f(c)$	Probability density function for c [L^{-1}].
$F(c)$	Cumulative density function for c [-].
g	Gravitational acceleration [LT^{-2}].
h	Water depth [L].
$H(x)$	Heaviside step function [-].
m	Hydraulic radius [L].
n	Manning's coefficient [$\text{L}^{-1/3}\text{T}$].
P	Wetted perimeter [L].
q	River flow rate per unit area of catchment [LT^{-1}].
$q_{\max}$	Maximum stable value of q [LT^{-1}].
q_d	Drainage to underlying aquifers [LT^{-1}].
q_p	Precipitation rate [LT^{-1}].
q_{ro}	Surface runoff [LT^{-1}].
q_s	Contribution to river flow [LT^{-1}].
q_v	Drainage of water stored within the vegetative canopy [LT^{-1}].
Q	River flow rate [L^3T^{-1}].
s	Dummy variable for studying numerical stability [-].
S	Volume of water stored within a unit area of catchment [L].
S_0	River channel slope [-].
$S_{\max}$	Scaling parameter for c [L].
S_s	Volume of water stored within a unit area of soil [L].
S_{trial}	Trial value of S [L].
S_v	Volume of water stored within a unit area of vegetative canopy [L].
t	Time [T].
Δt	Time-step duration [T].
u	Empirical exponent for the Pareto distribution [-].
v	Volume of water stored within the river channel network per unit area of catchment [L].
$v_{\max}$	Maximum stable value of v [L].
v_{trial}	Trial value of v [L].
V	Volume of water stored within the river channel network [L^3].
w	Dummy variable for studying numerical stability [T^{-1}].
α	Empirical coefficient for the river flow routing function [$\text{L}^{\frac{1}{b}-1}\text{T}^{-\frac{1}{b}}$].
β	Empirical exponent for the river flow routing function [-].
γ	Empirical exponent for the Pareto distribution [-].
ε	Error term for studying numerical stability [-].
μ	Dynamic viscosity [$\text{ML}^{-1}\text{T}^{-1}$].
ρ	Density of water [ML^{-3}].

20.1 Introduction

Rainfall runoff modelling is a process whereby precipitation and potential evapotranspiration data are transformed into a forecast of the flow rate in a river at some specified point. Such models are useful for water resource planning, flood forecasting and studying the effects of land-use change and/or climate change on hydrology in the future. The term runoff in this context is loosely used to refer to a river flow rate as opposed to surface runoff.

Broadly speaking there are three typical approaches to rainfall runoff modelling: (1) physics-based models, (2) empirical models and (3) conceptual models.

Physics-based models seek to describe a river catchment by discretising in space and solving physics-based equations to describe the various hydrological processes at each discretised point. The idea is that a site investigation can be undertaken and the model parameters for the relevant physics-based equations can be collected such that the model can then be used to forecast river flow rates. However, there are at least two significant problems with this approach.

The first problem is that the so-called physics-based equations are mostly not physics-based and are in fact semi-empirical, e.g., Richards' equation, Darcy's law and Manning's equation. Therefore, their parameters are not directly measurable and instead are determined by model calibration to observed data, e.g., moisture content, water table elevation and river flow data.

The second problem is that the relevant processes are not scale invariant, which means that if you parametrise the equations at some small scale, they are unlikely to accurately predict behaviour at a larger scale, such as a catchment scale. A consequence, is that many of the model parameters used are often obtained by model calibration to river flow data. Unfortunately, river flow data does not have sufficient information content for this purpose and so the problem is indeterminate.

In the past, physics-based models were considered unattractive because of their computational requirement; this is less of an issue nowadays because of significant development and cost reduction associated with computational equipment. Instead, an empirical model was preferred, referred to as the unit hydrograph method. This involved developing a transfer function between rainfall and river flow data using deconvolution. Whilst such an approach has a mathematical elegance, a significant downside is that it requires an assumption of a linear relationship between rainfall and river flow. It is also unclear how to incorporate the important effect of evapotranspiration.

So-called conceptual models seek to bridge the gap between physics-based models and empirical models. The idea is to split the catchment into conceptual stores of water, for example, the forest canopy, the soil, urban drainage systems, the river channel network, the underlying aquifer. Empirical non-linear equations can then be used to relate the storage level in a store to the outflow of the store. An advantage over the unit hydrograph method is that evapotranspiration is easily accounted for and more realistic non-linear relationships can be applied. An advantage over physics-based models is an associated reduction in unknown parameters values to be obtained by model calibration to observed river flow data.

There are many different conceptual models available in the literature for this purpose. The reader is directed to [1] for a thorough review and explanation. Nevertheless, most conceptual models have two important features, namely a water balance component and a river flow routing component. The water balance component is used to determine actual evapotranspiration from a combination of precipitation data and potential evapotranspiration data. But of particular importance in this context, the water balance component also determines how much precipitation contributes towards river flow. The river flow routing component accounts for the different travel pathways, water takes within the catchment, and translates contribution to river flow (from the water balance model) to a river flow rate.

In this chapter we will study representative examples of both a water balance model and a river flow routing model. Governing equations and numerical solutions are presented. A brief explanation about calibration and validation is provided. The problem sheet at the end of the chapter provides an opportunity to apply the described methods to hydro-meteorological data from the River Wear catchment upstream of Durham City.

20.2 Water Balance Modelling

When it rains, some of the rain lands on the soil surface where it will either infiltrate the soil or drain as surface runoff to a nearby stream or river channel. Some of the rain will land on overlying vegetative canopy where it will be evaporated back to the atmosphere. However, vegetative canopy has a finite storage capacity. Once this is exceeded, water will overspill and also drain to the underlying soil surface.

Water that infiltrates the soil will either drain to underlying aquifers or be abstracted by plant roots and transpired back to the atmosphere. Water that drains to underlying aquifers will in many cases drain out of the land surface through springs or up-well into groundwater fed river channels.

Here we will develop a water balance model that considers storage of water in both the vegetative canopy and the underlying soil. First we derive individual mass balance equations for the vegetative canopy and the underlying soil. These are then combined to form a single water balance equation for a given catchment. A probability distributed model is presented to incorporate stochastic spatial variations in storage capacity throughout a given catchment. Some example simulations are presented using hydro-meteorological data from the River Wear catchment upstream of Durham City. It is then shown how to solve the relevant equations using an Euler explicit time-stepping scheme.

20.2.1 Water Balance for the Vegetative Canopy

A water balance equation for the vegetative canopy takes the form

$$\frac{dS_v}{dt} = q_p - E_v - q_v \quad (20.1)$$

where S_v [L] is the volume of water stored within the canopy per unit area of canopy covered land, t [T] is time, q_p [LT^{-1}] is the precipitation rate, E_v [LT^{-1}] is the rate at which water is evaporated from the canopy and q_v [LT^{-1}] is the rate at which water drains through the canopy to the underlying land surface (see Fig. 20.1a).

The evaporation rate, E_v , is obtained from

$$E_v = H(S_v)E_p \quad (20.2)$$

where E_p [LT^{-1}] is the potential evapotranspiration rate and $H(x)$ is the Heaviside step function,

$$H(x) = \begin{cases} 0, & x \leq 0 \\ 1, & x > 0 \end{cases}$$

The idea behind Eq. (20.2) is that actual evaporation takes place at the potential rate unless there is no water to evaporate, in which case there is no evaporation. This also involves assuming that the potential evaporation rate from a vegetative surface is equal to the potential evapotranspiration rate.

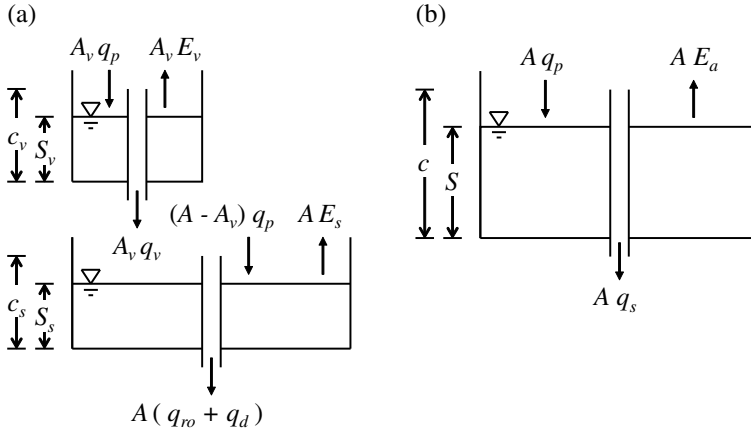


Fig. 20.1 **a** Water balance model with a vegetative canopy storage of capacity, c_v , and a soil water storage of capacity, c_s . **b** Water balance model with a combined vegetative canopy and soil water storage capacity, c

The drainage rate, q_v , is obtained from

$$q_v = H(S_v - c_v)q_p \quad (20.3)$$

where c_v [L] is the storage capacity of the vegetative canopy. The idea here is that once precipitation fills up the holding capacity of the vegetative canopy it overflows and drains on to the land surface below.

20.2.2 Water Balance for Soil

A water balance equation for the soil takes the form

$$\frac{dS_s}{dt} = \left(1 - \frac{A_v}{A}\right)q_p + \left(\frac{A_v}{A}\right)q_v - E_s - q_{ro} - q_d \quad (20.4)$$

where S_s [L] is the volume of water stored within the soil per unit area of land, A [L²] is the area of the catchment under consideration, A_v [L²] is the area of land (within the catchment) covered by vegetative canopy, E_s [LT⁻¹] is the rate of evapotranspiration from the land, q_{ro} [LT⁻¹] is the rate of surface runoff and q_d [LT⁻¹] is the rate of drainage to the water table below (see Fig. 20.1a).

The evapotranspiration rate, E_s , is obtained from

$$E_s = H(S_s) \left[E_p - \left(\frac{A_v}{A}\right)E_v \right] \quad (20.5)$$

The idea here is that actual evapotranspiration takes place at the potential rate unless there is no water to evaporate or transpire, in which case there is no evapotranspiration. Furthermore, the actual evapotranspiration rate will be reduced by loss of net incoming radiation to evaporation of water directly from the vegetative canopy, as determined by Eq. (20.2).

In practice, the runoff rate and drainage rate are often combined into a single river flow contribution rate, q_s [LT⁻¹], i.e., $q_s = q_{ro} + q_d$, which can be determined from

$$q_s = H(S_s - c_s) \left[\left(1 - \frac{A_v}{A}\right)q_p + \left(\frac{A_v}{A}\right)q_v \right] \quad (20.6)$$

where c_s [L] is the storage capacity of the soil. The idea here is that once precipitation and canopy drainage fills up the holding capacity of the soil it overflows and drains to a combined groundwater and river flow network.

20.2.3 Combined Water Balance

Challenge 20.1 Derive a simplified water balance equation for the combined storage, $S = S_s + (A_v/A)S_v$. Also, derive simplified expressions for the combined actual evapotranspiration rate, $E_a = E_s + (A_v/A)E_v$, and the combined drainage rate, q_s , by assuming (1) $S_s > 0$ when $S_v > 0$ and (2) $S_s < c_s$ when $S_v < c_v$.

Adding Eqs. (20.1) and (20.4) together leads to

$$\frac{dS}{dt} = q_p - E_a - q_s \quad (20.7)$$

where S is the combined volume of water stored within the land per unit area of land and E_a is the combined actual evapotranspiration rate found from

$$S = S_s + \left(\frac{A_v}{A}\right) S_v \quad (20.8)$$

and

$$E_a = E_s + \left(\frac{A_v}{A}\right) E_v \quad (20.9)$$

respectively.

Substituting Eqs. (20.2) and (20.5) into Eq. (20.9) leads to

$$E_a = \left\{ H(S_s) \left[1 - \left(\frac{A_v}{A}\right) H(S_v) \right] + \left(\frac{A_v}{A}\right) H(S_v) \right\} E_p \quad (20.10)$$

Assuming that $S_s > 0$ when $S_v > 0$, it further follows that $H(S_s)H(S_v) = H(S_v)$, $H(S) = H(S_s)$ and [2]

$$E_a = H(S)E_p \quad (20.11)$$

Substituting Eq. (20.3) into Eq. (20.6) leads to

$$q_s = H(S_s - c_s) \left[\left(1 - \frac{A_v}{A} \right) + \left(\frac{A_v}{A} \right) H(S_v - c_v) \right] q_p \quad (20.12)$$

Assuming that $S_s < c_s$ when $S_v < c_v$, it further follows that $H(S_s - c_s)H(S_v - c_v) = H(S_s - c_s)$, $H(S - c) = H(S_s - c_s)$ and [2]

$$q_s = H(S - c)q_p \quad (20.13)$$

where $c = c_s + (A_v/A)c_v$ represents the combined storage capacity (see Fig. 20.1b).

20.2.3.1 Example Simulation

Figure 20.2 shows results from an example simulation using the above model in conjunction with catchment averaged daily precipitation data (Fig. 20.2a) and daily potential evapotranspiration data (Fig. 20.2b) for the Sunderland Bridge gauging station on the River Wear, outside Durham City.

Figure 20.2c shows plots of the storage level, S , against time. Notice that S ranges from zero to 80 mm because the c parameter was set to 80 mm in this case. The storage level decreases in the summer due to the higher rates of evapotranspiration. The store fills again in the winter due to the reduced evapotranspiration rates and slightly higher precipitation rates. The storage level never goes below zero because the actual evapotranspiration, E_a , ceases when there is zero storage (see Fig. 20.2b). The storage level never goes over c because the store overflows to create contribution to river flow, q_s (see Fig. 20.2a).

A particular problem with the above model is that contribution to river flow is only predicted to occur when $S = c$. Therefore there are long periods during the summer when there is apparently no contribution to river flow. This is unrealistic in most cases, because many rivers, in a UK-type climate, show increases in flow rate due to high intensity summer rainfall events as well.

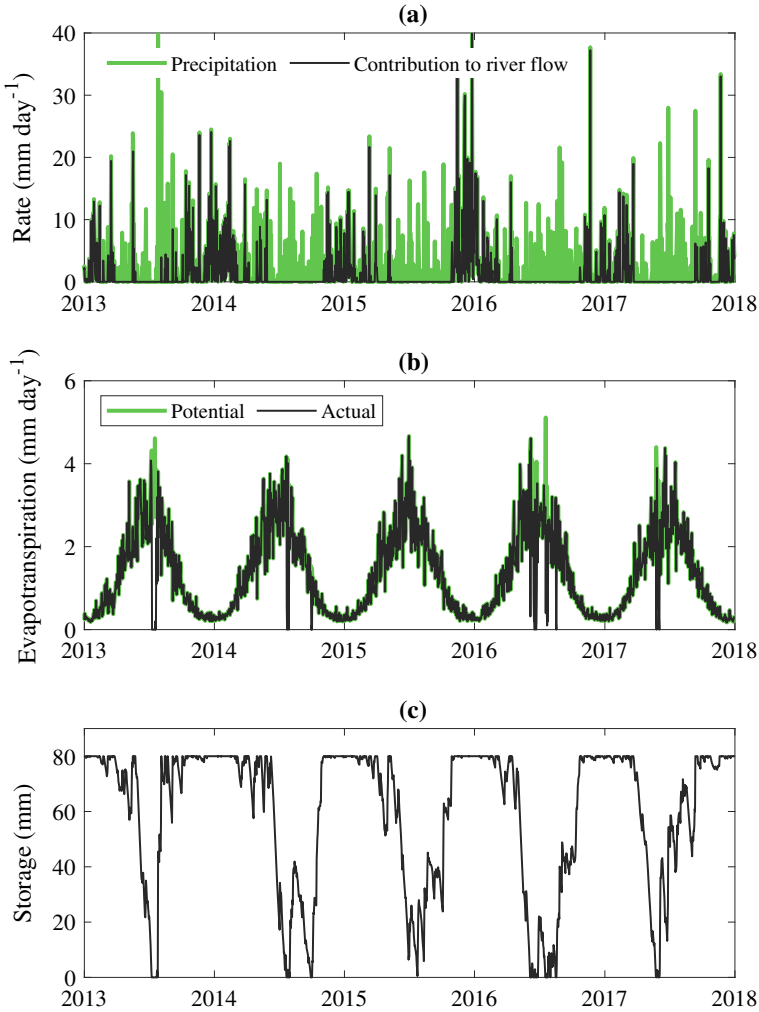


Fig. 20.2 Catchment water balance with a uniform storage capacity of 80 mm using catchment averaged daily precipitation data (acquired from [3]) and daily potential evapotranspiration data (determined using temperature data from [4]) for the Sunderland Bridge gauging station on the River Wear, outside Durham City

20.2.4 Probability Distributed Model (PDM)

The above model represents an oversimplification of reality. A more realistic model can be obtained by treating the capacity parameter, c , as a stochastic process that represents the spatial variability of c within the catchment as a whole. A widely applied approach in this context is the so-called probability distributed model (PDM) (attributed to [5]).

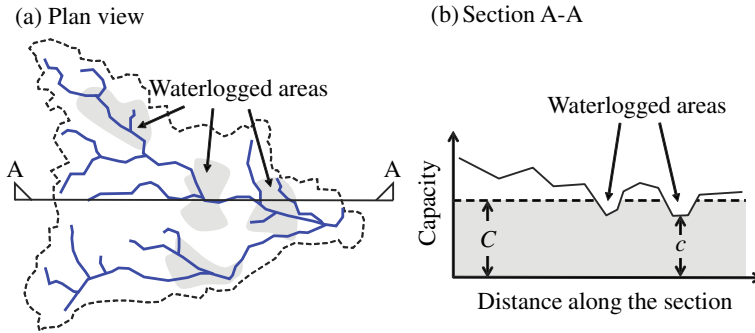


Fig. 20.3 Schematic diagram for the probability distributed model. **a** Plan view of the catchment with waterlogged regions denoted by the shaded areas. **b** Hypothetical plot of local storage capacity, c , against distance along the Section A-A, labelled on the plan view. The maximum capacity within the waterlogged region is denoted C . The shaded area represents the volume of water stored within the catchment

The idea behind the PDM is as follows. At any given time, an area within the catchment, A_w [L^2], contains waterlogged soil and canopy (Fig. 20.3a) such that additional precipitation, in this area, leads to the generation of river flow contribution. [5] considers the storage capacity at any point within the catchment, c [L], to be a random variable defined by a probability density function (PDF), $f(c)$ [L^{-1}]. Let C [L] be the maximum value of c observed within the area, A_w (Fig. 20.3b). It can then be stated that $A_w = F(C)A$ where $F(C)$ [-] is the probability of c not exceeding C (i.e., a cumulative distribution function (CDF)), defined as

$$F(C) = \int_{-\infty}^C f(c)dc \quad (20.14)$$

It can be further asserted that

$$q_s = F(C)q_p \quad (20.15)$$

However, to determine q_s as part of a water balance equation, such as Eq. (20.7), it is necessary to define a relationship between $F(C)$ and S . At any given time, the water storage level within the catchment is assumed equal to c within water-logged regions and equal to C outside of these regions (Fig. 20.3). It follows that the storage level, S , can be calculated from [5]

$$S = \int_{-\infty}^C cf(c)dc + C \int_C^{\infty} f(c)dc \quad (20.16)$$

Challenge 20.2 Use Eqs. (20.14) and (20.16) to derive an integral expression for S in terms of $f(c)$ and $F(c)$.

The first term in Eq. (20.16) can be expanded using integration by parts to get

$$\begin{aligned}\int_{-\infty}^C cf(c)dc &= [cF(c)]_{-\infty}^C - \int_{-\infty}^C F(c)dc \\ &= CF(C) - \int_{-\infty}^C F(c)dc\end{aligned}\quad (20.17)$$

The second term in Eq. (20.16) can be expanded by separating the limits to get

$$C \int_C^{\infty} f(c)dc = C \int_{-\infty}^{\infty} f(c)dc - C \int_{-\infty}^C f(c)dc \quad (20.18)$$

Note that

$$F(\infty) = \int_{-\infty}^{\infty} f(c)dc = 1 \quad (20.19)$$

Substituting Eqs. (20.14) and (20.19) into Eq. (20.18) leads to

$$C \int_C^{\infty} f(c)dc = C[1 - F(C)] \quad (20.20)$$

Substituting Eqs. (20.17) and (20.20) into Eq. (20.16) leads to

$$S = C - \int_{-\infty}^C F(c)dc$$

In practice, $c \geq 0$, which means that $f(c) = 0$ and $F(c) = 0$ for $c < 0$ and therefore

$$S = \int_0^C [1 - F(c)]dc$$

Applying of the chain rule leads to

$$S = \int_0^{F(C)} [1 - F(c)] \frac{dc}{dF} dF$$

Noting that $\frac{dF}{dc} = f(c)$ then gives us

$$S = \int_0^{F(C)} \left[\frac{1 - F(c)}{f(c)} \right] dF \quad (20.21)$$

20.2.4.1 Application of an Exponential Distribution Function

The simplest PDF that can be applied in this context is the one-parameter exponential distribution function

$$f(c) = \frac{1}{S_{\max}} \exp\left(-\frac{c}{S_{\max}}\right), \quad c \geq 0 \quad (20.22)$$

where $S_{\max}$ [L] represents a scaling parameter for c .

Challenge 20.3 Substitute Eq. (20.22) into Eq. (20.14) and use Eq. (20.21) to derive an explicit equation for the CDF, $F(C)$, in terms of the water storage level, S .

Substituting Eq. (20.22) into Eq. (20.14) leads to

$$\begin{aligned}
 F(C) &= \int_{-\infty}^C f(c)dc \\
 &= \int_0^C \frac{1}{S_{\max}} \exp\left(-\frac{c}{S_{\max}}\right) dc \\
 &= 1 - \exp\left(-\frac{C}{S_{\max}}\right) \\
 &= 1 - S_{\max} f(C)
 \end{aligned} \tag{20.23}$$

Solving Eq. (20.23) for $f(C)$ gives us

$$f(C) = \frac{1 - F(C)}{S_{\max}} \tag{20.24}$$

Substituting Eq. (20.24) into Eq. (20.21) and solving for $F(C)$ leads to

$$F(C) = \frac{S}{S_{\max}} \tag{20.25}$$

It can also be understood that $\lim_{C \rightarrow \infty} S = S_{\max}$. Therefore $S_{\max}$ actually represents the maximum possible value of S in this case.

20.2.4.2 Application of a Pareto Distribution Function

A more commonly used PDF in this context is the two parameter Pareto distribution

$$f(c) = \frac{u}{c_{\max}} \left(1 - \frac{c}{c_{\max}}\right)^{u-1}, \quad c \in [0, c_{\max}] \tag{20.26}$$

where u is an empirical exponent and $c_{\max}$ represents a maximum possible value of c .

Challenge 20.4 Substitute Eq. (20.26) into Eq. (20.14) and use Eq. (20.21) to derive an explicit equation for the CDF, $F(C)$, in terms of the water storage level, S .

Substituting Eq. (20.26) into Eq. (20.14) leads to

$$\begin{aligned}
 F(C) &= \int_{-\infty}^C f(c)dc \\
 &= \int_0^C \frac{u}{c_{\max}} \left(1 - \frac{c}{c_{\max}}\right)^{u-1} dc \\
 &= 1 - \left(1 - \frac{C}{c_{\max}}\right)^u \\
 &= 1 - \left[\frac{c_{\max}}{u} f(C)\right]^{\frac{u}{u-1}}
 \end{aligned} \tag{20.27}$$

Solving Eq. (20.27) for $f(C)$ gives us

$$f(C) = \frac{u}{c_{\max}} [1 - F(C)]^{1-\frac{1}{u}} \quad (20.28)$$

Substituting Eq. (20.28) into Eq. (20.21) leads to

$$\begin{aligned} S &= \frac{c_{\max}}{u} \int_0^{F(C)} (1 - F)^{\frac{1}{u}} dF \\ &= -\frac{c_{\max}}{u+1} \left[(1 - F)^{\frac{u+1}{u}} \right]_0^{F(C)} \\ &= \frac{c_{\max}}{u+1} \left\{ 1 - [1 - F(C)]^{\frac{u+1}{u}} \right\} \end{aligned} \quad (20.29)$$

Solving Eq. (20.29) for $F(C)$ gives us

$$F(C) = 1 - \left(1 - \frac{S}{S_{\max}} \right)^{\gamma} \quad (20.30)$$

where

$$S_{\max} = \frac{c_{\max}}{u+1} \quad \text{and} \quad \gamma = \frac{u}{u+1}$$

Note that $\lim_{C \rightarrow c_{\max}} S = S_{\max}$. Therefore $S_{\max}$ again represents the maximum possible value of S .

20.2.4.3 Link Between the Pareto Distribution, the Exponential Distribution and the Uniform Capacity Model

As $u \rightarrow \infty$, $\gamma \rightarrow 1$ and Eq. (20.30) reduces to Eq. (20.25). It can therefore be understood that the exponential PDF is a special case of the Pareto PDF when $u \rightarrow \infty$.

As $u \rightarrow 0$, $\gamma \rightarrow 0$ and Eq. (20.30) reduces to

$$F(C) = H(S - S_{\max}) \quad (20.31)$$

which, when substituted into Eq. (20.15) and setting $S_{\max} = c$, leads to Eq. (20.13), associated with the original uniform capacity model described in Sect. 20.2.3.

20.2.4.4 Example Simulation

Figure 20.4 shows results from an example simulation using the above PDM with an exponential distribution function. This should be compared with the results shown in Fig. 20.2, where we assumed a uniform storage capacity across the catchment. As in Fig. 20.2c, the storage level never goes below zero because the actual evapotranspiration, E_a , ceases when there is zero storage (see Fig. 20.4b). However, a significant difference is that a degree of contribution to river flow is maintained throughout the summer periods due to Eq. (20.15) (compare Figs. 20.2a and 20.4a), which is much more realistic in most cases.

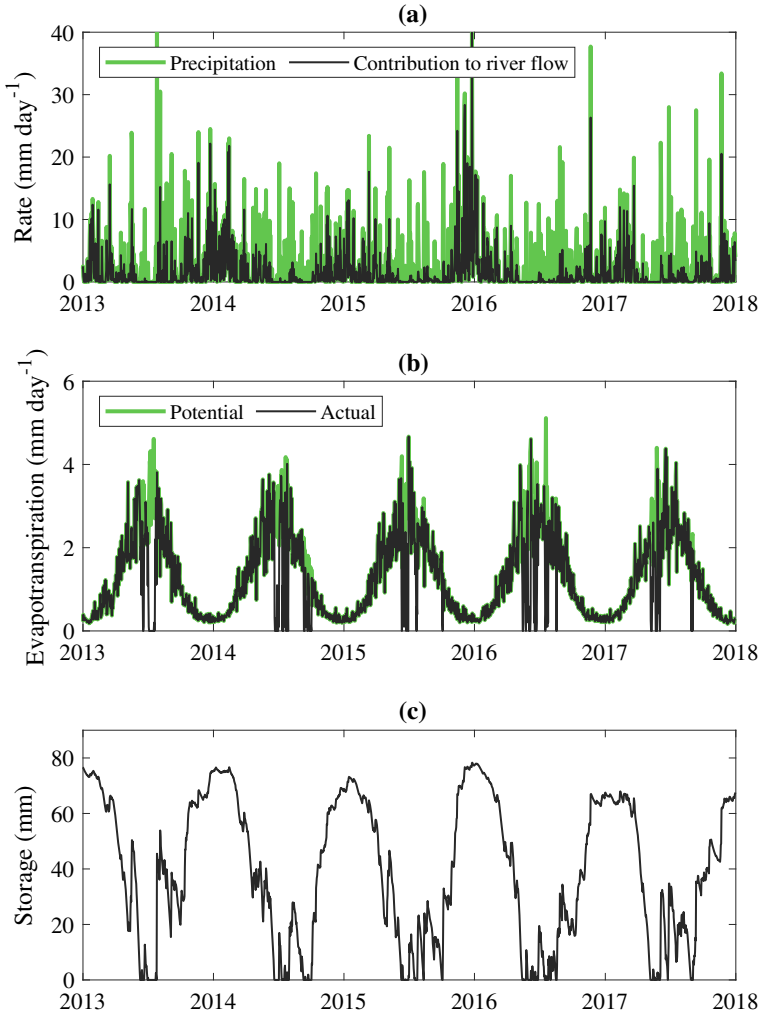


Fig. 20.4 Catchment water balance with the PDM with an exponential distribution function with $S_{\max} = 80$ mm and using catchment averaged daily precipitation data (acquired from [3]) and daily potential evapotranspiration data (determined using temperature data from [4]) for the Sunderland Bridge gauging station on the River Wear, outside Durham City

20.2.5 Numerical Solution

Estimates of river flow contribution, q_s , can be obtained for a given set of precipitation data, q_p , and potential evapotranspiration data, E_p , by numerical solution of Eq. (20.7). Here we will develop an Euler explicit solution, similar to as in Sects. 10.4.1 and 10.4.2.

Consider a Taylor series expansion for S [6, p. 901]

$$S(t + \Delta t) = S(t) + \Delta t \left. \frac{dS}{dt} \right|_t + O(\Delta t^2)$$

It follows that

$$\left. \frac{dS}{dt} \right|_t = \frac{S(t + \Delta t) - S(t)}{\Delta t} + O(\Delta t)$$

Consider a sequence of N discrete times, $t_1, t_2, \dots, t_N$, where each time is separated by the time interval Δt . The corresponding values of storage level, S , are $S_1, S_2, \dots, S_N$. It follows that

$$\left. \frac{dS}{dt} \right|_i = \frac{S_{i+1} - S_i}{\Delta t} + O(\Delta t), \quad i = 1, 2, \dots, N - 1$$

The corresponding values of q_p , E_a and q_s can be written as $q_{p,i}$, $E_{a,i}$ and $q_{s,i}$, respectively, where $i = 1, 2, \dots, N$. A discrete approximation of Eq. (20.7) can therefore be written as

$$\frac{S_{i+1} - S_i}{\Delta t} = q_{p,i} - E_{a,i} - q_{s,i} + O(\Delta t)$$

which can be rearranged to get

$$S_{i+1} \approx S_i + \Delta t(q_{p,i} - E_{a,i} - q_{s,i}) \quad (20.32)$$

20.2.5.1 Ensuring $S \leq S_{\max}$

Challenge 20.5 Determine a constraint for the river flow contribution, $q_{s,i}$, to ensure that $S_{i+1} \leq S_{\max}$.

Ordinarily $q_{s,i}$ should be calculated from Eq. (20.15), i.e., $q_{s,i} = F(S_i)q_{p,i}$. However, a consequence of our discrete approximation is that casual use of Eq. (20.15) may lead to S_{i+1} becoming greater than $S_{\max}$, which should not be permitted. Therefore a constraint is required on q_i to prevent this from happening. This can be determined as follows:

Consider Eq. (20.32) with $E_{a,i} = E_{p,i}$. Now let S_{trial} be an auxiliary variable calculated from

$$S_{\text{trial}} = S_i + \Delta t[(1 - F(S_i))q_{p,i} - E_{p,i}] \quad (20.33)$$

The constraint that $S \in [0, S_{\max}]$ implies that

$$S_{i+1} = \begin{cases} 0, & S_{\text{trial}} < 0 \\ S_{\text{trial}}, & S_{\text{trial}} \in [0, S_{\max}] \\ S_{\max}, & S_{\text{trial}} > S_{\max} \end{cases} \quad (20.34)$$

In the event that $S_{i+1} = S_{\max}$, Eq. (20.32), with $E_{a,i} = E_{p,i}$, can be solved to obtain an associated value of $q_{s,i}$ such that the water balance equation in Eq. (20.7) is maintained. It follows that

$$q_{s,i} = \begin{cases} F(S_i)q_{p,i}, & S_{\text{trial}} \leq S_{\max} \\ q_{p,i} - E_{p,i} - \left(\frac{S_{\max} - S_i}{\Delta t} \right), & S_{\text{trial}} > S_{\max} \end{cases} \quad (20.35)$$

20.2.5.2 Ensuring $S \geq 0$

Challenge 20.6 Determine a constraint for the actual evapotranspiration, $E_{a,i}$, to ensure that $S_{i+1} \geq 0$.

Ordinarily $E_{a,i} = E_{p,i}$ (consider Eq. (20.11)). However, from Eq. (20.34), it can be seen that $S_{i+1} = 0$ when $S_{\text{trial}} < 0$. Furthermore, during such a scenario, $q_{s,i} = F(S_i)q_{p,i}$. Considering again Eq. (20.32), it therefore follows that

$$E_{a,i} = \begin{cases} (1 - F(S_i))q_{p,i} + \frac{S_i}{\Delta t}, & S_{\text{trial}} \leq 0 \\ E_{p,i}, & S_{\text{trial}} > 0 \end{cases} \quad (20.36)$$

20.3 River Flow Routing

The river flow contribution, q_s , determined above, represents a mean response of the amount of river flow contribution that has been developed at each point in space across the catchment. However, often we require the river flow rate at the outlet of the catchment. It will take different amounts of time to travel from different points within the catchment to the catchment outlet. Therefore, a river flow rate time-series will take some delayed and attenuated form of a given q_s time-series.

A river flow routing function is a mathematical function used to translate a q_s time-series into a corresponding river flow rate time-series at a catchment outlet. There are many different approaches to designing and developing river flow routing functions. Here we will study one simple example involving treating the river channel network as a storage reservoir, where flow rate is treated as a power-law function of the reservoir storage level. For more discussion about different approaches to river flow routing the reader is again directed to [1].

20.3.1 Mass Conservation Statement

Let V [L^3] be the volume of water stored within the river channel network and Q [L^3T^{-1}] be the river flow rate at the catchment outlet. Mass conservation dictates that

$$\frac{dV}{dt} = Aq_s - Q \quad (20.37)$$

where q_s [LT^{-1}] is the contribution to river flow per unit area of catchment and A [L^2] is the catchment area.

It is convenient to normalise the above equation by dividing both sides by the catchment area to get

$$\frac{dv}{dt} = q_s - q \quad (20.38)$$

where $v = V/A$ and $q = Q/A$.

It can be understood that the dryer the catchment is, the smaller the flow rate out of the catchment. A simple but general empirical relationship to consider is

$$q = av^b \quad (20.39)$$

where a [$L^{1-b}T^{-1}$] and b [-] are empirical coefficients yet to be defined.

20.3.2 Sheet Flow Approximation

Imagine water flows as a sheet across the catchment with a uniform thickness, h [L]. A corresponding value of the exponent, b , can be determined under laminar and turbulent flow conditions.

20.3.2.1 Application of Poiseuille Equation

Under steady laminar flow conditions, the flow rate can be determined from the Poiseuille equation

$$Q = \frac{\rho g A_c m^2 S_0}{c_0 \mu} \quad (20.40)$$

where A_c [L^2] is the flowing cross-sectional area of the river channel, m [L] is the hydraulic radius, S_0 [-] is the slope of the river bed, ρ [ML^{-3}] is the fluid density, g [LT^{-2}] is gravitational acceleration, μ [$ML^{-1}T^{-1}$] is the dynamic viscosity and $c_0 \in [2, 3]$ [-] is a dimensionless geometrical factor.

(Equation (20.40) is obtained by substituting Eqs. (2.23) and (2.33) into Eq. (2.40), solving for the fluid velocity and multiplying the result by A_c to get an expression for Q .)

Challenge 20.7 Use the Poiseuille equation to derive expressions for the power law coefficients in Eq. (20.39) in terms of wetted perimeter, slope, catchment area, geometrical factor, density, gravitational acceleration, and dynamic viscosity.

The total volume of water in the sheet, $V = Ah$. It follows that $h = V/A = v$. The flowing cross-sectional area of the catchment is found from $A_c = Ph = Pv$ where P [L] is the wetted perimeter of the flowing channel. Furthermore, the hydraulic radius, $m = A_c/P = v$.

Substituting the above expressions into Eq. (20.40) leads to

$$q = \frac{\rho g P S_0 v^3}{A c_0 \mu} \quad (20.41)$$

Comparing Eq. (20.41) with Eq. (20.39) then suggests that

$$a = \frac{\rho g P S_0}{A c_0 \mu} \quad \text{and} \quad b = 3$$

20.3.2.2 Application of Manning's Equation

Under turbulent flow conditions Manning's equation can be used where

$$Q^2 = \frac{A_c^2 m^{4/3} S_0}{n^2} \quad (20.42)$$

and n [$L^{-1/3}T$] is Manning's coefficient.

(Equation (20.42) is obtained by substituting Eq. (2.37) into Eq. (2.40), solving for the square of the fluid velocity and multiplying the result by A_c^2 to get an expression for Q^2 .)

Challenge 20.8 Use Manning's equation to derive expressions for the power law coefficients in Eq. (20.39) in terms of wetted perimeter, slope, catchment area and Manning's coefficient.

Again, $A_c = P v$ and $m = A_c / P = v$.

Substituting the above expressions into Eq. (20.42) leads to

$$q = \frac{P S_0^{1/2} v^{5/3}}{A n} \quad (20.43)$$

Comparing Eq. (20.43) with Eq. (20.39) then suggests that

$$a = \frac{P S_0^{1/2}}{A n} \quad \text{and} \quad b = \frac{5}{3}$$

20.3.3 Behaviour During Recession

When the contribution to the river is zero (i.e., $q_s = 0$), the river is said to be in recession. Whilst the above analysis has provided some simple ideas about likely values of the power law exponent, b , the sheet flow assumption is quite unrealistic, and both a and b are better found by calibration against observed river flow rates [7]. Nevertheless, further insight into the meaning of a and b can be gained by studying how the above model behaves during recession events.

Challenge 20.9 Use Eqs. (20.38) and (20.39) to determine a relationship between $\frac{dq}{dt}$ and q when $q_s = 0$.

Applying the chain rule to Eq. (20.38) leads to

$$\frac{\partial v}{\partial q} \frac{dq}{dt} = q_s - q \quad (20.44)$$

Solving Eq. (20.39) for v gives us

$$v = \left(\frac{q}{a}\right)^{\frac{1}{b}} \quad (20.45)$$

Differentiating Eq. (20.45) with respect to q leads to

$$\frac{\partial v}{\partial q} = \frac{q^{\frac{1}{b}-1}}{a^{\frac{1}{b}}b} \quad (20.46)$$

Substituting Eq. (20.46) into Eq. (20.44) gives us

$$\frac{dq}{dt} = a^{\frac{1}{b}}bq^{1-\frac{1}{b}}(q_s - q) \quad (20.47)$$

During a recession event $q_s = 0$ so

$$\frac{dq}{dt} = -\alpha q^{\beta} \quad (20.48)$$

where

$$\alpha = a^{\frac{1}{b}}b \quad \text{and} \quad \beta = 2 - \frac{1}{b}$$

from which it can be understood that during a recession event, $\frac{dq}{dt}$ is a power law of q with β being its exponent.

Note that $\lim_{b \rightarrow \infty} \beta = 2$. Furthermore, it can be appreciated that β is unlikely to be less than one. Therefore it follows that b is also unlikely to be less than one.

20.3.4 Numerical Solution

Estimates of river flow rate per unit area of catchment at the catchment outlet, q , can be obtained for a given set of river flow contribution data, q_s , by numerical solution of Eq. (20.38). An Euler explicit solution for the river channel storage per unit area of catchment, v , takes the form

$$v_{i+1} \approx v_i + \Delta t(q_{s,i} - q_i) \quad (20.49)$$

Unlike Eq. (20.32), Eq. (20.49) is unconstrained because there is no natural upper-bound for v . A consequence is that the explicit solution scheme in Eq. (20.49) can become unstable if an appropriate check is not put in place. Such a check can be obtained as follows.

20.3.4.1 Stability Analysis for Euler Explicit Schemes

Consider a differential equation of the form

$$\frac{ds}{dt} = -w \quad (20.50)$$

Applying an Euler explicit time-stepping scheme leads to a discrete solution of the form

$$s_{i+1} = s_i - \Delta t w_i \quad (20.51)$$

where $\Delta t = t_{i+1} - t_i$.

The approximate solution, $s(t_i) = s_i$, is related to an exact solution, s_0 , by

$$s = s_0 + \varepsilon \quad (20.52)$$

where ε is the error associated with the approximation.

Substituting Eq. (20.52) into Eq. (20.50) leads to

$$\frac{ds_0}{dt} + \frac{d\varepsilon}{dt} = -w(s_0 + \varepsilon)$$

and applying a Taylor series expansion to $w(s_0 + \varepsilon)$ gives us

$$\frac{ds_0}{dt} + \frac{d\varepsilon}{dt} = -w(s_0) - \varepsilon \frac{\partial w}{\partial s_0} + O(\varepsilon^2) \quad (20.53)$$

Recalling that s_0 satisfies Eq. (20.50) exactly, Eq. (20.53) reduces to

$$\frac{d\varepsilon}{dt} = -\varepsilon \frac{\partial w}{\partial s_0} + O(\varepsilon^2) \quad (20.54)$$

Applying an Euler explicit time-stepping scheme to Eq. (20.54) and rearranging then leads to

$$\frac{\varepsilon_{i+1}}{\varepsilon_i} = 1 - \Delta t \left[\frac{\partial w}{\partial s_0} \right]_i + O(\varepsilon_i)$$

from which it can be understood that Eq. (20.51) will remain stable providing

$$\frac{\partial w}{\partial s} < \frac{1}{\Delta t} \quad (20.55)$$

20.3.4.2 Development of a Stability Constraint

Challenge 20.10 Compare Eqs. (20.38) and (20.50) and use Eq. (20.55) to derive an expression for the maximum stable value of v in terms of a , b and Δt .

Given Eqs. (20.38) and (20.55) and noting that $\partial q_s / \partial v = 0$, a stability constraint for our routing function can be obtained by imposing

$$\frac{\partial q}{\partial v} < \frac{1}{\Delta t}$$

Given $q = av^b$, it follows that stability should be ensured providing

$$abv^{b-1} < \frac{1}{\Delta t} \quad (20.56)$$

So the maximum stable value of v is found from

$$v_{\max} = (ab\Delta t)^{\frac{1}{1-b}} \quad (20.57)$$

20.3.4.3 Application of a Stability Constraint

To force the stability criterion in Eq. (20.56) we can impose that $v < v_{\max}$ where $v_{\max} = (ab\Delta t)^{\frac{1}{1-b}}$, which can be achieved as follows [7]:

Consider the auxiliary variables, q_{trial} [LT^{-1}] and v_{trial} [L], found from

$$q_{\text{trial}} = av_i^b \quad \text{and} \quad v_{\text{trial}} = v_i + \Delta t(q_{s,i} - q_{\text{trial}}) \quad (20.58)$$

The $v_{\max}$ constraint can be applied by calculating q_i from

$$q_i = \begin{cases} q_{\text{trial}}, & v_{\text{trial}} < v_{\max} \\ q_{s,i} - \frac{(v_{\max} - v_i)}{\Delta t}, & v_{\text{trial}} \geq v_{\max} \end{cases} \quad (20.59)$$

and v_{i+1} from

$$v_{i+1} = \begin{cases} v_{\text{trial}}, & v_{\text{trial}} < v_{\max} \\ v_{\max}, & v_{\text{trial}} \geq v_{\max} \end{cases} \quad (20.60)$$

In this way, stability is ensured by routing excess river flow contribution direct to the catchment outlet during exceptionally wet periods.

20.3.4.4 A $q_{\max}$ Formulation

The development and application of a stability constraint in Sects. 20.3.4.2 and 20.3.4.3 points towards an alternative formulation for the non-linear routing function model defined by Eqs. (20.38) and (20.39). Let $q_{\max}$ [LT^{-1}], be the threshold value of q_s beyond which q_s bypasses the routing function directly to the catchment outlet as in Eq. (20.59). Substituting Eq. (20.57) into Eq. (20.39) suggests that

$$q_{\max} = a^{\frac{1}{1-b}} (b\Delta t)^{\frac{b}{1-b}} \quad (20.61)$$

Substituting Eq. (20.61) into Eq. (20.47) and implementing the threshold concept defined above leads to

$$\frac{dq}{dt} = \begin{cases} \frac{1}{\Delta t} \left(\frac{q}{q_{\max}} \right)^{1-\frac{1}{b}} (q_s - q), & q_s < q_{\max} \\ \frac{dq_s}{dt}, & q_s \geq q_{\max} \end{cases} \quad (20.62)$$

20.3.5 Example Simulations

Figure 20.5 shows some example simulation results using the above flood routing function. All the models shown used the river flow contribution data, q_s , presented in Fig. 20.4a. For comparison, the simulation results are compared to observed river flow rates (per unit area of catchment) measured at the Sunderland Bridge gauging station on the River Wear outside Durham City.

The b parameter was taken arbitrarily to be 5/3. The $q_{\max}$ parameter was set as stated in the subtitles shown in Fig. 20.5. For low $q_{\max}$ values, the modelled flow rates are highly reactive to individual storm events with periods of zero flow in the summer. As $q_{\max}$ increases, the flow rate becomes more attenuated and there is a base-flow component ensuring non-zero flow throughout the year.

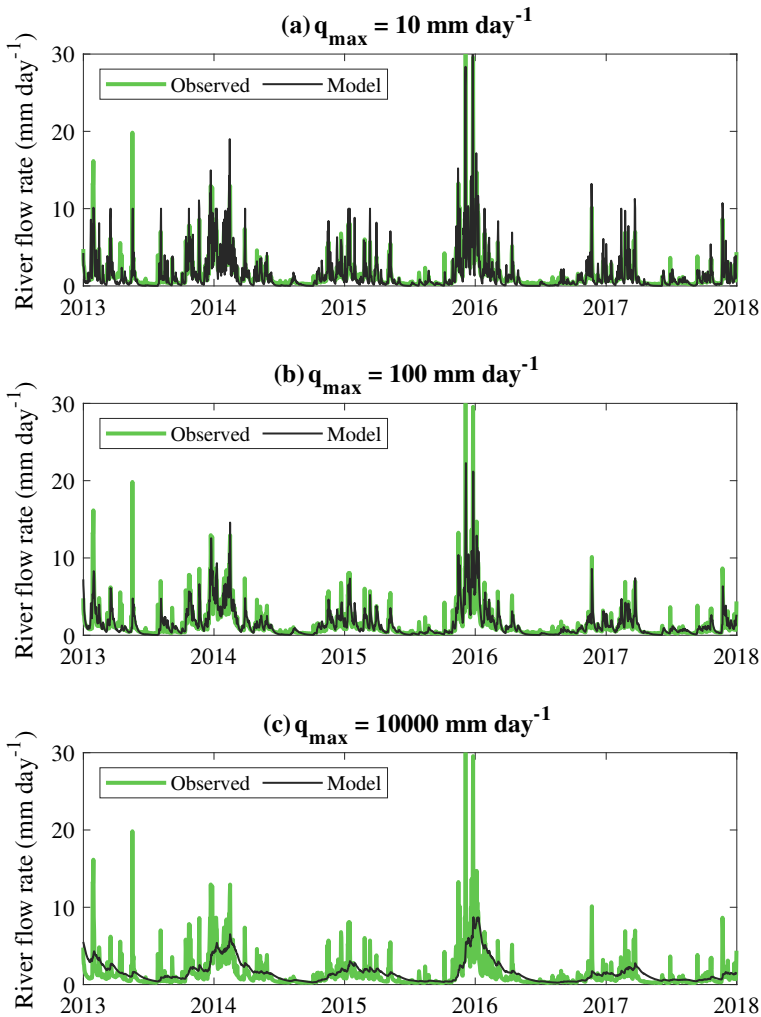


Fig. 20.5 River flow routing with different $q_{\max}$ values. The observed data is from the Sunderland Bridge gauging station on the River Wear outside Durham City (acquired from [3])

20.4 Calibration and Validation

The rainfall runoff model described above has four empirical parameters including $S_{\max}$, γ , $q_{\max}$ and b . Such parameters are often found by calibrating a model to observed river flow rate data as follows:

1. An initial guess is made about the unknown parameters values.
2. An objective function is specified, for example the mean absolute error between the simulated and observed flow rates.

3. The parameter values are iteratively changed until the objective function is minimised.

Ordinarily, a portion of historic flow observation data is excluded from the calibration exercise so that it can be subsequently used for a validation comparison with the best fitting models.

When the number of parameters is small (less than four), a local optimisation scheme, such as MATLAB's `fminsearch` function, can be used. However, where more parameters are required, there are multiple minimum points in the parameter-objective function space. In this case a global optimisation routine is required, which normally involves some form of probabilistic analysis.

In practice it is found that multiple combinations of model parameter values provide modelled flow rates with equally good correspondence with associated flow observations, hence it is often necessary to consider the response of an ensemble of different models. The phenomenon, of multiple models providing a close to similar response, is commonly referred to as equifinality. The reader is directed to [8] for a more in depth discussion on this topic.

20.5 Problem Sheet

Problem 20.1 (see Worked Solution 20.1)

The following two-monthly mean precipitation, q_p , and potential evapotranspiration, E_p , data are observed:

Period	(i)	(ii)	(iii)	(iv)	(v)	(vi)
q_p (mm day ⁻¹)	2.70	2.65	2.10	1.50	3.10	2.89
E_p (mm day ⁻¹)	0.28	0.67	2.50	2.70	2.68	0.80

(a) Use the PDM with the Pareto distribution function and $\gamma = 0$, to determine contribution to river flow and actual evapotranspiration for each of the six periods. Assume each 2-month period is 62 days long, $S_{\max} = 70$ mm and that the storage level, S , is initially at $S_{\max}$.

(b) Repeat the exercise above but with $\gamma = 1$.

Problem 20.2 (see Worked Solution 20.2)

Tables 20.1 and 20.2 contain daily precipitation, q_p , and potential evapotranspiration, E_p , data for 845 consecutive days. Each column of data follows the previous column.

(a) Write a MATLAB script to determine corresponding values of contribution to river flow, q_s , actual evapotranspiration, E_a , and catchment storage level, S , using the PDM with the Pareto distribution function. Assume $\gamma = 1$, $S_{\max} = 80$ mm and that S is initially zero. Generate plots of q_p , q_s , E_p , E_a and S against time.

(b) Extend your MATLAB script by providing a river flow routing model, as described in Sect. 20.3. Assume $b = 5/3$, $q_{\max} = 10,000$ mm day⁻¹ and that the river channel storage, v , is initially zero. Determine a corresponding value for a from Eq. (20.61). Determine river flow rate per unit area of catchment, q , and plot this against time. Once you have done this, experiment by changing γ , $S_{\max}$, b and $q_{\max}$.

20.6 Worked Solutions

Worked Solution 20.1 (see Problem 20.1)

(a) (i) The period of January and February.

If $\gamma = 0$ then the PDM-CDF, $F(S) = 0$. From Eq. (20.33), we then have

$$S_{\text{trial}} = S_1 + (q_{p,1} - E_{p,1})\Delta t = 70 + (2.70 - 0.28) \times 62 = 220.0 \text{ mm}$$

Because $S_{\text{trial}} > S_{\max}$ it follows that:

$$S_2 = S_{\max} = 70 \text{ mm}$$

$$\begin{aligned} q_{s,1} &= q_{p,1} - E_{p,1} - \frac{(S_{\max} - S_1)}{\Delta t} \\ &= 2.7 - 0.28 - \frac{(70 - 70)}{62} = 2.42 \text{ mm day}^{-1} \end{aligned}$$

$$E_{a,1} = E_{p,1} = 0.28 \text{ mm day}^{-1}$$

(ii) The period of March and April.

$$S_{\text{trial}} = S_2 + (q_{p,2} - E_{p,2})\Delta t = 70 + (2.65 - 0.67) \times 62 = 192.8 \text{ mm}$$

Because $S_{\text{trial}} > S_{\max}$ it follows that:

$$S_3 = S_{\max} = 70 \text{ mm}$$

$$\begin{aligned} q_{s,2} &= q_{p,2} - E_{p,2} - \frac{(S_{\max} - S_2)}{\Delta t} \\ &= 2.65 - 0.67 - \frac{(70 - 70)}{62} = 1.98 \text{ mm day}^{-1} \end{aligned}$$

$$E_{a,2} = E_{p,2} = 0.67 \text{ mm day}^{-1}$$

Table 20.1 Daily precipitation data acquired from [3]

Daily precipitation (mm)												
0.4	0.1	4.1	0.1	0	0	6.3	2.2	0.1	0.4	0.1	0	0.4
7.9	0.1	11.6	1.3	0	12.7	0.7	0.1	1.7	0.6	0.1	0	0.2
2.8	0	1.8	0.4	0	0.5	0	0	4.1	5.1	7.5	4.6	0.1
2.1	0	33.2	0.1	0.1	0	0	0	5.1	14.8	0.4	3	0.4
6.5	6.4	4	0	0.3	0	0.1	0	0.8	6.3	0	0.8	0
0.1	6.5	0.1	0	0	0	4.3	0.7	0.1	0.1	0.2	1	0
1.6	0.1	9.6	3.9	8.5	0	8.1	0	0	0.2	0	0	0.1
1.6	3.5	17.1	3	5.9	0.6	2.3	1.2	1.6	0.4	0.4	0	0
1.6	2	0.2	2.2	0.4	0.3	0.1	1.1	1	0.5	0	9.4	0
2.9	0.7	5.2	0.6	1.5	0	0.4	2	0	0.1	1.4	8	2.7
0.3	2.6	0.8	3.8	0.2	0.1	3.7	3.9	1.4	0.2	0.2	28	0.1
0	0.4	0.9	13.6	0	0	0	6.7	0.1	0.1	3	3.7	0
1.8	0	3.4	4.3	1.5	0	4.5	8.6	0.3	1	0.3	0.8	0.2
0.3	3.3	0.7	8.6	2.8	0.3	7.9	1.6	0	6.9	2.2	0	8.9
2.5	2.8	0.1	2.3	4	7.9	1.1	0.2	0.3	14.2	0.1	0.3	1.3
0.6	0.3	0	0.4	1.9	0	0.9	4.4	1.6	5.3	0	0.9	0.1
2.1	0.6	3.2	4.2	1.5	2.2	0.1	5.6	9.7	2.7	0	13.6	4.9
1.6	1.7	11.9	3	2.6	5	0	1.6	2.6	3	0	2.1	1.2
0.4	0	7.4	0.4	2.9	5	0	2.5	9.1	6.6	0	3	3.4
0	0	11	2	2.5	1.2	0	0.9	1.3	2.4	0	0.4	7.8
0.6	0	2.7	0.6	2.7	0.9	0	1.5	5	0	0	0.1	0.6
0.4	0.1	1.6	2.5	0	0.2	0	5.7	0.3	0.4	0	3.2	27.5
12.1	0	19.8	7.8	6.7	0.8	6.6	4.4	0	0.9	0	4	1.5
12.5	0	28.3	6.5	17	0.2	13	2.4	0.1	14	0	2.1	3.1
7	0	30.2	7	0.8	0.8	4.6	0.3	0.1	0.5	0	0	1.8
3.8	0	0.4	0.2	0.2	0	4.1	0	0	1.3	0	1.1	2.2
0.4	0	6	0	8.1	6.1	0.1	1.8	11.9	0.2	0	2.9	7.1
1.8	0	4.8	0	1.2	0.2	4.5	0	2.6	9.2	0	1.7	1.7
1.8	13.3	13.8	0.5	0	0	4.2	0	0.1	1.1	0.7	0	0
1.9	18.9	3.7	4.6	0	0	0	0.1	0.1	0.1	1.3	0	0.6
0.5	9.7	2.3	2.1	0	0.2	21.6	0.9	0	0.5	0.7	0	0.3
1.6	0.1	20	0.2	0	1	0.5	0.1	0.3	4.5	6.4	4.1	2.2
0.7	0	2.5	5.5	0	4.4	0	0	1.8	0	0.8	1	0.1
0.6	0.8	1.8	3.5	0	3.5	0	1.2	0.1	0.1	0	5.2	1.8
0	0.1	4.2	0.4	0.1	0.2	0	4.6	1.8	0	0.6	7.9	0.7

(continued)

Table 20.1 (continued)

Daily precipitation (mm)												
0.8	2.6	0.2	2	0	9.5	0.7	3	2.1	0	1.7	11	0.1
0	0.1	1.4	1.8	0.4	12.5	0	10.8	0.8	1.8	2.8	0.1	11.1
1.8	0.1	1.2	2.4	4.9	7.8	19.2	1.3	1.5	6.1	0.1	1.3	1.5
0	0.4	19.5	0.1	3.3	2.1	0.7	7.9	2.3	7.9	0	7.7	2.8
0	0.2	8	0.1	7	0.9	0	3.1	0.1	3.2	0	3.7	2.3
17.6	0	17.3	0	5.8	0	0	0.6	6.7	3	0	3.1	2.1
12.7	0.1	8	0	0.6	7.7	0	9.3	2.7	10.2	0	1.3	1.1
0	0.2	4.6	0	1.4	0.1	2	0.1	0.4	19.9	0	3.5	0.3
0	8.5	3.5	0.1	2.4	0.9	2	4.3	0.1	0.1	6.6	0.4	7
0.2	0.1	42.2	0.1	0.1	0.5	0.2	0.4	0	0	1.2	0.4	0
6	0	21.5	8.5	0	1	0	2.2	0.1	0	2.7	11.6	1.1
2.1	0.2	0.9	1.3	0	3.2	0	4	0	0	0.2	4.4	0.2
0.6	0.9	0.8	1.5	0	4.8	8.2	8.7	0.3	0	0	0	0.3
6.9	0	1	10.4	0	0.2	0.1	0.6	0	0.7	1.3	0.2	2.6
9.5	0.1	7.2	10.7	0	0	5.3	0.4	0	2.1	0.3	4.7	2.3
7.8	0.8	4.9	4.6	0	2.2	0.5	0.2	0	3	0	0.1	7.1
0	10.2	11.8	0.3	0	0	0	37.7	0	0.6	4	10.1	0.9
2.1	12.4	11.7	0.1	0	3.5	1.8	2.8	0	2.2	22.3	0	3.4
1.8	7.2	11.7	2.5	0	0	0	0	3.2	0	16.1	0.1	1
0.5	0.2	17.7	3.4	0	0	0	0	1.7	0	2.3	1.9	0.3
1.4	0.1	9.7	0	0	0.1	1.4	0	0.2	0	4.4	3.2	1.4
1.8	0.1	11.5	0.1	0	0.4	0.2	1.2	0.2	0	7.1	0.7	0.2
0.8	1.4	2.9	0	0	3.9	0	0.3	4.9	0	2.7	6.2	0.5
1.7	0.2	6.5	0	0.2	0.4	5.1	0	0.5	0	2.7	0.1	19.6
1.9	2.8	16.9	0.1	2.5	0.4	1	0.1	0.9	0	0	3.8	2.5
1.3	6	3.8	0.3	1.3	0.1	2	0	5.5	0	0	1	7.3
1	8.4	1.3	0.1	2.1	1.4	0.1	0	0.4	0	0	2.5	0.8
1.3	15.1	2.6	0.1	0.7	0.2	5	0.9	0	1.1	1.7	0.5	1.5
0	3.8	3.8	0	1	10.2	3.2	0	8.2	0.2	0	0	3.7
0	2.7	1.4	0	0.8	0.1	0.8	0	2.1	0.1	0	1.2	0

(iii) The period of May and June.

$$S_{\text{trial}} = S_3 + (q_{p,3} - E_{p,3})\Delta t = 70 + (2.10 - 2.50) \times 62 = 45.20 \text{ mm}$$

Because $S_{\text{trial}} \in (0, S_{\text{max}})$ it follows that:

$$S_4 = S_{\text{trial}} = 45.20 \text{ mm}$$

$$q_{s,3} = 0 \text{ mm day}^{-1}$$

Table 20.2 Daily potential evapotranspiration data determined using temperature data from [4]

Daily potential evapotranspiration (mm)												
3.43	2.39	0.334	0.285	1.41	3.1	2.44	1.13	0.308	0.309	1.5	4.03	2.38
3.48	1.59	0.508	0.278	1.54	1.93	2.66	1.23	0.349	0.268	1.53	4.38	1.51
2.45	1.53	0.283	0.238	1.19	1.93	2.52	1.34	0.43	0.292	1.55	2.8	1.89
2.15	2.03	0.341	0.254	0.703	2.69	2.5	1.36	0.264	0.397	1.63	4.19	1.6
1.86	1.97	0.665	0.27	1.14	3.03	2.7	0.909	0.396	0.298	1.85	1.96	1.92
2.99	1.23	0.277	0.312	1.44	3.36	2.4	1.03	0.244	0.469	1.61	2.1	2.14
3.92	1.75	0.537	0.354	1.4	3.17	1.6	0.739	0.275	0.592	1.68	2.55	1.82
2.09	1.61	0.498	0.463	1.14	2.4	1.95	0.802	0.236	0.56	1.64	2.59	1.2
2.2	1.26	0.295	0.359	1.21	1.97	2.3	0.874	0.251	0.502	1.79	2.99	1.98
2.55	1.84	0.256	0.5	1.28	2.99	3.2	0.889	0.312	0.557	2.19	1.67	1.98
2.6	1.66	0.206	0.376	1.48	3.98	1.5	0.731	0.286	0.502	1.21	1.11	2.28
3.03	1.42	0.375	0.574	1.74	2.9	1.99	0.716	0.247	0.546	1.7	2.1	2.33
3.33	1.8	0.405	0.436	1.29	4.3	2.37	0.649	0.24	0.683	1.61	1.97	1.76
2.24	1.33	0.265	0.526	0.915	4.44	2.27	0.628	0.365	0.751	2.11	2.43	1.93
2.21	1.03	0.34	0.401	1.54	4.61	2.26	0.728	0.248	0.46	1.93	2.41	1.23
1.91	1.49	0.408	0.259	0.946	3.32	1.58	0.822	0.211	0.641	1.77	2.42	1.53
2.95	1.36	0.28	0.423	1.33	4.13	1.78	0.689	0.257	0.618	1.97	2.15	1.28
2.03	1.11	0.319	0.608	0.927	2.73	1.78	0.541	0.308	0.799	1.98	2.11	1.34
2.35	1.19	0.366	0.304	1.74	2.18	3.06	0.677	0.324	0.703	2.14	3.45	1.53
2.25	1.37	0.234	0.419	1.64	2.78	3.18	0.583	0.264	0.523	2.51	2.39	1.58
2.58	1.62	0.596	0.593	1.42	1.78	2.81	0.662	0.358	0.7	2.32	3.25	1.55
2.68	1.74	0.298	0.351	2.06	2.98	2.77	0.664	0.213	0.809	2.37	3.12	1.35
2.59	1.69	0.428	0.633	1.95	2.74	1.55	0.501	0.236	0.725	2.16	2.31	1.29
1.5	1.64	0.431	0.42	0.958	2.02	1.58	0.641	0.247	0.704	2.07	2.31	1.4
1.56	1.9	0.259	0.45	1.2	1.88	1.71	0.803	0.268	0.85	1.74	3.33	1.4
2.26	1.57	0.279	0.33	1.2	2.65	2.39	0.594	0.369	0.771	2.36	3.35	1.18
2.21	0.976	0.529	0.44	1.22	3.14	2.99	0.545	0.254	0.87	2.86	2.51	1.47
2.51	1.05	0.265	0.523	1.58	2.51	2.31	0.454	0.204	0.841	3.18	2.72	0.996
2.26	1.38	0.427	0.503	2.01	3.22	1.48	0.804	0.218	0.995	2.71	2.54	1.65
2.37	0.946	0.306	0.397	1.58	3.52	1.99	0.622	0.344	0.823	1.69	3.73	1.52
2.15	0.491	0.239	0.373	2.34	4.05	2.61	0.619	0.229	1	2.2	4.04	0.786
2.27	1.2	0.204	0.404	2.77	2.88	1.43	0.383	0.285	0.658	2.61	3.06	1.47
2.39	1.23	0.216	0.598	3.09	3.53	2.21	0.553	0.382	0.696	1.56	1.41	1.31
2.05	0.915	0.257	0.593	1.93	2.95	1.9	0.48	0.286	1.24	1.91	3.13	1.39
2.85	0.786	0.261	0.676	1.94	2.3	1.51	0.405	0.288	1.01	2.81	2.05	1.03
2.97	0.966	0.362	0.665	1.98	2.79	1.85	0.342	0.263	1.28	2.07	2.68	1.21
2.19	0.822	0.282	0.449	1.55	2.25	1.57	0.346	0.342	0.9	1.9	2.07	0.979

(continued)

Table 20.2 (continued)

Daily potential evapotranspiration (mm)												
2.38	0.964	0.263	0.628	1.66	2.68	1.15	0.324	0.238	0.969	2.59	2.57	1.12
2.22	0.909	0.353	0.666	1.55	2.47	1.61	0.325	0.204	0.856	3.07	2.49	1.06
3.19	0.655	0.255	0.687	1.72	2.8	2.03	0.264	0.27	0.985	3.11	2.19	1
2.87	0.7	0.275	0.745	1.42	2.78	1.84	0.427	0.327	0.82	3.06	2.21	1.49
1.07	0.585	0.374	0.575	2.25	2.98	1.94	0.404	0.524	0.88	4.4	2.18	0.744
2.19	0.845	0.232	0.537	1.97	2.66	1.08	0.464	0.268	0.941	3.89	2.31	0.83
2.51	0.739	0.279	0.623	1.4	3.04	1.65	0.434	0.302	1.02	3.9	2.23	0.749
2.69	1.02	0.214	0.706	2.1	2.65	1.72	0.505	0.266	1.61	2.78	2.37	0.997
1.9	0.517	0.422	0.625	2.37	2.62	1.95	0.325	0.272	2.09	1.4	2.53	0.949
2.23	0.776	0.27	1.31	2.86	2.79	2.21	0.374	0.294	1.78	2.12	2.14	0.909
2.04	0.491	0.388	0.738	3.1	2.2	2.34	0.255	0.288	1.56	3.6	1.81	0.874
2.01	0.646	0.243	0.887	2.66	2.27	1.76	0.263	0.223	1.6	2.92	2.34	0.765
2.08	0.712	0.384	0.615	3.99	2.83	2.31	0.295	0.339	1.37	2.33	2.49	0.684
2.57	0.655	0.234	0.698	3.84	2.82	1.19	0.3	0.378	1.15	3.16	1.87	0.764
2.16	0.438	0.244	0.752	3.26	3.48	1.78	0.366	0.313	1.02	2.65	2.04	0.832
1.94	0.631	0.304	0.924	2.94	2.95	1.76	0.279	0.329	1.29	2.37	2.22	1.03
1.71	0.805	0.243	1.07	2.95	2.31	1.29	0.276	0.383	1.6	1.32	2.83	0.704
1.67	0.491	0.229	0.591	1.65	2.67	1.58	0.312	0.342	1.71	2.38	2.44	0.685
1.81	0.592	0.238	0.855	2.75	3.88	1.48	0.329	0.377	1.19	2.59	1.93	1.09
1.7	0.728	0.23	1.06	2.99	5.11	0.951	0.538	0.455	1.3	2.54	2.62	0.527
1.93	0.676	0.234	1.11	3.14	2.52	1.5	0.274	0.389	1.57	2.83	2.12	0.746
1.57	0.493	0.29	1.17	3.36	3.41	1.43	0.284	0.389	1.44	1.75	1.87	0.688
1.87	0.53	0.289	1.37	2.23	3.47	0.862	0.313	0.464	2.52	1.75	2.37	0.707
1.68	0.48	0.237	1.09	2.15	2.84	1.13	0.389	0.363	2.2	2.72	2.2	0.632
1.42	0.41	0.244	1.1	2.51	2.46	1.39	0.3	0.373	1.77	3.54	1.6	0.481
1.7	0.596	0.252	1.44	2.39	2.34	1.4	0.302	0.418	1.52	2.48	1.73	0.87
1.52	0.687	0.239	1.06	2.95	2.64	0.775	0.234	0.505	1.31	2.48	1.89	0.757
2.27	0.388	0.203	0.802	3.32	2.52	1.15	0.251	0.467	1.54	3.53	2.69	0.587

$$E_{a,3} = E_{p,3} = 2.50 \text{ mm day}^{-1}$$

(iv) The period of July and August.

$$S_{\text{trial}} = S_4 + (q_{p,4} - E_{p,4})\Delta t = 45.20 + (1.50 - 2.70) \times 62 = -29.20 \text{ mm}$$

Because $S_{\text{trial}} \leq 0$ it follows that:

$$S_5 = 0 \text{ mm}$$

$$q_{s,4} = 0 \text{ mm day}^{-1}$$

$$E_{a,4} = q_{p,4} + \frac{S_4}{\Delta t} = 1.50 + \frac{45.2}{62} = 2.229 \text{ mm day}^{-1}$$

(v) The period of September and October.

$$S_{\text{trial}} = S_5 + (q_{p,5} - E_{p,5})\Delta t = 0 + (3.10 - 2.68) \times 62 = 26.04 \text{ mm}$$

Because $S_{\text{trial}} \in (0, S_{\text{max}})$ it follows that:

$$S_6 = S_{\text{trial}} = 26.04 \text{ mm}$$

$$q_{s,5} = 0 \text{ mm day}^{-1}$$

$$E_{a,5} = E_{p,5} = 2.68 \text{ mm day}^{-1}$$

(vi) The period of November and December

$$S_{\text{trial}} = S_6 + (q_{p,6} - E_{p,6})\Delta t = 26.04 + (2.89 - 0.80) \times 62 = 155.6 \text{ mm}$$

Because $S_{\text{trial}} > S_{\text{max}}$ it follows that:

$$S_7 = S_{\text{max}} = 70 \text{ mm}$$

$$\begin{aligned} q_{s,6} &= q_{p,6} - E_{p,6} - \frac{(S_{\text{max}} - S_6)}{\Delta t} \\ &= 2.89 - 0.8 - \frac{(70 - 26.04)}{62} = 1.38 \text{ mm day}^{-1} \end{aligned}$$

$$E_{a,6} = E_{p,6} = 0.8 \text{ mm day}^{-1}$$

The results can be summarised as follows:

Period	(i)	(ii)	(iii)	(iv)	(v)	(vi)
q_p (mm day ⁻¹)	2.70	2.65	2.10	1.50	3.10	2.89
E_p (mm day ⁻¹)	0.28	0.67	2.50	2.70	2.68	0.80
S (mm)	70	70	70	45.20	0	26.04
S_{trial} (mm)	220.0	192.8	45.20	-29.20	26.04	155.6
q_s (mm day ⁻¹)	2.42	1.98	0	0	0	1.38
E_a (mm day ⁻¹)	0.28	0.67	2.50	2.23	2.68	0.80

(b) (i) The period of January and February.

If $\gamma = 1$ then the PDM-CDF, F , is found from

$$F_1 = \frac{S_1}{S_{\text{max}}} = \frac{70}{70} = 1$$

From Eq. (20.33), we then have

$$\begin{aligned} S_{\text{trial}} &= S_1 + [(1 - F_1)q_{p,1} - E_{p,1}]\Delta t \\ &= 70 + (0 \times 2.70 - 0.28) \times 62 = 52.64 \text{ mm} \end{aligned}$$

Because $S_{\text{trial}} \in (0, S_{\text{max}})$ it follows that:

$$S_2 = S_{\text{trial}} = 52.64 \text{ mm}$$

$$q_{s,1} = F_1 q_{p,1} = 2.70 \text{ mm day}^{-1}$$

$$E_{a,1} = E_{p,1} = 0.28 \text{ mm day}^{-1}$$

(ii) The period of March and April.

$$F_2 = \frac{S_2}{S_{\max}} = \frac{52.64}{70} = 0.7520$$

and

$$\begin{aligned} S_{\text{trial}} &= S_2 + [(1 - F_2)q_{p,2} - E_{p,2}]\Delta t \\ &= 52.64 + (0.2480 \times 2.65 - 0.67) \times 62 = 51.85 \text{ mm} \end{aligned}$$

Because $S_{\text{trial}} \in (0, S_{\max})$ it follows that:

$$S_3 = S_{\text{trial}} = 51.85 \text{ mm}$$

$$q_{s,2} = F_2 q_{p,2} = 0.7520 \times 2.65 = 1.99 \text{ mm day}^{-1}$$

$$E_{a,2} = E_{p,2} = 0.67 \text{ mm day}^{-1}$$

(iii) The period of May and June.

$$F_3 = \frac{S_3}{S_{\max}} = \frac{51.85}{70} = 0.7407$$

and

$$\begin{aligned} S_{\text{trial}} &= S_3 + [(1 - F_3)q_{p,3} - E_{p,3}]\Delta t \\ &= 51.85 + (0.2593 \times 2.10 - 2.50) \times 62 = -69.39 \text{ mm} \end{aligned}$$

Because $S_{\text{trial}} \leq 0$ it follows that:

$$S_4 = 0 \text{ mm}$$

$$q_{s,3} = F_3 q_{p,3} = 0.7407 \times 2.10 = 1.56 \text{ mm day}^{-1}$$

$$E_{a,3} = (1 - F_3)q_{p,3} + \frac{S_3}{\Delta t} = 0.2593 \times 2.10 + \frac{51.85}{62} = 1.38 \text{ mm day}^{-1}$$

(iv) The period of July and August.

$$F_4 = \frac{S_4}{S_{\max}} = \frac{0}{70} = 0$$

and

$$\begin{aligned} S_{\text{trial}} &= S_4 + [(1 - F_4)q_{p,4} - E_{p,4}]\Delta t \\ &= 0 + (1.50 - 2.70) \times 62 = -74.40 \text{ mm} \end{aligned}$$

Because $S_{\text{trial}} \leq 0$ it follows that:

$$S_5 = 0 \text{ mm}$$

$$q_{s,4} = F_4 q_{p,3} = 0 \text{ mm day}^{-1}$$

$$E_{a,4} = (1 - F_4)q_{p,4} + \frac{S_4}{\Delta t} = 1.50 + 0 = 1.50 \text{ mm day}^{-1}$$

(v) The period of September and October.

$$F_5 = \frac{S_5}{S_{\max}} = \frac{0}{70} = 0$$

and

$$\begin{aligned} S_{\text{trial}} &= S_5 + [(1 - F_5)q_{p,5} - E_{p,5}]\Delta t \\ &= 0 + (3.10 - 2.68) \times 62 = 26.04 \text{ mm} \end{aligned}$$

Because $S_{\text{trial}} \in (0, S_{\max})$ it follows that:

$$\begin{aligned} S_6 &= S_{\text{trial}} = 26.04 \text{ mm} \\ q_{s,5} &= F_5 q_{p,5} = 0 \text{ mm day}^{-1} \\ E_{a,2} &= E_{p,2} = 2.68 \text{ mm day}^{-1} \end{aligned}$$

(vi) The period of November and December

$$F_6 = \frac{S_6}{S_{\max}} = \frac{26.04}{70} = 0.3720$$

and

$$\begin{aligned} S_{\text{trial}} &= S_6 + [(1 - F_6)q_{p,6} - E_{p,6}]\Delta t \\ &= 26.04 + (0.6280 \times 2.89 - 0.80) \times 62 = 88.97 \text{ mm} \end{aligned}$$

Because $S_{\text{trial}} \geq S_{\max}$ it follows that:

$$\begin{aligned} S_7 &= S_{\max} = 70 \text{ mm} \\ q_{s,6} &= q_{p,6} - E_{p,6} - \frac{(S_{\max} - S_6)}{\Delta t} \\ &= 2.89 - 0.8 - \frac{(70 - 26.04)}{62} = 1.38 \text{ mm day}^{-1} \\ E_{a,6} &= E_{p,6} = 0.80 \text{ mm day}^{-1} \end{aligned}$$

The results can be summarised as follows:

Period	(i)	(ii)	(iii)	(iv)	(v)	(vi)
q_p (mm day ⁻¹)	2.70	2.65	2.10	1.50	3.10	2.89
E_p (mm day ⁻¹)	0.28	0.67	2.50	2.70	2.68	0.80
S (mm)	70	52.64	51.85	0	0	26.04
S_{trial} (mm)		52.64	51.85	-69.39	-74.40	26.04
q_s (mm day ⁻¹)	2.70	1.99	1.56	0	0	1.38
E_a (mm day ⁻¹)	0.28	0.67	1.38	1.50	2.68	0.80

Worked Solution 20.2 (see Problem 20.2)

(a) A MATLAB script to determine the contribution to river flow and actual evapotranspiration is given below.

```
%Concatenate input data:
qp=qp(:); %Precipitation (mm/day)
Ep=Ep(:); %Potential evapotranspiration (mm/day)
%Specify input parameters:
Smax=80; %Maximum storage for PDM (mm)
gamma=1; %Exponent for Pareto distribution
%Initialisation steps:
N=size(qp,1); %Determine number of data points
S=0; %Specify initial catchment storage (mm)
dt=1; %Time step is one day
for i=1:N; %Step through each day
    F=1-(1-S(i)/Smax)^gamma; %Pareto CDF
    %Trial value for S
    Strial=S(i)+(1-F)*qp(i)-Ep(i)*dt;
    %To start with try the following:
    S(i+1)=Strial; %Catchment storage
    qs(i)=F*qp(i); %River flow contribution
    Ea(i)=Ep(i); %Actual evapotranspiration
    if Strial<=0 %Force S>=0
        S(i+1)=0;
        Ea(i)=(1-F)*qp(i)+S(i)/dt;
    elseif Strial>=Smax %Force S<=Smax
        S(i+1)=Smax;
        qs(i)=qp(i)-Ep(i)-(Smax-S(i))/dt;
    end
end
```

The plotted results should look similar to the last two years shown in Fig. 20.4.

(b) A MATLAB script to determine the flow rate is given below, which should be appended to the script given in response to part (a) above.

```
%Specify input parameters:
qmax=10000; %Flow rate Scaling parameter (mm/day)
b=5/3; %Exponent in  $q=a*v^b$ 
%Initialisation steps:
a=qmax^(1-b)*(b*dt)^-b; %Determine a for  $q=a*v^b$ 
vmax=(a*b*dt)^(1/(1-b)); %Limit on v for stability
v=0; %Specify initial river storage (mm)
for i=1:N; %Step through each day
    %Trial values for q and v:
```



```

qtrial=a*v(i)^b;
vtrial=v(i)+(qs(i)-qtrial)*dt;
if vtrial<vmax %Ordinarily use trial values
q(i)=qtrial; %River flow (mm/day)
v(i+1)=vtrial; %River storage (mm)
else %Force v<=vmax
q(i)=qs(i)-(vmax-v(i))/dt;
v(i+1)=vmax;
end
end

```

The plotted results should look similar to the last two years shown in Fig. 20.5c.

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Part III
Environmental Engineering

Cost Benefit Analysis

21

Abstract

This chapter develops simple mathematical methods for cost benefit analysis. The need for quantifying environmental benefits is explained using the tragedy of the commons concept. Opportunity cost, discounting and minimum acceptable rate of return (MARR) are explained. Simple closed-form cash flow equations are derived for a uniform payment model, an exponentially increasing payment model and a linearly increasing payment model. Project evaluation methods are developed including net present value (NPV), internal rate of return (IRR) and equivalent annual cost (EAC). The importance of capital expenditure (CapEx) and operating expenses (OpEx) are explained. Inflation rate is incorporated using “real” rates of return. Practical applications are presented through worked examples and a problem sheet with worked solutions.

Notation

A	Uniform annual payment.
B	Annual benefit.
C	Current cost.
C_0	Initial value of an annual payment (current value).
C_n	Annual payment (current value).
d	Depreciation rate.
f	Inflation rate.
F	Net future value (current value).
g	Growth rate for exponentially increasing annual payment model.
i	Rate of return (current value).
i_R	Rate of return (real value).
I	Initial CapEx.
M	An amount of money.
n	Year of consideration.

N	Project lifetime in years.
P	Net present value.
R_0	Initial value of an annual payment (real value).
R_n	Annual payment (real value).
λ	Auxiliary variable for geometric series.
CapEx	Capital expenditure.
EAB	Equivalent annual benefit.
EAC	Equivalent annual cost.
GBP	Great Britain Pound.
IRR	Internal rate of return.
NFC	Net future cost.
NFV	Net future value.
NPC	Net present cost.
NPV	Net present value.
MARR	Minimum acceptable rate of return.
OpEx	Operating expenses.
USD	United States Dollars.

21.1 Introduction

Economics is the study of how and why individuals and groups make decisions about the use and distribution of valuable resources [1]. Environmental economics is concerned with the impact of the economy on the environment and developing appropriate ways of regulating economic activity to balance environmental management and economic goals [2].

The first part of this chapter seeks to establish the concepts of common-pool resources and public goods, which are a significant reason as to why conventional cost benefit analyses often overlook environmental impacts and benefits. The second part of the chapter seeks to introduce engineering students to key concepts concerning cash flow analysis. It is necessary to properly understand these foundation topics to enable further study of how to incorporate external environmental impacts and benefits (the topic of the next chapter).

The outline of this chapter is as follows. The concepts of excludability and rivalry are introduced so as to identify common pool resources and public goods. These are used to explain the so-called tragedy of the commons, which in turn helps to explain why environmentally damaging and unsustainable activity so often takes place. Following from this we look at some conventional economics tools associated with cash flow analysis. First we look at the concept of discounting and learn about how industry sectors value time in different ways depending on minimum acceptable rates of return. We then derive some useful annual payment models which are subsequently used to develop three project evaluation methods: net-present value, internal rate of return and equivalent annual cost. We also look at inflation and how to incorporate it into our calculations. Finally some practical calculation exercises are provided.

21.2 Common-Pool Resources and Public Goods

Some questions that often arise in the field of environmental engineering include:

- Why do we pollute rivers, lakes and oceans even though we benefit from ecosystem services provided by healthy aquatic environments?
- Why do we pollute the atmosphere even though we require clean air to breathe?
- Why do we unsustainably harvest fisheries even though we understand this will lead to irreversible depletion?

The reason is in part due to the qualities of common-pool resources and public goods.

21.2.1 Excludability, Rivalry, Goods and Bads

In economics a good is an object or service that provides a positive value to a consumer. In contrast, a bad is an object or service that provides a negative value to a consumer. Two fundamental characteristics of goods and bads are excludability and rivalry [2]. Excludability is the degree to which a supplier can prevent free consumption of a good. Rivalry is the degree to which consumption of a good by one consumer reduces the availability of that good to other consumers. These two characteristics are used to distinguish between the four following categories of goods [2]:

1. **Private goods**, which are excludable and rival;
2. **Club goods**, which are excludable and non-rival;
3. **Common pool resources**, which are non-excludable and rival;
4. **Public goods**, which are non-excludable and non-rival.

Each category has a bad counterpart. Some relevant examples are provided in Table 21.1.

Challenge 21.1 Assess the following items in terms of excludability and rivalry and determine whether they are private goods, club goods, common pool resources, public goods or any bad counterpart:

- Bottled water.
- Subscription internet content.
- Water pollution in a small lake.
- Producing water from a groundwater well.
- A pod of whales in the ocean to whale hunters.
- A pod of whales in the ocean to whale watchers.
- Poor air quality.

Table 21.1 Some examples demonstrating the use of the terms excludable and rival

Item	Excludable	Rival	Type
Bottled water	✓	✓	Private good
Subscription internet content	✓	✗	Club good
Water pollution in a small lake	✓	✗	Club bad
Producing water from a groundwater well	✗	✓	Common-pool resource
A pod of whales in the ocean to whale hunters	✗	✓	Common-pool resource
A pod of whales in the ocean to whale watchers	✗	✗	Public good
Poor air quality	✗	✗	Public bad

21.2.2 The Tragedy of the Commons

Hardin [3] provides the following important example to explain the tragedy of the commons:

“Picture a pasture open to all. It is to be expected that each herdsman will try to keep as many cattle as possible on the commons. Such an arrangement may work reasonably satisfactorily for centuries because tribal wars, poaching, and disease keep the numbers of both man and beast well below the carrying capacity of the land. Finally, however, comes the day of reckoning, that is, the day when the long-desired goal of social stability becomes a reality. At this point, the inherent logic of the commons remorselessly generates tragedy.

As a rational being, each herdsman seeks to maximize his gain. Explicitly or implicitly, more or less consciously, he asks, “What is the utility to me of adding one more animal to my herd?” This utility has one negative and one positive component.

1. The positive component is a function of the increment of one animal. Since the herdsman receives all the proceeds from the sale of the additional animal, the positive utility is nearly +1.
2. The negative component is a function of the additional overgrazing created by one more animal. Since, however, the effects of overgrazing are shared by all the herdsmen, the negative utility for any particular decision-making herdsman is only a fraction of −1.

Adding together the component partial utilities, the rational herdsman concludes that the only sensible course for him to pursue is to add another animal to his herd. And another; and another... But this is the conclusion reached by each and every rational herdsman sharing a commons. Therein is the tragedy. Each man is locked

into a system that compels him to increase his herd without limit—in a world that is limited. Ruin is the destination toward which all men rush, each pursuing his own best interest in a society that believes in the freedom of the commons. Freedom in a commons brings ruin to all.”

Hardin [3] goes on to relate this problem to pollution:

“In a reverse way, the tragedy of the commons reappears in problems of pollution. Here it is not a question of taking something out of the commons, but of putting something in—sewage, or chemical, radioactive, and heat wastes into water; noxious and dangerous fumes into the air, and distracting and unpleasant advertising signs into the line of sight. The calculations of utility are much the same as before. The rational man finds that his share of the cost of the wastes he discharges into the commons is less than the cost of purifying his wastes before releasing them. Since this is true for everyone, we are locked into a system of “fouling our own nest,” so long as we behave only as independent, rational, free-enterprisers.”

21.2.3 More Difficult Questions

So why do we manage our environment so badly? The answer to this question can be understood further by asking some more difficult questions. For example:

- What is the benefit of a farmer reducing their groundwater production from a scarce resource in the knowledge that a neighbouring farmer will continue to produce groundwater until the aquifer is depleted?
- What is the benefit of a coal-fired power plant removing CO₂ from their flue gas if other plants are not doing the same but still equally benefiting from the incremental reduction in greenhouse gas emissions to the atmosphere?
- What is the benefit of a gold miner treating their wastewater stream if only communities downstream of the mine benefit from reduced pollution in their river?
- What is the benefit of choosing an expensive renewable energy supplier if almost everyone else in the world continues to use fossil fuels?

The problem is that damaging the environment appears to be free and therefore there is commonly insufficient motivation to stop doing it.

21.3 Cash Flow Analysis

21.3.1 Discounting

If you were to pay me £10 next year, that £10 would be worth less to me than if you were to pay me £10 today. Notwithstanding inflation, this is because I have lost the opportunity to utilise that £10 through the coming year. This loss of opportunity to do something with the £10 is referred to as the opportunity cost of waiting one year.

If I am to understand the value of that £10 you are planning to give me next year as compared to £10 I have in my pocket today, I need to apply a discount factor to account for this opportunity cost.

The value of an amount of money in the present, P , can be related to its value, N years in the future, F , using the compound interest formula [4, p. 48]

$$F = P(1 + i)^N \quad (21.1)$$

where i is the rate of return expected to be paid each year on the money.

The rate of return, i , is often referred to as the discount rate. If the money was being stored in a bank account, the discount rate would correspond to the interest rate. For an organisation considering a potential investment, the discount rate typically reflects their minimum acceptable rate of return (MARR).

The MARR of an investor will represent some idea of how much they think they can ordinarily make out of an investment. Some idea about the value of MARR for different industries can be understood by considering average returns on investment (RoI) from the past. Average RoI for the period of 2012 to 2020 for various US industries are presented in Table 21.2. It can be seen that there is a wide range of variation of RoI indicating that MARR will also vary widely for different industries.

Table 21.2 Average returns on investment for the period of 2012 to 2020 for various US industries (sourced from www.csimarket.com 26/01/2021)

Industry	Return on investment (%)
Tobacco	89.4
Legal Marijuana	74.4
Casinos and gambling	26.4
Forestry and wood products	16.3
Software and programming	15.0
Internet services and social media	13.4
Aerospace and defence	12.9
Consumer electronics	9.24
Environmental services	8.63
Construction services	8.57
Educational services	6.75
Agricultural production	5.66
Investment services	3.38
Water supply	2.82
Iron and steel	2.68

21.3.2 Sequences of Annual Payments

The cash-flow of a project includes a sequence of annual payments made each year. Let C_n be the annual payment made at the end of the n -th year. For a discount rate, i , the total future value of the annual payments at the end of the N -th year, F , is found from

$$\begin{aligned} F &= C_1(1+i)^{N-1} + C_2(1+i)^{N-2} + \dots + C_N \\ &= \sum_{n=1}^N C_n(1+i)^{N-n} \end{aligned} \quad (21.2)$$

21.3.2.1 Uniform Annual Payments

Challenge 21.2 Let C_n be a uniform annual payment, A . Determine a closed-form expression relating F to A , N and i .

For a uniform annual payment, $C_n = A$,

$$F = \sum_{n=1}^N A(1+i)^{N-n} \quad (21.3)$$

A closed-form expression can be obtained by considering the sum of a geometric series [5, p. 772]

$$\sum_{n=0}^N \lambda^n = \frac{1 - \lambda^{N+1}}{1 - \lambda} \quad (21.4)$$

Shifting the index in Eq. (21.3) gives us

$$F = A(1+i)^N \left[\sum_{n=0}^N (1+i)^{-n} - 1 \right] \quad (21.5)$$

Substituting Eq. (21.4) into Eq. (21.5) leads to

$$F = A(1+i)^N \left[\frac{1 - (1+i)^{-N-1}}{1 - (1+i)^{-1}} - 1 \right] \quad (21.6)$$

After some further rearrangement we have [4, p. 51]

$$F = A \left[\frac{(1+i)^N - 1}{i} \right] \quad (21.7)$$

21.3.2.2 Exponentially Increasing Annual Payments

Let C_n be an exponentially increasing annual payment, i.e.,

$$C_n = C_0(1 + g)^{n-1}. \quad (21.8)$$

where C_0 is the initial value of the annual payment and g is the growth rate.

Challenge 21.3 Determine a closed-form expression relating F to C_0 , g , N and i .

Substituting Eq. (21.8) into Eq. (21.2) leads to

$$F = \sum_{n=1}^N C_0(1 + g)^{n-1}(1 + i)^{N-n} \quad (21.9)$$

Shifting the index in Eq. (21.9) gives us

$$F = \frac{C_0(1 + i)^N}{1 + g} \left[\sum_{n=0}^N \left(\frac{1 + g}{1 + i} \right)^n - 1 \right] \quad (21.10)$$

Substituting Eq. (21.4) into Eq. (21.10) leads to

$$F = \frac{C_0(1 + i)^N}{1 + g} \left[\frac{1 - \left(\frac{1+g}{1+i} \right)^{N+1}}{1 - \frac{1+g}{1+i}} - 1 \right] \quad (21.11)$$

After some further rearrangement we have

$$F = C_0 \left[\frac{(1 + i)^N - (1 + g)^N}{i - g} \right] \quad (21.12)$$

The growth rate, g , is often used to model the way maintenance costs increase as equipment gets older and more challenging to keep going. The growth rate can also be used to model the effect of monetary inflation, which is discussed in more detail in Sect. 21.3.5.

21.3.2.3 Linearly Increasing Annual Payments

Let C_n be a linearly increasing annual payment, increasing by a constant amount C_0 each year, i.e.,

$$C_n = nC_0 \quad (21.13)$$

Challenge 21.4 Determine a closed-form expression relating F to C_0 , N and i .

Substituting Eq. (21.13) into Eq. (21.2) leads to

$$F = \sum_{n=1}^N nC_0(1+i)^{N-n} \quad (21.14)$$

Substituting $\lambda = (1+i)^{-1}$ into Eq. (21.14) give us

$$F = C_0\lambda^{-N}S_N \quad (21.15)$$

where

$$S_N = \sum_{n=1}^N n\lambda^n = \lambda + 2\lambda^2 + 3\lambda^3 + \dots + (N-1)\lambda^{N-1} + N\lambda^N \quad (21.16)$$

Multiplying both sides of Eq. (21.16) by λ give us

$$\lambda S_N = \lambda^2 + 2\lambda^3 + 3\lambda^4 + \dots + (N-1)\lambda^N + N\lambda^{N+1} \quad (21.17)$$

Subtracting Eq. (21.17) from Eq. (21.16) leads to

$$\begin{aligned} (1-\lambda)S_N &= \lambda + \lambda^2 + \lambda^3 + \dots + \lambda^N - N\lambda^{N+1} \\ &= \sum_{n=1}^N \lambda^n - N\lambda^{N+1} \\ &= \sum_{n=0}^N \lambda^n - 1 - N\lambda^{N+1} \end{aligned} \quad (21.18)$$

Substituting Eq. (21.4) into Eq. (21.18) and dividing both sides of the result by $(1-\lambda)$ gives us

$$S_N = \frac{\lambda - [N(1-\lambda) + 1]\lambda^{N+1}}{(1-\lambda)^2} \quad (21.19)$$

Substituting Eq. (21.19) into Eq. (21.15) leads to

$$F = \frac{C_0\lambda[\lambda^{-N} - N(1-\lambda) - 1]}{(1-\lambda)^2} \quad (21.20)$$

Reversing the $\lambda = (1+i)^{-1}$ substitution in Eq. (21.20) yields

$$F = \frac{C_0[(1+i)^{N+1} - i(N+1) - 1]}{i^2} \quad (21.21)$$

21.3.3 Project Evaluation Methods

The total cost of a different project can often be separated into two important categories:

1. Capital expenditure (CapEx).
2. Operating expenses (OpEx).

CapEx typically occurs at the start of a project and mostly includes assets (land, buildings, machines, etc.), which sometimes have a salvage value that can be recovered at the end of the project.

OpEx occur at regular intervals throughout the project and mostly include consumable expenses (wages, maintenance costs, energy, raw materials, etc.).

Different project options will have costs distributed to CapEx and OpEx in different proportions and will therefore be more or less attractive to different organisations, depending on their MARR. Companies with high MARR prefer projects with low CapEx. High CapEx is less of an issue for companies with low MARR and therefore they may prefer an option with a particularly low OpEx.

There are many financial approaches for evaluating different project options. Here we will explore three important measures:

1. Net present value (NPV)
2. Internal rate of return (IRR)
3. Equivalent annual cost (EAC).

21.3.3.1 Net Present Value (NPV)

Net present value (NPV) is often used for comparing different project options in terms of cost and benefit. An important criterion is that a successful project should have a positive NPV for a given MARR.

Consider the following example. A desalination project is required to supply 150 ML day⁻¹ of fresh water to a power station in Abu Dhabi for 25 years. The annual benefit of the project is 57,000,000 USD (US Dollars). The CapEx and annual OpEx for the two options are given in Table 21.3. The CapEx for both projects is assumed salvageable with a depreciation rate of 30%.

Table 21.3 CapEx and annual OpEx values for a desalination project option comparison example

	Option 1	Option 2
Technology	MSF distillation	Reverse osmosis
CapEx (USD)	550,000,000	410,000,000
Annual OpEx (USD)	18,000,000	25,000,000

Table 21.4 NPV for the desalination project options described in Table 21.3

MARR (%)	Option 1	Option 2
1.5	\$258,100,000	\$253,100,000
4	\$59,290,000	\$89,930,000

Challenge 21.5 Determine the NPV for both options and choose which one should be used assuming a MARR of 1.5% and then again assuming a MARR of 4.0%.

The net future cost (NFC) of the project, F , can be determined from a combination of the compound interest formula, Eq. (21.1), and the uniform payment model, Eq. (21.7), as follows

$$F = (A - B) \left[\frac{(1 + i)^N - 1}{i} \right] + I(1 + i)^N - I(1 - d)^N \quad (21.22)$$

where A is the annual OpEx, B is the annual benefit, I is the initial CapEx, i is the MARR, N is the number of years and d is the depreciation rate used to calculate the salvage value.

The net present cost (NPC) of the project, P , is found by substituting Eq. (21.22) into the compound interest formula, Eq. (21.1), to get

$$P = (A - B) \left[\frac{1 - (1 + i)^{-N}}{i} \right] + I \left[1 - \left(\frac{1 - d}{1 + i} \right)^N \right] \quad (21.23)$$

The NPV is equal to the minus of the NPC (i.e., $\text{NPV} = -P$). The resulting NPV for options 1 and 2 assuming a MARR of 1.5% and 4% are given in Table 21.4. When the MARR is 1.5%, Option 1 is preferred and when MARR is 4%, Option 2 is preferred.

Note that MSF distillation only works in this context because the power station is implicitly assumed to provide the necessary thermal energy required for free. Without free thermal energy reverse osmosis is more likely to be a preferable option.

21.3.3.2 Internal Rate of Return (IRR)

A problem with NPV is that it biases towards larger projects and is therefore only suitable for comparing projects of similar size. Where projects of different size are to be compared, an internal rate of return (IRR) comparison may be more useful.

IRR involves iteratively solving for the rate of return that leads to a zero NPC for a given project option. An important criterion is that a successful project should have an IRR greater than or equal to the MARR.

Sometimes people prefer NPV comparisons because they avoid the need for iterative solution.

Challenge 21.6 Determine the IRR of the two desalination options detailed in Table 21.3.

The IRR of the two desalination options detailed in Table 21.3 can be found by searching for a value of i such that P from Eq. (21.23) is equal to zero. This can be done using MATLAB's `fzero` function as follows:

```
B=57e6; %Annual benefit (USD)
N=25; %Number of years
d=0.3; %Depreciation rate
I=550e6; %Initial CapEx (USD)
A=18e6; %Annual OpEx (USD)
MARR=0.015; %Minimum acceptable rate of return
%Find the internal rate of return (IRR)
%using fzero with MARR as an initial guess
FUN=@(i) (A-B)*(1-(1+i)^-N)/i+I*(1-((1-d)/(1+i))^N);
IRR=fzero(FUN,MARR)
```

The MATLAB function, `fzero`, requires an initial estimate of IRR to search from. The MARR under consideration can be a good place to start.

The IRRs for Options 1 and 2 turn out to be 4.99% and 5.98%, respectively. The IRR comparison suggests that Option 2 is better than Option 1. However, this analysis misses the idea that Option 1 gives a better NPV when the MARR is 1.5%.

21.3.4 Equivalent Annual Cost (EAC)

Consider a situation where a sequence of payments are distributed non-uniformly with time over a project lifetime. The equivalent annual cost (EAC) of the project can be determined by evaluating the NFC at the end of the project lifetime, F , and then using Eq. (21.7) to derive an equivalent uniform annual cost, A . EAC is often used to determine when to replace existing machinery and infrastructure.

Consider car ownership. The CapEx is due to the initial purchase of the car. The OpEx includes maintenance costs. As the car gets older it becomes more expensive to maintain due to increasing numbers of components wearing out and requiring replacement. Eventually, maintenance costs become prohibitively expensive and the owner may choose to replace the car with a new model. Nevertheless, the owner will be able to salvage some value from the car at the end of ownership by selling it to a new owner at a reduced price, dictated by the car's depreciation rate. When to replace the car will be dependent on the owner's MARR.

Consider a car purchased for £15,000. The maintenance of the car costs £100 at the end of the first year and doubles every year thereafter. The resale value depreciates at an annual rate of 20%. The car owner has a MARR of 5% (this could be a loan rate for instance).

Challenge 21.7 Determine the EAC of the car assuming the car is resold after 1, 2, 3, 4, 5, 6, 7 and 8 years and select the optimal year to replace the car with a new identical model.

The NFC of the car, F , can be determined from a combination of the compound interest formula, Eq. (21.1), and the exponentially increasing annual payment model, Eq. (21.12), as follows

$$F = I(1+i)^N + C_0 \left[\frac{(1+i)^N - (1+g)^N}{i-g} \right] - I(1-d)^N \quad (21.24)$$

where I is the initial CapEx, i is the MARR, N is the year the car is sold on, C_0 is the annual maintenance cost in the first year, g is the growth rate of the annual maintenance cost and d is the depreciation rate.

The first term in Eq. (21.24) represents the purchase of the car. The second term in Eq. (21.24) represents the total maintenance cost. The final term in Eq. (21.24) represents funds salvaged by reselling the car. The EAC, A , is obtained by substituting Eq. (21.24) into the uniform annual payment model, Eq. (21.7), to get

$$A = A_{\text{cap}} + A_{\text{op}}$$

where A_{cap} and A_{op} are the EAC of the CapEx and OpEx, respectively, found from

$$A_{\text{cap}} = \frac{iI[(1+i)^N - (1-d)^N]}{(1+i)^N - 1}$$

$$A_{\text{op}} = \frac{iC_0}{(1+i)^N - 1} \left[\frac{(1+i)^N - (1+g)^N}{i-g} \right]$$

In our case, $i = 0.05$ (for the MARR), $g = 1$ (for the doubling of the maintenance each year), $d = 0.2$ (for the depreciation), $I = £15000$ (for the purchase cost), $C_0 = £100$ (for the first annual maintenance payment). Corresponding values of A_{cap} , A_{op} and EAC are given in Table 21.5.

The CapEx component of EAC decreases with increasing years of use. In contrast the OpEx component of EAC increases. The overall EAC decreases with increasing years prior to 5 years and then increases with increasing years. The reason is that after 5 years, the rate at which the OpEx contribution increases is greater than the rate at which the CapEx decreases. The best time to sell the car is after 5 years because this gives the lowest overall EAC (£3160). So the car should be replaced after 5 years.

21.3.5 Inflation Rates

The price of goods and services change over time due to changes in the way we value money at a given time. Inflation is when prices go up. Deflation is when prices go down. Usually people measure inflation by comparing the cost of things today with how much they cost a year ago. The average increase in price is known as the inflation rate.

Table 21.5 Equivalent annual cost (EAC) of a car for different replacement times with A_{cap} and A_{op} representing the CapEx and OpEx components, respectively

N (years)	A_{cap}	A_{op}	EAC
1	£3750	£100	£3850
2	£3384	£148.8	£3533
3	£3072	£228.5	£3300
4	£2805	£361.1	£3166
5	£2575	£585.3	£3160
6	£2377	£969.7	£3347
7	£2206	£1637	£3843
8	£2057	£2806	£4863

Inflation occurs when consumers preferentially value goods and services more than money. Deflation occurs when consumers preferentially value money more than goods and services.

High inflation rates are undesirable because they lead to unsustainable price rises and excessive devaluation of savings. As prices go up, consumers purchase goods and services earlier than necessary to avoid future higher prices. This in turn leads to further devaluing of money (since more of it is now available to the market) and hence further inflation.

However, deflation is also undesirable because this leads to consumers seeking to purchase goods and services as late as possible so as to benefit from future lower prices. The associated reduction in consumption is bad for business and can lead to a shrinkage of the economy, referred to as a recession. Recessions are bad because they lead to reduced economic activity, unemployment and poverty.

Most stable nations aim to have a small but stable inflation rate. This encourages people to consume slightly sooner and enables companies to pay higher wages, both of which lead to economic growth. UK monetary policy includes a target of keeping inflation at 2%. The Bank of England (BoE) seeks to control inflation by varying the national interest rate, known as the base rate. If inflation goes over 2%, the BoE increases the base rate making it harder to borrow money for spending on more goods and making it more desirable not to spend savings. If inflation goes below 2%, the BoE decreases the base rate to cause the opposite effect.

At the beginning of 2021, the UK inflation rate was 0.3% and the base rate was 0.1%. To increase the inflation rate, the BoE could reduce the base rate further; then we would be getting into a negative base rate, which could mean you might get paid to borrow money. In 1980, the UK inflation rate was around 18% and the base rate was held at 15% to help reduce inflation; that would have been a difficult time to have a large bank loan.

21.3.5.1 The Effect of Inflation on Purchasing Power

Let C_0 be the price of a chocolate bar today. The inflation rate is f . The price of a chocolate bar next year is therefore $C_0(1 + f)$.

Let M be an amount of money. The number of chocolate bars that can be purchased with M today is $\frac{M}{C_0}$. The number of chocolate bars that can be purchased with M next year is $\frac{M}{C_0(1+f)}$. So the purchasing power of our money has reduced by a factor of $(1 + f)^{-1}$.

Sometimes we talk about how much money from a given year is worth in terms of today's money. For example, let us assume that the inflation rate is 2% and look at how much 1000 GBP₂₀₂₅ is worth in GBP₂₀₂₁. GBP is an acronym for Great Britain Pound. The term 1000 GBP₂₀₂₅ means the purchasing power of £1000 in 2025. The term 1000 GBP₂₀₂₁ means the purchasing power of £1000 in 2021.

The number of years of inflation to consider is 4. Therefore

$$\frac{1000 \text{ GBP}_{2025}}{(1 + 0.02)^4} = 923.85 \text{ GBP}_{2021}$$

Algebraically, the above calculation takes the form

$$\frac{C_n}{(1 + f)^n} = R_n \quad (21.25)$$

where C_n is the value of a payment made in n years time, f is the inflation rate and R_n is the value of C_n in today's money. In this context, C_n is referred to as the “current” value of the payment and R_n is referred to as the “real” value of the payment [4, p. 309].

21.3.5.2 The Effect of Inflation on Real Rate of Return

Consider a sequence of N annual payments, C_n . The NFC of the sequence is found from Eq. (21.2). Combining Eq. (21.2) with the compound interest formula, Eq. (21.1), leads to the following expression for the NPC of the sequence:

$$P = \sum_{n=1}^N \frac{C_n}{(1 + i)^n} \quad (21.26)$$

where i is the rate of return.

In the presence of inflation, C_n represents the value of the annual payment made in the n -th year in terms of the current value of cash in the n -th year. In this context, C_n is referred to as the current annual payment and i is referred to as the current rate of return.

Equation (21.26) can be written in terms of real annual payments, R_n , by substituting Eq. (21.25) to get

$$P = \sum_{n=1}^N \frac{(1 + f)^n R_n}{(1 + i)^n} \quad (21.27)$$

Let us consider an equivalent rate of return, i_R , such that

$$P = \sum_{n=1}^N \frac{R_n}{(1 + i_R)^n} \quad (21.28)$$

Equating Eqs. (21.27) and (21.28) it can be understood that [4, p. 312]

$$i_R = \frac{1 + i}{1 + f} - 1 \quad (21.29)$$

In fact, this equivalent rate of return, i_R , represents the real rate of return.

Suppose an investor wants to achieve a real MARR of i_R and the inflation rate is f , they need to find an investment with a return rate of i that satisfies Eq. (21.29).

21.3.5.3 Exponentially Increasing Annual Payments Revisited

Challenge 21.8 Consider a set of current annual payments that increase with inflation, $C_n = C_0(1 + f)^{n-1}$. Use Eq. (21.8) to obtain an expression for the current NFC of N years of payments, F , assuming a current rate of return, i . Once you have done this, obtain an expression for the real NFC, F_R , written in terms of the real rate of return, i_R . Finally, determine an expression for the NPC of the payment sequence, P , using the current NFC and then the real NFC.

Consider a set of current annual payments that increase with inflation, $C_n = C_0(1 + f)^{n-1}$. Analogous to Eq. (21.12), the current NFC of N years of payments, F , is found from

$$F = C_0 \left[\frac{(1 + i)^N - (1 + f)^N}{i - f} \right] \quad (21.30)$$

Considering Eq. (21.25), the real NFC, F_R , is obtained by dividing Eq. (21.30) by $(1 + f)^N$ to get

$$F_R = \frac{C_0}{(1 + f)^N} \left[\frac{(1 + i)^N - (1 + f)^N}{i - f} \right] \quad (21.31)$$

Substituting Eq. (21.29) into Eq. (21.31) give us

$$\begin{aligned} F_R &= C_0 \left[\frac{(1 + i_R)^N - 1}{i - f} \right] \\ &= C_0 \left[\frac{(1 + i_R)^N - 1}{(1 + i) - (1 + f)} \right] \\ &= \frac{C_0}{1 + f} \left[\frac{(1 + i_R)^N - 1}{i_R} \right] \end{aligned} \quad (21.32)$$

The NPC, P , of the sequence of payments can be found by substituting Eq. (21.30) into Eq. (21.1) with the current rate of return, i , to get

$$P = \frac{F}{(1+i)^N} = C_0 \left[\frac{1 - \left(\frac{1+i}{1+f}\right)^{-N}}{i-f} \right]$$

Alternatively, P can be found by substituting Eq. (21.32) into Eq. (21.1) with the real rate of return, i_R , to get

$$P = \frac{F_R}{(1+i_R)^N} = \frac{C_0}{1-f} \left[\frac{1 - (1+i_R)^{-N}}{i_R} \right] = C_0 \left[\frac{1 - \left(\frac{1+i}{1+f}\right)^{-N}}{i-f} \right]$$

Both approaches lead to identical results.

Interestingly, if we substitute $R_0 = \frac{C_0}{1+f}$ into Eq. (21.32), where R_0 represents the real value of C_0 , we get

$$F_R = R_0 \left[\frac{(1+i_R)^N - 1}{i_R} \right]$$

which is identical in form to the uniform payment model given by Eq. (21.7).

21.3.5.4 Accounting for Inflation in Cash Flow Analysis

There are two ways of accounting for inflation in cash flow analysis [4, p. 316]:

1. Use current values for cash flows and current rates of return.
2. Use real values for cash flows and real rates of return.

Both methods lead to the same NPV. The latter method is often more straightforward to apply. The important thing is not to mix the two approaches.

21.4 Problem Sheet

Problem 21.1 (see Worked Solution 21.1)

A chemical recovery system costs £200,000 and saves £25,000 each year of its ten-year life. The salvage value of the system (i.e., the amount the equipment can be sold for at the end of 10 years) is estimated at £60,000.

- (a) Determine the equivalent annual benefit of the chemical recovery system for a company in the water supply industry.
- (b) Determine the equivalent annual benefit of the chemical recovery system for a company in the consumer electronics industry.

(c) Discuss the difference between the two answers.

Problem 21.2 (see Worked Solution 21.2)

A brewery is planning to construct a private wastewater treatment plant to reduce the cost of their trade effluent. They are considering two schemes. The brewery has a MARR of 5%. Both treatment plants will achieve annual savings of £35,000 and have a design life of 15 years.

Scheme A has an initial CapEx of £270,000, an annual OpEx of £2000 increasing by 15% each year thereafter and a salvage value of £20,000.

Scheme B has an initial CapEx cost of £190,000, an annual OpEx of £1000 increasing by 35% each year thereafter and a salvage value of £15,000.

(a) Determine (i) the net present value, (ii) the equivalent annual benefit and (iii) the internal rate of return for Scheme A.

(b) Determine (i) the net present value, (ii) the equivalent annual benefit and (iii) the internal rate of return for Scheme B.

(c) Recommend your preferred scheme and provide an explanation for your choice.

Problem 21.3 (see Worked Solution 21.3)

The purchase cost of a new water pump is £10,000. The installation cost is £1000. Annual operation and maintenance costs are initially £500 and then increase by £300 per year thereafter. The resell value of the pump depreciates at a rate of 20% per year. The MARR for the company of concern is 10%.

(a) Determine the equivalent annual cost (EAC) of the pump assuming it is replaced after 1, 2, 3, 4, 5, 6, 7, 8, 9 and 10 years and decide (giving explanation) which year would be best to replace it.

(b) The water pump from part (a) is being considered to replace an existing water pump. The existing pump currently has a salvage value of £1000 and will retain this salvage value indefinitely. Operation and maintenance costs are currently £2500 per year and rise by £400 per year. Should the current pump be replaced and if so when?

Problem 21.4 (see Worked Solution 21.4)

A farming cooperative is considering constructing a new irrigation system. The initial CapEx is £200,000 and the annual (current) OpEx is expected to be £2000. The irrigation system is expected to bring £22,000 per year in additional (current) revenue due to better crop production and has an anticipated operation life of 20 years. Determine the real IRR of the project assuming an inflation rate of 3%.

21.5 Worked Solutions

Worked Solution 21.1 (see Problem 21.1)

The NFC of the project, F , can be determined from a combination of the compound interest formula, Eq. (21.1), and the uniform payment model, Eq. (21.7) as follows

$$F = I(1+i)^N - B \left[\frac{(1+i)^N - 1}{i} \right] - S \quad (21.33)$$

where I is the initial cost of the system, i is the MARR, N is the number of years, B is the annual saving and S is the salvage value of the system.

The EAC of the project, A , is found by substituting Eq. (21.33) into Eq. (21.7) to get

$$\begin{aligned} A &= \frac{iF}{(1+i)^N - 1} \\ &= \frac{i}{(1+i)^N - 1} \left\{ I(1+i)^N - B \left[\frac{(1+i)^N - 1}{i} \right] - S \right\} \\ &= \frac{i[I(1+i)^N - S]}{(1+i)^N - 1} - B \end{aligned} \quad (21.34)$$

The equivalent annual benefit (EAB) is equal to the minus of the EAC (i.e., $EAB = -A$). From the information given in Problem 21.1, we have that $I = £200,000$, $S = £60,000$, $B = £25,000$ and $N = 10$.

(a) For a company in the water supply industry we can assume $i = 0.0282$ (see Table 21.2). In this case, $A = -£7046$. So the EAB is £7046.

(b) For a company in the consumer electronics industry we can assume $i = 0.0924$ (see Table 21.2). In this case, $A = £2590$, so there is no net benefit and instead an EAC (including the savings) of £2590.

(c) The results suggest that it is worthwhile investing in the chemical recovery system for a water company but not for an electronics company. The reason is that the savings associated with chemical recovery are presumably not as much as the electronics company can make by investing the same funds into manufacturing more electronic goods.

Worked Solution 21.2 (see Problem 21.2)

Consider the uniform annual payment model, Eq. (21.7), the compound interest formula, Eq. (21.1), and the exponentially increasing annual payment model, Eq. (21.12). The NFC of each scheme after N years, F , can be determined from

$$F = I(1+i)^N + C_0 \left[\frac{(1+i)^N - (1+g)^N}{i-g} \right] - B \left[\frac{(1+i)^N - 1}{i} \right] - S \quad (21.35)$$

Table 21.6 Results for Problem 21.2

	Scheme A	Scheme B
(i) NPV	£44,630	£39,280
(ii) EAB	£4299	£3784
(iii) IRR	7.44%	9.65%

where I is the initial CapEx, i is the MARR, C_0 is the annual OpEx for the first year, g is the growth rate for the OpEx, B is the annual saving and S is the salvage value.

The NPC, P , is obtained by substituting Eq. (21.35) into the compound interest formula, Eq. (21.1), to get

$$P = I + C_0 \left[\frac{1 - \left(\frac{1+g}{1+i} \right)^N}{i-g} \right] - B \left[\frac{1 - (1+i)^{-N}}{i} \right] - S(1+i)^{-N} \quad (21.36)$$

The NPV = $-P$.

The EAC, A , is obtained from P by substituting Eq. (21.1) into the uniform payment model, Eq. (21.7), to get:

$$A = P \left[\frac{i}{1 - (1+i)^{-N}} \right] \quad (21.37)$$

The EAB = $-A$.

The internal rate of return (IRR) is obtained by finding a value of i such that $P = 0$. This can be achieved (with values from Problem 21.2(a) using MATLAB's solver, `fzero`, with the following code:

```
B=35000; %Annual saving (GBP)
N=15; %Number of years
MARR=0.05; %Minimum annual rate of return
I=270000; %Initial CapEx (GBP)
C0=2000; %Initial annual OpEx (GBP)
g=0.15; %OpEx growth rate
S=20000; %Salvage value (GBP)
%Find the internal rate of return (IRR)
%using fzero with MARR as an initial guess
FUN=@(i) I+C0*(1-((1+g)/(1+i))^N)/(i-g)...
-B*(1-(1+i)^-N)/i-S/(1+i)^N;
IRR=fzero(FUN,MARR)
```

The results for part (a) and (b) are given in Table 21.6.

(c) Although Scheme B has a higher IRR, Scheme A should be chosen because this has a higher NPV and EAB when considering the MARR of the organisation.

Worked Solution 21.3 (see Problem 21.3)

The operation and maintenance costs, C_n , are best dealt with by splitting them into two parts, a uniform annual cost, A_A , and a linearly increasing annual cost, nA_B , such that $C_n = A_A + nA_B$. Considering the compound interest formula, Eq. (21.1), the uniform annual payment model, Eq. (21.7), and the linearly increasing annual payment cost model, Eq. (21.21), the NFC of the project is found from

$$F = (I_A + I_B)(1+i)^N + A_A \left[\frac{(1+i)^N - 1}{i} \right] + \frac{A_B[(1+i)^{N+1} - i(N+1) - 1]}{i^2} - I_A(1-d)^N \quad (21.38)$$

where I_A is the purchase cost, I_B is the installation cost, i is the MARR, N is the number of years and d is the depreciation rate associated with the salvage value of the items initially purchased.

The EAC, A , is obtained by substituting Eq. (21.38) into Eq. (21.7) and solving for A to get

$$A = A_A + \frac{A_B[(1+i)^{N+1} - i(N+1) - 1] + i^2[(I_A + I_B)(1+i)^N - I_A(1-d)^N]}{i[(1+i)^N - 1]} \quad (21.39)$$

(a) The EAC of the new pump, if it is replaced after 1, 2, 3, 4, 5, 6, 7, 8, 9 and 10 years, is found using Eq. (21.39). From the information about the new water pump given in Problem 21.3a: $I_A = £10,000$, $I_B = £1,000$, $A_A = 500 - 300 = £200$, $A_B = £300$, $d = 0.2$, $i = 0.1$ and $N = 1, 2, 3, \dots, 10$ years. EAC values for the new pump are shown in Table 21.7. The best time to replace the pump is after 8 years because this gives the minimum EAC, which is £3317. Note that this means the EAC of the water pump is £3317 for each year providing the pump is replaced after 8 years.

(b) The EAC for continuing to use the old pump can also be found using Eq. (21.39). From the information given about the existing pump: $I_A = £1000$, $I_B = £0$, $A_A = 2500 - 400 = £2100$, $A_B = £400$, $d = 0$, $i = 0.1$ and $N = 1, 2, 3, \dots, 10$ years. EAC values for the existing pump are also shown in Table 21.7. The EAC for using the existing pump for four years is £3152, which is less than the optimal EAC for the new pump, which is £3317. The EAC for using the existing pump for five years is £3324, which is greater than the optimal EAC for the new pump. Therefore the existing pump should be replaced by the new pump after four years.

Worked Solution 21.4 (see Problem 21.4)

The real IRR can be determined from the current IRR using Eq. (21.29). The current IRR can be determined by determining the IRR using all current prices.

Table 21.7 Comparison of equivalent annual cost for an old and new water pump (see Problem 21.3)

N (years)	(a) EAC new pump	(b) EAC old pump
1	£4600	£2600
2	£3933	£2790
3	£3657	£2975
4	£3502	£3152
5	£3408	£3324
6	£3353	£3489
7	£3325	£3649
8	£3317	£3802
9	£3323	£3949
10	£3340	£4090

Considering the uniform annual payment model, Eq. (21.7), and the compound interest formula, Eq. (21.1), the NFC (current) of the project, F , can be determined from

$$F = I(1+i)^N + (A - B) \left[\frac{(1+i)^N - 1}{i} \right] \quad (21.40)$$

where I is the initial CapEx, i is the current IRR, N is the number of years the project runs for, A is the annual (current) OpEx and B is the annual (current) benefit. The NPC, P , is found by substituting Eq. (21.40) into Eq. (21.1) to get

$$P = I + (A - B) \left[\frac{1 - (1+i)^{-N}}{i} \right] \quad (21.41)$$

From the information given in Problem 21.4, we have that $I = £200,000$, $A = £2000$, $B = £22,000$ and $N = 20$ years. The current IRR, i , is found by iterative solution of the above equation with $P = 0$. We will arbitrarily consider an initial guess for i of 0.02. The exact value of the current IRR can then be obtained from the following MATLAB code:

```
I=200000; %Initial CapEx (GBP)
A=2000; %Annual OpEx (GBP)
B=22000; %Annual benefits (GBP)
N=20; %Number of years
i0=0.02; %Initial guess for IRR
%Find current internal rate of return (IRR)
IRR=fzero(@(i) I+(A-B)*(1-(1+i)^-N)/i,i0)
```

This gives a current IRR, $i = 0.07755$ or 7.76%.

The real IRR, i_R , is found from Eq. (21.29). Given that the inflation rate, $f = 0.03$ it follows that the real IRR is 0.04616 or 4.62%.

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Abstract

This chapter develops simple mathematical methods to explore the concepts of market efficiency and environmental externalities. The concepts of marginal cost, consumer surplus, producer surplus and social surplus are introduced. Linear supply and demand schedules are used to derive equilibrium conditions for monopoly controlled and competitive markets. A Pigouvian tax is derived to force market efficiency in the presence of external costs. A range of relevant environmental policy options are discussed including private ownership, command control regulation and pollution permit trading. Linear abatement cost models are used to demonstrate the equimarginal principle of optimality. Practical applications are presented through a problem sheet with worked solutions.

Notation

A	Abatement quantity.
A_i	Abatement quantity for the i th polluter.
A_t	Total abatement quantity of a collective.
c_{ai}	MAC schedule constant parameter for the i th polluter.
c_c	Demand schedule constant parameter.
c_p	Supply schedule constant parameter.
m_{ai}	MAC schedule gradient parameter for the i th polluter.
m_c	Demand schedule gradient parameter.
m_e	Marginal external cost gradient parameter.
m_p	Supply schedule gradient parameter.
p_{ai}	Marginal abatement cost (MAC) for the i th polluter.
p_c	Marginal benefit of consuming another unit of a commodity.
p_{co}	Optimal marginal benefit of consuming another unit of a commodity.
p_e	Marginal external cost associated with the production of a commodity.
p_p	Marginal cost of producing another unit of a commodity.

p_{po}	Optimal marginal cost of producing another unit of a commodity.
p_t	Pigouvian tax.
q	Quantity of a commodity.
S_{ai}	Total abatement cost for the i th polluter.
S_{as}	Actual social surplus.
S_{at}	Total abatement cost for the collective.
S_c	Consumer surplus.
S_e	Total cost an externality.
S_p	Producer surplus.
S_s	Social surplus.
δS_{as}	Dead-weight loss.

22.1 Introduction

In Chap. 3 we looked at the problem of common-pool resources and public goods and learnt about how conventional cash flow analysis is often used to compare the benefits of different engineering project options. Incorporation of common-pool resources and public goods requires methodologies for quantifying their value, which is the focus of the next chapter. A necessary prerequisite includes an understanding of market efficiency.

The first part of this chapter looks at supply and demand modelling. Mathematical definitions for producer, consumer and social surplus are provided; these are explicitly used in the next chapter to quantify environmental benefits. Equilibrium conditions for monopoly controlled and competitive markets are derived using simple linear models. It is then explained how externalities lead to market inefficiencies and a “Pigouvian tax” is derived to force efficiency by reducing supply.

The second part of this chapter looks at alternative environmental policy options for improving market efficiency. First we discuss the benefits of private ownership. We then look at command and control regulations including ambient standards, emission standards and technology standards. Finally we look at how increased cost effectiveness can be achieved using pollution permit trading and the equimarginal principle of optimality.

22.2 Modelling Supply and Demand

The supply of a commodity, in this context, refers to the quantity of a commodity, q , that a producer is willing to sell at a given price, p_p [1, p. 60]. As the price of a commodity increases, producers will be willing to supply more of that commodity. The relationship between supply and price is referred to as a supply schedule. The supply price is a measure of the marginal cost of producing another unit of the commodity.

The demand of a good is the quantity of a commodity, q , that a consumer is willing to buy at a given price, p_c [1, p. 55]. As the price of a commodity is increased, the demand for the commodity will generally decrease. The relationship between demand and price is referred to as a demand schedule. The demand price is a measure of the marginal benefit associated with consuming another unit of the commodity.

22.2.1 Producer, Consumer and Social Surplus

Producer surplus, S_p , represents the total profit available to a producer for a given commodity when it is supplied at a quantity, q [1, p. 62]. Consumer surplus, S_c , represents the total benefit available to a consumer for a given commodity when it is supplied at a quantity, q [1, p. 56]. Both quantities can be illustrated as shaded areas on a combined plot of the supply and demand schedules (see Fig. 22.1).

The producer surplus, S_p , and consumer surplus, S_c , are described by the following integral equations:

$$S_p = p_c q - \int_0^q p_p dq \quad (22.1)$$

$$S_c = \int_0^q p_c dq - p_c q \quad (22.2)$$

The social surplus, $S_s = S_c + S_p$, represents the total benefit to society that can be derived from a given commodity when it is supplied at a quantity, q [1, p. 62].

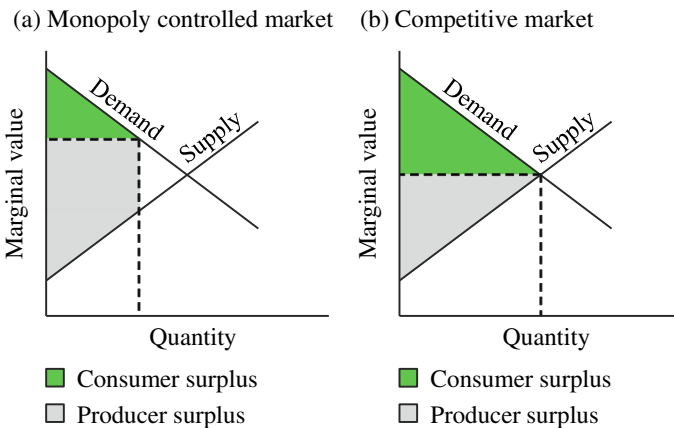


Fig. 22.1 Schematic diagram illustrating consumer and producer surplus as shaded areas on a combined plot of supply and demand schedules. **a** Supply is controlled by a monopoly. **b** Supply is dictated by a competitive market

22.2.2 Linear Supply and Demand Schedules

Many different functional forms can be used to represent supply and demand schedules. For simplicity we will limit ourselves to the following linear functions for the supply schedule and demand schedule, respectively:

$$p_p = c_p + m_p q \quad (22.3)$$

$$p_c = c_c - m_c q \quad (22.4)$$

where c_p , m_p , c_c and m_c are empirical parameters that can be obtained by linear regression with relevant survey data.

Challenge 22.1 Use linear supply and demand schedules to derive closed-form expressions for the producer surplus, consumer surplus and social surplus, in terms of q .

Closed form expressions for the producer and consumer surplus can be found by substituting Eqs. (22.3) and (22.4) into Eqs. (22.1) and (22.2), respectively, to get

$$\begin{aligned} S_p &= (c_c - m_c q)q - \int_0^q (c_p + m_p q) dq \\ &= (c_c - c_p)q - \left(m_c + \frac{m_p}{2}\right) q^2 \end{aligned} \quad (22.5)$$

and

$$\begin{aligned} S_c &= \int_0^q (c_c - m_c q) dq - (c_c - m_c q)q \\ &= \frac{m_c q^2}{2} \end{aligned} \quad (22.6)$$

For the social surplus

$$\begin{aligned} S_s &= S_p + S_c \\ &= (c_c - c_p)q - (m_c + m_p) \frac{q^2}{2}. \end{aligned} \quad (22.7)$$

22.2.3 Monopoly Controlled Market

A pure monopoly occurs when there is only one organisation producing a certain commodity. Such a producer will naturally seek to maximise their profit [1, p. 125].

Challenge 22.2 Determine an expression for q that maximises the producer surplus, S_p . Following on from this determine simplified expressions for the corresponding supply price, demand price, producer surplus, consumer surplus and social surplus.

Differentiating Eq. (22.5) with respect to q leads to

$$\frac{dS_p}{dq} = (c_c - c_p) - (2m_c + m_p)q \quad (22.8)$$

It is clear that the derivative of Eq. (22.8) will be negative for positive q . Therefore S_p will be maximised when $\frac{dS_p}{dq} = 0$. It follows that an expression for q that maximises S_p is

$$q = \frac{c_c - c_p}{2m_c + m_p} \quad (22.9)$$

Substituting Eq. (22.9) into Eqs. (22.3) and (22.4) leads to the following expressions for the corresponding supply and demand prices:

$$p_p = \frac{2m_c c_p + m_p c_c}{2m_c + m_p} \quad (22.10)$$

$$p_c = \frac{m_c(c_c + c_p) + m_p c_c}{2m_c + m_p} \quad (22.11)$$

Generally speaking, $c_c > c_p$. Not surprisingly, Eqs. (22.10) and (22.11), therefore tell us that maximising profit generally requires the supply price to be less than the demand price.

Substituting Eq. (22.9) into Eqs. (22.5)–(22.7) leads to the following expressions for the corresponding producer, consumer and social surpluses:

$$S_p = \frac{(c_c - c_p)^2}{2(2m_c + m_p)} \quad (22.12)$$

$$S_c = \frac{m_c}{2} \left(\frac{c_c - c_p}{2m_c + m_p} \right)^2 \quad (22.13)$$

$$S_s = \frac{(3m_c + m_p)}{2} \left(\frac{c_c - c_p}{2m_c + m_p} \right)^2 \quad (22.14)$$

The producer and consumer surpluses for a monopoly controlled market are illustrated graphically as shaded areas in Fig. 22.1a.

22.2.4 Competitive Market

When a market is truly competitive, the supply should exactly equal demand. The reason is that if there are enough producers, they will continue to produce until the marginal cost of production becomes greater than the marginal benefit associated with consuming another unit of the commodity [1, p. 63]. Whereas monopolies maximise producer profit, competitive markets tend to maximise social surplus.

Challenge 22.3 Determine an expression for q that maximises the social surplus, S_s . Following on from this determine simplified expressions for the corresponding supply price, demand price, producer surplus, consumer surplus and social surplus.

Differentiating Eq. (22.7) with respect to q leads to

$$\frac{dS_s}{dq} = (c_c - c_p) - (m_c + m_p)q \quad (22.15)$$

It is clear that the derivative of Eq. (22.15) will be negative for positive q . Therefore S_s will be maximised when $\frac{dS_s}{dq} = 0$. It follows that an expression for q that maximises S_s is

$$q = \frac{c_c - c_p}{m_c + m_p} \quad (22.16)$$

Given that all the coefficients are positive it can be understood that the q from Eq. (22.16) is greater than the q from Eq. (22.9), when the producer surplus is maximised.

Substituting Eq. (22.16) into Eqs. (22.3) and (22.4) leads to the following expressions for the corresponding supply and demand prices:

$$p_p = \frac{m_c c_p + m_p c_c}{m_c + m_p} \quad (22.17)$$

$$p_c = \frac{m_c c_p + m_p c_c}{m_c + m_p} \quad (22.18)$$

It can be seen that maximising the social surplus leads to the supply and demand prices being equal, which is a key characteristic of a competitive market.

Substituting Eq. (22.16) into Eqs. (22.5), (22.6) and (22.7) leads to the following expressions for the corresponding producer, consumer and social surpluses:

$$S_p = \frac{m_p}{2} \left(\frac{c_c - c_p}{m_c + m_p} \right)^2 \quad (22.19)$$

$$S_c = \frac{m_c}{2} \left(\frac{c_c - c_p}{m_c + m_p} \right)^2 \quad (22.20)$$

$$S_s = \frac{(c_c - c_p)^2}{2(m_c + m_p)} \quad (22.21)$$

The producer and consumer surpluses for a competitive market are illustrated graphically as shaded areas in Fig. 22.1b. The producer surplus given by Eq. (22.19) is less than that given by Eq. (22.14), when the producer profit was maximised. However, both the consumer surplus and social surplus given by Eqs. (22.20) and (22.21) are greater than those given by Eqs. (22.13) and (22.14).

Our analysis demonstrates that monopolies preferentially benefit producers whereas competitive markets benefit both the consumer and society as a whole. Consequently national governments often concern themselves with breaking up monopolies and encouraging the development of competitive markets.

22.2.5 Market Efficiency and Externalities

In the previous section we established that maximising producer profit does not lead to optimal social surplus and that a characteristic of maximised social surplus is that supply equals demand. Maximising producer profit is likely to happen when the market is controlled by a monopoly. Maximising social welfare is likely to happen when the market is competitive. When the social surplus is optimised the market is said to be efficient [2, p. 61].

The problem with most so-called competitive markets is that they often only consider private benefits and private costs. There are often external benefits and external costs that are unaccounted for. These are referred to as externalities. When externalities are unaccounted for the market is inefficient and social welfare is not maximised [2, p. 66].

Let p_e be the marginal external cost associated with the production of the commodity described in the previous section. Assuming again a linear function of q

$$p_e = m_e q \quad (22.22)$$

where m_e is another parameter.

The total cost of the externality, S_e (analogous to a surplus term), in this case is found by integrating to get

$$S_e = \int_0^q p_e dq = \frac{m_e q^2}{2}. \quad (22.23)$$

22.2.5.1 Competitive Market That Ignores Externalities

Suppose a competitive market operates without knowledge of this externality and reaches the equilibrium quantity given by Eq. (22.16). The apparent social surplus is given by Eq. (22.21). However, substituting Eq. (22.16) into Eq. (22.23) gives that the total cost of the externality will be

$$S_e = \frac{m_e}{2} \left(\frac{c_c - c_p}{m_c + m_p} \right)^2 \quad (22.24)$$

The actual (i.e., accounting for the externality) social surplus, S_{as} , is found from

$$S_{as} = S_s - S_e = \frac{1}{2} \left(\frac{c_c - c_p}{m_c + m_p} \right)^2 (m_c + m_p - m_e) \quad (22.25)$$

22.2.5.2 Efficient Market That Considers Externalities

This competitive market described above is not the most efficient solution. The actual social surplus can be maximised by forcing $p_c = p_p + p_e$. The quantity that this occurs is

$$q = \frac{c_c - c_p}{m_c + m_p + m_e} \quad (22.26)$$

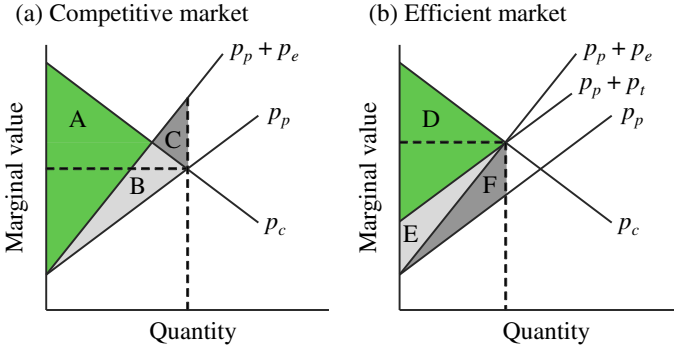


Fig. 22.2 Schematic diagram illustrating social surplus in the presence of an externality. The line, p_c , represents the marginal benefit of consumption. The line, p_p , represents the the marginal cost of production excluding the externalities. The line, $p_p + p_e$, represents the the marginal cost of production including the externalities. The line, $p_p + p_t$, represents the marginal cost of production plus a constant Pigouvian tax designed to force the market to an efficient equilibrium. **a** A competitive market that ignores externalities. **b** An efficient market that accounts for externalities using a Pigouvian tax

and the actual social surplus is

$$S_{as} = \frac{(c_c - c_p)^2}{2(m_c + m_p + m_e)} \quad (22.27)$$

The above result is shown graphically in Fig. 22.2a. The actual social surplus for an efficient market (i.e., $p_c = p_p + p_e$) is shown as the green triangle labelled A. The apparent social surplus for a competitive market that ignores externalities ($p_c = p_p$), is represented by the combined area of triangles A and B.

22.2.5.3 Dead-Weight Loss

The difference between the actual social surplus that arises by markets that consider or ignore externalities is known as a dead-weight loss [3, p. 49]. The dead-weight loss, δS_{as} , for the scenario described above is found by subtracting Eq. (22.25) from Eq. (22.27):

$$\begin{aligned} \delta S_{as} &= \frac{(c_c - c_p)^2}{2(m_c + m_p + m_e)} - \frac{1}{2} \left(\frac{c_c - c_p}{m_c + m_p} \right)^2 (m_c + m_p - m_e) \\ &= \frac{m_e^2}{2(m_c + m_p + m_e)} \left(\frac{c_c - c_p}{m_c + m_p} \right)^2 \end{aligned} \quad (22.28)$$

The dead-weight loss is represented graphically in Fig. 22.2a as the dark grey triangle, labelled C. It can now be understood that the actual social surplus for a competitive market (i.e., $p_c = p_p$) is represented by the area of triangle A minus the area of triangle C.

22.2.5.4 Pigouvian Tax

The British economist, Pigou, proposed that this dead-weight loss to society can be reduced by charging the producers a tax, now referred to as a Pigouvian tax.

Challenge 22.4 For the supply, demand and externality schedules, given by Eqs. (22.3), (22.4) and (22.22), respectively, determine an optimal Pigouvian tax such that there is zero dead-weight loss when the market is competitive.

The optimal price, p_{co} , for a product, including a Pigouvian tax, is found by substituting Eq. (22.26) into the demand schedule, Eq. (22.4), to get

$$p_{co} = c_c - \frac{m_c(c_c - c_p)}{m_c + m_p + m_e}$$

The marginal cost of production at this quantity, p_{po} , is found by substituting Eq. (22.26) into the supply schedule, Eq. (22.3):

$$p_{po} = c_p + \frac{m_p(c_c - c_p)}{m_c + m_p + m_e}$$

The optimal Pigouvian tax, p_t , is therefore found from

$$\begin{aligned} p_t &= p_{co} - p_{po} \\ &= \frac{m_e(c_c - c_p)}{m_c + m_p + m_e} \end{aligned} \quad (22.29)$$

The good thing about the Pigouvian tax is that it forces a reduction in production to the efficient level [3, p. 100]. This idea is shown graphically in Fig. 22.2b. In this case, the actual social surplus is found from the combined areas of triangles D and E, which will be equal to the area of triangle A in Fig. 22.2a. The total tax collected is shown by the combined area of triangles E and F. Triangle F represents the portion of tax payment that compensates for the external costs. Triangle E contributes towards the total social surplus.

There are at least two issues, leading to Pigouvian tax not being generally favoured by economists. The first issue concerns the difficulty in correctly quantifying marginal external cost. The second issue is the implicit assumption that externalities can only be reduced by directly reducing the production of the commodity of concern [3, p. 101]. Pigouvian tax does not allow for the possibility of abating (reducing or removing) external costs by changing the production process (introducing carbon capture and storage, increasing water efficiency etc.).

22.3 Environmental Policy Options

Alternative policy options for regulating environmental pollution include private ownership, command and control regulation and pollution permit trading.

22.3.1 Private Ownership

The Coase Theorem (attributed to British economist, Ronald Coase) states that as long as a good is properly and completely owned by an organisation or individual, an efficient market equilibrium will arise, even in the presence of externalities, regardless of whom owns the good [2, p. 193].

22.3.1.1 An Example Using a Lake

As an example, let us consider a paper factory discharging wastewater into a lake, which is also enjoyed by an angling club. The wastewater from the factory will be high in biochemical oxygen (BOD) and an increase in BOD in the lake will lead to a reduction in the fish population.

Nobody owns the lake If nobody owns the lake, the factory will likely discharge untreated wastewater without cost and save money on wastewater treatment, which in turn reduces the marginal cost of paper production and leads to a higher quantity of paper being produced. Meanwhile the fish will die due to high levels of BOD and the angling club will lose out.

The angling club owns the lake If the angling club own the lake they may at first prohibit discharge of wastewater from the paper factory. However, the factory will offer payment to the club to allow them to discharge wastewater. Providing the club properly understands the marginal benefit of catching the next fish, they will be able to negotiate the maximum possible wastewater discharge licence such that the tariff for waste disposal is just high enough to forfeit the next fish they wanted to catch and just low enough such that the factory is not better off treating an extra load of wastewater using a private wastewater treatment plant. In this way, an efficient market equilibrium should be reached.

The factory owns the lake If the factory owns the lake, they may at first discharge all of their wastewater without regard to the fish population. However, the angling club may choose to pay the factory to fish in the lake. In that case, as long as the tariff for the next fish caught is higher than the marginal cost of treating another unit of wastewater, the factory will continue to treat more wastewater. In this way, an efficient market equilibrium should also be reached.

Other parties concerned with the lake Suppose other interested groups are concerned about additional externalities due to the wastewater discharge. They too should be able to negotiate with whoever owns the lake such that they can pay the appropriate price to have their interest properly protected.

22.3.1.2 Important Assumptions

Important assumptions include [2, p. 193]:

1. Property rights must be well defined, enforceable and transferable.
2. An efficient and competitive system must be available that allows stakeholders to negotiate about how an environmental asset will be used.
3. A complete set of markets must be present that capture all social values associated with the environmental asset.
4. Transaction costs, associated with the negotiations, must be small compared to economic benefits.

22.3.2 Command and Control Regulation

Command and control environmental regulations typically take the form of standards, which state some idea about how things should be. Field and Field [2, p. 203] distinguish between three different types of standard: (1) ambient standards, (2) emission standards and (3) technology standards.

22.3.2.1 Ambient Standards

Ambient standards are used to specify limits on how the environment more broadly should be. Ambient standards might include maximum limits on pollutants such as nitrogen dioxide or minimum levels of dissolved oxygen in rivers and lakes. The EU Water Framework Directive comprises many ambient standards and aims for 'good status' for all ground and surface waters in the EU.

Ambient standards cannot be enforced directly. Instead additional emission standards are required that collectively lead to ambient quality levels. Ambient standards often refer to average quantities such that short-term ambient quality levels may be worse than the standard qualities as long as they are not persistent and are balanced by periods when the ambient quality is better than that specified by the standard [2, p. 203].

22.3.2.2 Emission Standards

Emission standards target specific sources of pollution and might include limits on pollutants leaving the flue gas of a factory or power station or limits on contaminants dissolved in wastewater effluents that are discharged to natural watercourses [2, p. 204]. The EU Urban Waste Water Treatment Directive comprises many emission standards and aims to "to protect the environment from the adverse effects of urban waste water discharges and discharges from certain industrial sectors". Organisations can decide for themselves how they plan to meet emission standards, whether it is through changes in production process or application of treatment works. Nevertheless, emission standards can be enforced directly by government agencies and there are penalties for non-compliance.

22.3.2.3 Technology Standards

Technology standards seek to reduce pollution by enforcing the use of a specific technology where a pollutant is likely to be produced [2, p. 205]. For example, vehicles in the UK are legally required to use catalytic converters to reduce carbon monoxide production. The disadvantage of technology standards over emission standards is that they limit the ability for organisations to innovate more economic solutions.

22.3.2.4 Disadvantage of Command and Control Regulation

Command and control regulations tend not to be cost effective due to an inability to recognise that abatement costs (cost of reducing emissions) are not uniform across polluting sectors [3, p. 92]. For example, cost of CO₂ capture from steel works, power stations and fertiliser plants vary considerably. With a uniform standard on emission levels, different sectors will target the same level regardless of cost when instead it would be economically beneficial to focus on reducing emissions more where it is cheaper.

22.3.3 Pollution Permit Trading

An alternative approach is for governments to decide how much pollution they are willing to tolerate at a regional scale and then to distribute tradable permits, to emit that pollution, to organisations of concern [2, p. 246]. Organisations can choose to:

1. Use their permits and invest in abatement strategies to eliminate additional emissions.
2. Buy more permits to reduce the cost of abatement.
3. Sell their permits and reduce their emissions further by abatement.

Whether organisations will choose to buy or sell pollution permits will depend on the market price of the permits and their marginal cost of abatement.

Many such schemes have been set up to control greenhouse gas emissions including the EU Emission Trading Scheme, the UK Emission Trading Scheme and the California Trading Program. Similar trading schemes have also been used to manage waterborne mercury (San Francisco Bay Offset Program), waterborne nutrients (nitrogen and phosphorous) (Chesapeake Bay Agreement) and acres of wetlands (Ohio Wetlands Mitigation Program) [2, p. 250].

22.3.3.1 Equimarginal Principle of Optimality

The equimarginal principle of optimality states that if each polluter were to abate to the point where the corresponding level of marginal abatement cost (MAC) is equal across firms, the targeted environmental standard would have been met at minimum cost [3, p. 93].

To explore this idea further let us consider two polluters characterised by the following two linear MAC schedules:

$$p_{a1} = c_{a1} + m_{a1}A \quad (22.30)$$

$$p_{a2} = c_{a2} + m_{a2}A \quad (22.31)$$

where p_{a1} and p_{a2} are the MACs for Polluter 1 and Polluter 2, respectively, at an abatement level of A , and c_{a1} , m_{a1} , c_{a2} and m_{a2} are empirical parameters characterising the linear MAC schedules.

Suppose that a total abatement of $A_t = A_1 + A_2$ is required where A_1 is the abatement level to be achieved by Polluter 1 and A_2 is the abatement level to be achieved by Polluter 2. The total abatement costs for each polluter, S_{a1} and S_{a2} are found from:

$$S_{a1} = \int_0^{A_1} p_{a1} dA \quad (22.32)$$

$$S_{a2} = \int_0^{A_2} p_{a2} dA \quad (22.33)$$

The total abatement cost for the collective as a whole, $S_{at} = S_{a1} + S_{a2}$.

Substituting the MAC schedules, Eqs. (22.30) and (22.31), into Eqs. (22.32) and (22.33) leads to:

$$S_{a1} = c_{a1}A_1 + \frac{m_{a1}A_1^2}{2}$$

$$S_{a2} = c_{a2}A_2 + \frac{m_{a2}A_2^2}{2}$$

The total abatement cost for the collective as a whole is therefore

$$S_{at} = c_{a1}A_1 + \frac{m_{a1}A_1^2}{2} + c_{a2}A_2 + \frac{m_{a2}A_2^2}{2}$$

Recall that $A_t = A_1 + A_2$ therefore

$$S_{at} = c_{a1}A_1 + \frac{m_{a1}A_1^2}{2} + c_{a2}(A_t - A_1) + \frac{m_{a2}(A_t - A_1)^2}{2} \quad (22.34)$$

Differentiating the Eq. (22.34) with respect to A_1 leads to

$$\frac{dS_{at}}{dA_1} = c_{a1} + m_{a1}A_1 - c_{a2} - m_{a2}(A_t - A_1) \quad (22.35)$$

It is clear that the derivative of Eq. (22.35) will be positive for positive A_1 . Therefore S_{at} will be minimised when $\frac{dS_{at}}{dA_1} = 0$. Given that $A_t = A_1 + A_2$, it follows that S_{at} is minimised when

$$c_{a1} + m_{a1}A_1 - c_{a2} - m_{a2}A_2 = 0 \quad (22.36)$$

Substituting Eqs. (22.30) and (22.31) into Eq. (22.36) reveals that S_{at} is minimised when

$$p_{a1} = p_{a2}$$

which satisfies the equimarginal principle of optimality.

22.4 Problem Sheet

Problem 22.1 (see Worked Solution 22.1)

Consumers are willing to buy 4 bottles of Durham ale per week at £1.25 per bottle. At £1.75 per bottle they are likely only to buy 2 bottles per week.

(a) Assuming there are 10,000 regular real ale drinkers in county Durham, determine a linear demand schedule that approximates demand for bottles of Durham ale each year.

(b) The annual supply schedule for Durham ale is described by $p_p = 0.60 + 3.1 \times 10^{-7}q$ where p_p is in GBP (Great Britain Pounds) and q is number of bottles of beer produced in a year.

(i) Determine the equilibrium demand price, producer surplus and social surplus assuming only one brewery exists in county Durham. Also determine how many bottles of beer the average drinker will consume each week.

(ii) Determine the equilibrium demand price, producer surplus and social surplus assuming that multiple breweries exist and there is a competitive market producing Durham beer. Also determine how many bottles of beer the average drinker will consume each week.

(c) There are many externalities associated with alcohol consumption relating to healthcare, policing, social services and loss in productivity. Suppose that the external cost of drinking, $p_e = 1.2 \times 10^{-6}q$. Determine the actual social surplus that is obtained by a competitive market.

(d) Determine an appropriate Pigouvian tax along with the actual social surplus once it is applied to a competitive market and the dead-weight loss that occurs if the externalities are ignored. Also determine the efficient equilibrium cost of a bottle of beer and the number of bottles an average drinker will consequently consume each week.

Problem 22.2 (see Worked Solution 22.2)

A car factory in Tyne and Wear releases pollution into a nearby wetland and the consequential loss of biodiversity is not considered in the private market. The supply and demand of the cars produced is modelled by:

$$p_p = 10,200 + 0.0036q \quad \text{and} \quad p_c = 12,000$$

where p_p is the marginal cost of producing a car (in GBP), p_c is the marginal benefit of owning a car (in GBP) and q is the number of cars being produced. It is assumed that the car factory is not big enough to affect the demand of cars.

Currently the factory produces 450,000 cars per year. They would like to expand their plant to maximise their profit. The annual marginal cost of biodiversity destruction in the wetland, p_e , (in GBP) is modelled by

$$p_e = 0.0004q$$

The car factory owns the right to pollute the wetland as they wish (this is fiction of course). An international environmental protection group is planning to negotiate with the car factory to halt plant expansion and conserve existing biodiversity.

- (a) Determine the minimum annual payment the factory would be willing to accept to halt further expansion.
- (b) Determine the maximum annual tariff an environmental protection group would be willing to pay to prevent further pollution.

Problem 22.3 (see Worked Solution 22.3)

The local authority at Teeside is seeking to halve CO₂ emissions from major industrial sources. A local fertilizer plant emits 1.2 Mt CO₂ per year whilst a nearby steel works emits 1.0 Mt CO₂ per year. The following marginal abatement cost (MAC) functions apply:

$$p_{a1} = 50 + 20 \times 10^{-6}A \quad \text{and} \quad p_{a2} = 70 + 30 \times 10^{-6}A$$

where p_{a1} represents the MAC for the fertilizer plant (in GBP), p_{a2} represents the MAC for the steel works (in GBP) and A is the quantity of CO₂ emissions that has been abated (in tonnes).

- (a) Determine the total annual abatement cost if both the fertilizer plant and the steel works each reduce their own CO₂ emissions by 50%.
- (b) Determine the minimum possible total abatement cost if the fertilizer plant and the steel works collaboratively reduce their CO₂ emissions as a collective.
- (c) The local authority plan to incentivise CO₂ reduction by allocating a set of tradable CO₂ emission permits worth 10 kt CO₂ each. The fertilizer plant and steel works are allocated 60 and 50 permits, respectively. Determine the number of permits the fertilizer plant is likely to sell to the steel works and the range of payment likely to be made.

22.5 Worked Solutions

Worked Solution 22.1 (see Problem 22.1)

(a) Let q_i be the number of bottles of Durham ale consumed by a Durham beer drinker in a week at a price, p_c per bottle. Assuming a linear demand schedule

$$q_i = a + bp_c$$

Given the information about beer drinking behaviour, $4 = a + 1.25b$ and $2 = a + 1.75b$. It follows that $a = 9$ and $b = -4$. Given that there are 52 weeks in a year and 10,000 consumers, it follows that the number of bottles of beer that will be drunk in a year, q , at a price p_c , is found from

$$q = 52 \times 10,000 \times q_i = 5.2 \times 10^5 \times (9 - 4p_c)$$

Solving for p_c then leads to

$$p_c = 2.25 - 4.808 \times 10^{-7} q$$

(b) (i) If there is only one brewery, they will have a monopoly on the market and will restrict supply such that their profit is maximised. The equilibrium demand price, p_{ce} , producer surplus, S_p , and social surplus, S_s , will therefore be found from Eqs. (22.11), (22.12) and (22.14).

From the originally given information and the answer to part (a) above, $c_c = 2.25$, $m_c = 4.808 \times 10^{-7}$, $c_p = 0.60$ and $m_p = 3.1 \times 10^{-7}$. It follows that:

$$p_{ce} = \frac{m_c(c_c + c_p) + m_p c_c}{2m_c + m_p} = \text{£}1.63$$

$$S_p = \frac{(c_c - c_p)^2}{2(2m_c + m_p)} = \text{£}1,071,000$$

$$S_s = \frac{(3m_c + m_p)}{2} \left(\frac{c_c - c_p}{2m_c + m_p} \right)^2 = \text{£}1,475,000$$

The number of bottles to be consumed in a year, q_e , is found from Eq. (22.9)

$$q_e = \frac{c_c - c_p}{2m_c + m_p} = 1,298,000 \text{ bottles}$$

Assuming there are 10,000 consumers and that there are 52 weeks in a year, each consumer gets to drink a mean of 2.50 bottles of Durham beer per week.

(ii) If there is a competitive market then the marginal cost of production will be equal to the marginal benefit of consumption and the social surplus will be maximized. The equilibrium demand price, p_{ce} , producer surplus, S_p , and social surplus, S_s , will therefore be found from Eqs. (22.18), (22.19) and (22.21).

Again, from the originally given information and the answer to part (a) above, $c_c = 2.25$, $m_c = 4.808 \times 10^{-7}$, $c_p = 0.60$ and $m_p = 3.1 \times 10^{-7}$. It follows that:

$$p_{ce} = \frac{m_c c_p + m_p c_c}{m_c + m_p} = £1.25$$

$$S_p = \frac{m_p}{2} \left(\frac{c_c - c_p}{m_c + m_p} \right)^2 = £674,800$$

$$S_s = \frac{(c_c - c_p)^2}{2(m_c + m_p)} = £1,721,000$$

The number of bottles to be consumed in a year, q_e , is found from Eq. (22.16)

$$q_e = \frac{c_c - c_p}{m_c + m_p} = 2,086,000 \text{ bottles}$$

Assuming there are 10,000 consumers and that there are 52 weeks in a year, each consumer gets to drink a mean of 4.01 bottles of Durham beer per week.

(c) Assuming a competitive market, the actual social surplus, S_{as} , can be determined from Eq. (22.25), where $m_e = 1.2 \times 10^{-6}$. So

$$S_{as} = \frac{1}{2} \left(\frac{c_c - c_p}{m_c + m_p} \right)^2 (m_c + m_p - m_e) = -£890,700$$

(d) An appropriate Pigouvian tax, p_t , can be found from Eq. (22.29):

$$p_t = \frac{m_e(c_c - c_p)}{m_c + m_p + m_e} = £0.9946$$

If such a tax was applied, the actual social surplus can be calculated from Eq. (22.27)

$$S_{as} = \frac{(c_c - c_p)^2}{2(m_c + m_p + m_e)} = £683,800$$

so the dead-weight loss that comes about from not accounting for external costs is

$$683,800 + 890,700 = £1,575,000$$

The equilibrium price resulting from adding the £1 per bottle tax is found from (consider Eq. (22.18) but with the Pigouvian tax added to the marginal cost of production)

$$p_{ce} = \frac{m_c(c_p + p_t) + m_p c_c}{m_c + m_p} = £1.85$$

The number of bottles to be consumed in a year, q_e , is found from Eq. (22.26)

$$q_e = \frac{c_c - c_p}{m_c + m_p + m_e} = 828,800 \text{ bottles}$$

Assuming there are 10,000 consumers and that there are 52 weeks in a year, each consumer gets to drink a mean of 1.59 bottles of Durham beer per week.

Worked Solution 22.2 (see Problem 22.2)

(a) To determine the minimum annual payment the factory should accept, we need to determine the maximum possible gain in producer surplus the factory can hope to achieve by expansion. According to Eq. (22.9), the maximum producer surplus is achieved when

$$q = \frac{c_c - c_p}{2m_c + m_p}$$

where, from the information given, $c_p = 10,200$, $m_p = 0.0036$, $c_c = 12,000$ and $m_c = 0$. So the factory is likely to expand until $q = 500,000$ cars.

The producer surplus as a function of q is given by Eq. (22.5)

$$S_p = (c_c - c_p)q - \left(m_c + \frac{m_p}{2}\right)q^2$$

At $q = 450,000$ cars, $S_p = £445,500,000$. At $q = 500,000$ cars, $S_p = £450,000,000$. Therefore the maximum possible gain in producer surplus is £4,500,000. It follows that the minimum annual payment that the factory would be willing to accept to halt expansion is £4,500,000.

(b) The additional cost of the pollution caused by maximum possible plant expansion is found from

$$\int_{450,000}^{500,000} p_e dq = \left[0.0004 \frac{q^2}{2}\right]_{450,000}^{500,000} = £9,500,000$$

It follows that the maximum annual tariff the environmental protection group would be willing to pay to prevent further pollution is £9,500,000.

Worked Solution 22.3 (see Problem 22.3)

(a) If both facilities cut their emissions by 50% each, the fertilizer plant will reduce their emissions by 0.6 Mt per year and the steel works will reduce their emissions by 0.5 Mt per year. The total abatement cost for the fertilizer plant is

$$\begin{aligned} S_{a1} &= \int_0^{600,000} p_{a1} dt \\ &= [50A + 10 \times 10^{-6} A^2]_0^{600,000} \\ &= £33,600,000 \end{aligned}$$

The total abatement cost for the steel works is

$$\begin{aligned} S_{a2} &= \int_0^{500,000} p_{a2} dt \\ &= [70A + 15 \times 10^{-6} A^2]_0^{500,000} \\ &= £38,750,000 \end{aligned}$$

The total abatement cost for the two plants as a collective is therefore £72,350,000.

(b) The minimum possible abatement cost will be achieved if the total emission target is distributed between the two facilities in a way that both facilities have equal marginal abatement costs. The total emissions from both facilities is 2.2 Mt per year. So the total abatement target, $A_t = 1.1 \times 10^6$ tonnes per year.

Let A_1 and A_2 be the abatement target for the fertilizer plant and the steel works, respectively. The total abatement, $A_t = A_1 + A_2 = 1.1 \times 10^6$.

Since the marginal abatement costs must be equal, $p_{a1} = p_{a2}$ and

$$50 + 20 \times 10^{-6} A_1 = 70 + 30 \times 10^{-6} A_2$$

It follows that $A_1 = 1.06 \times 10^6$ tonnes and $A_2 = 4 \times 10^4$.

The total abatement cost for the fertilizer plant is therefore

$$\begin{aligned} S_{a1} &= \int_0^{1,060,000} p_{a1} dt \\ &= [50A + 10 \times 10^{-6} A^2]_0^{1,060,000} \\ &= £64,236,000 \end{aligned}$$

The total abatement cost for the steel works is therefore

$$\begin{aligned} S_{a2} &= \int_0^{40,000} p_{a2} dt \\ &= [70A + 15 \times 10^{-6} A^2]_0^{40,000} \\ &= £2,824,000 \end{aligned}$$

The total abatement cost for the two plants as a collective is therefore £67,060,000. This represents a 7.31% saving as compared to our answer in part (a).

(c) The optimal scenario is obviously when the fertilizer plant abates 1.06 Mt per year and the steel works abates 0.04 Mt per year. This means that the fertilizer plant will only be emitting 0.14 Mt per year and only needs 14 of its 60 CO₂ emission permits. It can therefore sell the other 46 permits to the steel works.

This will enable the steel works to save

$$£38,750,000 - £2,824,000 = £35,926,000$$

so it should be willing to pay $\leq$ £35,926,000 for 46 permits.

The fertilizer plant will have spent an additional

$$£64,236,000 - £33,600,000 = £30,636,000$$

so it should be willing to accept $\geq$ £30,636,000 for 46 permits.

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Abstract

This chapter explores various methods for evaluating the environment including cost based methods, revealed preference methods and stated preference methods. Ecosystem services are used to quantify the value of different biomes. Value of statistical life (VSL) and disability-adjusted life year (DALY) are used to quantify the cost of pollution on health. Detailed examples involving hedonic pricing, travel cost method, VSL and DALY are presented through a problem sheet with worked solutions.

Notation

c_k	Coefficients from a hedonic pricing function.
$DW_{n,k}$	Disability weighting factor for the k th condition that occurred in the n th year.
DALY	Disability-adjusted life year.
EDW_n	Effective disability weighting factor.
i	Discount rate.
M_n	Number of disabilities that affected a subject during the n th year.
N	Average number of remaining years of life for the population.
N_{LD}	Number of years lived with disability.
N_{LL}	Undiscounted YLL.
p	House price or salary.
q_k	Quantity of the k th characteristic.
GBP	Great Britain Pounds.
NPV	Net present value.
USD	United States Dollars.
VLY	Value of a life year.

VSL	Value of statistical life.
WTA	Willingness to accept.
WTP	Willingness to pay.
YLD	Years of healthy life lost due to disability.
YLL	Years of life lost due to premature death.

23.1 Introduction

In this chapter we look at how to evaluate external environmental costs. We can consider the impact of pollution on the environment and the cost of losing ecosystem services. Alternatively, we can consider the health effects of pollution and the associated cost of dealing with that.

There are three different types of evaluation methods commonly applied. These include cost based methods, revealed preference methods and stated preference methods. Cost based methods involve determining the cost incurred by society to mitigate or remediate damage caused by pollution. Revealed preference methods look at people's habits and infer their willingness to pay (WTP) to avoid different types of pollution or experience different types of environmental benefits (scenic views, forests etc.). Stated preference methods involve surveying people directly about their WTP for different environmental aspects. These latter two methods can also be used to determine the value of a statistical life, which, in turn, is often used to derive the monetary value of costs associated with mortality and morbidity due to pollution.

The outline of this chapter is as follows. The three different evaluation methods, mentioned above, are explained. The concept of an ecosystem service is explained and some literature values for different biomes are presented. Health costs of different types of pollution are explored using value of statistical life and disability adjusted life years. Finally, some exercises are provided to practice a selection of evaluation methods.

23.2 Evaluation Methods

Three categories of evaluation methods commonly used to evaluate external environmental costs include:

1. Cost based methods.
2. Revealed preference methods.
3. Stated preference methods.

23.2.1 Cost Based Methods

Cost based methods involve seeking to evaluate costs incurred as a consequence of pollution happening or of an ecosystem service being destroyed. These are discussed in more detail in Sects. 23.3.2 and 23.4.1 below.

23.2.2 Revealed Preference Methods

Revealed preference methods involve the study of choices made by individuals so as to uncover the implied values that have led them to make their decisions. The assumption is that when people make market choices concerning items that have different characteristics related to the environment, they are revealing the value they place on those environmental factors [1, p. 138]. Two revealed preference methods include the hedonic pricing method and the travel cost method.

23.2.2.1 Hedonic Pricing Method

House prices are often used to infer willingness to pay (WTP) for environmental benefits (being close to a lake, access to unpolluted air, etc.). Salaries are often used to infer willingness to accept (WTA) risk to health. The hedonic pricing method involves collecting large amounts of data on house prices or salaries and characteristics of the houses (number of bedrooms, proximity to green space, distance to roads etc.) or jobs (qualifications required, training provision, health and safety risk, etc.). Multiple regression analysis is then used to obtain a “hedonic price function” [2].

In terms of house price, the idea is that buyers will choose levels of each characteristic so that its implicit price is just equal to their marginal WTP for that level in each characteristic. The slope of the hedonic price function with respect to each characteristic is equal to the implicit price. Typically used hedonic pricing functions take the form

$$\ln p = c_0 + \sum_{k=1}^M c_k q_k \quad (23.1)$$

where p is the house price, q_k , is the quantity of the k th characteristic, c_k is the associated regression coefficient and M is the number of characteristics under consideration. The slope of such a function is found from

$$\frac{\partial p}{\partial q_k} = p c_k$$

This represents the WTP for an incremental increase in a particular characteristic.

23.2.2.2 Travel Cost Method

Many people choose to spend their recreational time in natural areas, which typically do not demand an entry tariff (forests, wetlands, beaches, etc.). The travel cost method

is frequently used to estimate the recreational value of such areas. The idea is to use the cost of travelling to such an area as a proxy for the value of accessing the site [2].

Two pieces of information are required:

1. The frequency of visits that an individual makes to a particular recreational site.
2. The total cost incurred by the individual to travel to that site, which includes two important components:
 - (a) The direct costs of travelling to and from the site (train fares, operational cost of car, etc.).
 - (b) The opportunity cost of time spent travelling.

This latter opportunity cost refers to the value the individual could have derived by spending the time spent travelling doing something else instead. Empirical work has shown that time spent travelling is valued at around 40% of an individual's wage rate [2,3].

Data used for the travel cost method is usually collected using surveys carried out at the recreational site of concern. Data collected is used to make a demand schedule for accessing the site. The recreational value of the site is inferred from the consumer surplus assuming a zero supply cost.

23.2.3 Stated Preference Methods

Stated preference methods involve asking people directly what their WTP would be for different environmental scenarios [1, p. 144]. Contingent valuation is a commonly used such method. A contingent proposition is neither necessarily true nor necessarily false.

Contingent valuation involves the following four steps [1, p. 144]

1. Identification and description of the environmental quality characteristic or health outcome to be evaluated;
2. Identification of respondents to be approached;
3. Design and application of a survey questionnaire, interview, or focus group;
4. Analysis of results and aggregation of individual responses to estimate values for the group affected by the environmental change.

From a valuation perspective it is important to consider that consumers engage with environmental goods in different ways [1, p. 152]. In some cases they will consider the direct use value (e.g., how much they would value cycling in a forest). In other cases they might consider the option value (e.g., how much they value the fact that they could cycle in a forest sometime in the future, if they choose to). Alternatively, they might consider the bequest value (e.g., how much they value a forest being available for future generations). Finally, they might be considering the

existence value (e.g., how much they value just knowing a forest exists, with no intention of visiting it either now or in the future).

Problems with stated preference methods include that respondents to questions maybe insufficiently informed to respond in a meaningful way and also that they might be incentivised to misrepresent their true response to the investigator (e.g., they may be embarrassed to admit their true WTP). Another problem concerns when questions look more at WTA as opposed to WTP. People generally need to be paid more to accept that a nearby wetland would be destroyed compared to their WTP to ensure it is maintained.

23.3 Ecosystem Services

The term “ecosystem services” is used to describe the many benefits humans derive from natural environments. These enable us to contemplate and prescribe values to existing environmental states, such that they can be accounted for within cost benefit analyses when project proposals potentially put them under threat in the future.

23.3.1 Categories of Services and Biomes

Ecosystem services are generally categorised into four different classes including [4]:

1. **Provisioning services:** These are where ecosystems provide specific market goods (food, water, timber, etc.).
2. **Regulating services:** Ecosystems provide environmental functioning that leads to monetary savings to societies. For example, natural flood protection might mean an artificial flood wall is not needed.
3. **Habitat services:** Ecosystems provide natural breeding grounds and nurseries. Without these, many species would not be in abundance for exploitation (salmon, tuna, etc.).
4. **Cultural services:** Many landscapes and ecosystems are beautiful and offer tranquility, inspiration and opportunities for sport and recreation.

A detailed list of different services often considered is provided in Table 23.1. Ten main biomes are typically considered for studying ecosystem services. A biome is a large naturally occurring community of flora and fauna occupying a major habitat. A detailed list of different biomes often considered is provided in Table 23.2.

Table 23.1 List of ecosystem services considered by [4]. The descriptions were adapted from a combination of text provided by [5] and [6]

Provisioning services: 1. <i>Food</i>: Any food products derived from plants, animals, and microbes 2. <i>Water</i>: Any source of freshwater 3. <i>Raw materials</i>: Includes materials such as wood, jute, hemp, silk and fuels such as wood, dung and peat 4. <i>Genetic resources</i>: Genes and genetic information used for animal and plant breeding and biotechnology 5. <i>Medicinal resources</i>: Many medicines, biocides, food additives such as alginates, and biological materials are derived from ecosystems 6. <i>Ornamental resources</i>: Animal products, such as skins and shells, and flowers used for decorations	12. <i>Erosion prevention</i>: Vegetative cover plays an important role in soil retention and the prevention of landslides 13. <i>Soil formation</i>: Healthy ecosystems compost and generate new soils, retaining more carbon than is depleted, boosting biodiversity, and maintaining water and nutrient cycling processes 14. <i>Pollination</i>: Ecosystem changes affect the distribution, abundance, and effectiveness of pollinators 15. <i>Biological control</i>: Changes in ecosystems can directly change the abundance of human pathogens, such as cholera, and can alter the abundance of disease vectors, such as mosquitoes. Ecosystem changes also affect the prevalence of crop and livestock pests and diseases
Regulating services: 7. <i>Air quality regulation</i>: Ecosystems both contribute chemicals to and extract chemicals from the atmosphere, influencing many aspects of air quality 8. <i>Climate regulation</i>: Ecosystems influence climate both locally and globally. For example, at a local scale, changes in land cover can affect both temperature and precipitation. At the global scale, ecosystems play an important role in climate by either sequestering or emitting greenhouse gases 9. <i>Natural hazard mitigation</i>: Forests and wetlands dampen flood events and provide protection against flood damage. Mangroves and coral reefs can reduce damage caused by hurricanes or large waves 10. <i>Water regulation</i>: Changes to land use (especially urban development and/or conversion of wetlands or forests to farmland) can lead to significant changes to the timing and magnitude of runoff, flooding, and aquifer recharge 11. <i>Waste treatment</i>: Some ecosystems help filter out and decompose organic wastes introduced into inland waters and coastal and marine ecosystems	Habitat services: 16. <i>Nursery service</i>: Ecosystems often provide breeding, feeding and resting habitat for transient species 17. <i>Genetic diversity</i>: Maintaining ecological balance and evolutionary processes Cultural services: 18. <i>Aesthetic</i>: Many people find beauty or aesthetic value in various aspects of ecosystems, as reflected in the support for parks, “scenic drives,” and the selection of housing locations 19. <i>Recreational</i>: People often choose where to spend their leisure time based in part on the characteristics of the natural or cultivated landscapes in a particular area 20. <i>Inspiration</i>: Ecosystems provide a source of inspiration for art, folklore, national symbols, architecture, and advertising. Many religions attach spiritual and religious values to ecosystems or their components. Many societies place high value on the maintenance of either historically important landscapes or culturally significant species

Table 23.2 Ecosystem biome descriptions [4]

1. <i>Marine</i>, which includes the largest area of the marine ecosystem, including deep sea (water and sea floor below 200 m). Excluded from this biome-section are shelf sea, coral reefs, ocean islands and atolls which are included in other biomes 2. <i>Coral reefs</i>, an underwater ecosystem characterized by reef-building corals 3. <i>Coastal systems</i>, which includes several distinct ecosystems such as sea-grass fields, shallow seas of continental shelves, rocky shores and beaches, which are found in the terrestrial near-shore as well as the intertidal zones – i.e., until the 200 m bathymetric line with open oceans 4. <i>Coastal wetlands</i>, which includes two main types of ecosystem, tidal marshes and mangroves 5. <i>Inland wetlands</i>, which includes (fresh-water) floodplains, swamps/marshes and peat lands. It explicitly does not include coastal wetlands and rivers and lakes 6. <i>Fresh water</i>, which includes freshwater rivers and lakes. Saline lakes, and wetlands and floodplains are not included in this biome 7. <i>Tropical forest</i>, which includes various types of forests in the tropical	- and subtropical regions, e.g., rainforests, deciduous/semi-deciduous broadleaf forest and tropical mountain forests 8. <i>Temperate forest</i>, which includes temperate deciduous forest, temperate broadleaf and mixed forest, temperate coniferous forest and temperate rainforest 9. <i>Woodlands</i>, which includes a large range of vegetation types including savannas, shrublands, scrublands and chaparral interleaved with one another in mosaic landscape patterns distributed along the western coasts of North and South America, areas around the Mediterranean Sea, South Africa, and Australia, jointly representing about 5% of the planets surface 10. <i>Grasslands</i>, which includes tropical grasslands (savannas), temperate grasslands (including the European and Central Asian steppe and North American prairie), boreal grasslands (tundra's) and mountainous grasslands (such as the Latin American Paramo highlands). The largest continuous stretch of tropical grassland is the North African Sahel, that stretches from Senegal to the Horn of Africa

23.3.2 Evaluating Ecosystem Services

Global estimates for monetary values for ecosystem services in different biomes, obtained by [4], are provided in Table 23.3. Such average values provide a general idea about where components of value lie. It is particularly striking to see the regulating service values of coral reefs and coastal wetlands. However, consideration of local factors (population density, degree of development of the region, etc.) are needed, if ecosystem services are to be meaningfully included in a cost benefit analysis [7].

A wide range of methods are used to determine the value of different ecosystem services [4]. Provisioning services are mostly evaluated using direct market value methods. Regulating services are mostly evaluated using cost based methods. Habitat services are often evaluated using a combination of direct market value and stated preference methods. Cultural services are evaluated using a combination of direct market value methods, revealed preference methods and stated preference methods.

Direct market value methods are particularly applicable to provisional services that lead to the production of commonly sold goods [4]. For example, if a forest can

Table 23.3 Global estimates of ecosystem values for different biomes (USD₂₀₀₇ ha⁻¹ year⁻¹) [4]

	Marine	Coral reefs	Coastal systems	Coastal wetlands	Inland wetlands	Fresh water	Tropical forest	Temperate forest	Woodlands	Grasslands
Provisioning services	101	55725	2396	2997	1660	1914	1828	671	254	1306
1. Food	93	677	2384	1111	614	106	200	299	52	1192
2. Water	0	0	0	1217	408	1808	27	191	0	60
3. Raw materials	8	21528	12	358	425	0	84	181	170	53
4. Genetic resources	0	33048	0	10	0	0	13	0	0	0
5. Medicinal resources	0	0	0	301	99	0	1504	0	0	1
6. Ornamental resources	0	472	0	0	114	0	0	0	32	0
Regulating services	65	171478	25847	171515	17363	187	2529	492	51	159
7. Air quality regulation	0	0	0	0	0	0	12	0	0	0
8. Climate regulation	65	1188	479	65	488	0	2044	152	7	40
9. Natural hazard mitigation	0	16991	0	5351	2986	0	66	0	0	0
10. Water regulation	0	0	0	0	5606	0	342	0	0	0

(continued)

Table 23.3 (continued)

	Marine	Coral reefs	Coastal systems	Coastal wetlands	Inland wetlands	Fresh water	Tropical forest	Temperate forest	Woodlands	Grasslands
11. Waste treatment	0	85	0	162125	3015	187	6	7	0	75
12. Erosion prevention	0	153214	25368	3929	2607	0	15	5	13	44
13. Soil formation	0	0	0	45	1713	0	3	93	0	0
14. Pollination	0	0	0	0	0	0	30	0	31	0
15. Biological control	0	0	0	0	948	0	11	235	0	0
Habitat services	5	16210	374	17138	2455	0	39	862	1276	1214
16. Nursery service	0	0	194	10648	1287	0	16	0	1273	0
17. Genetic diversity	5	16210	180	6490	1168	0	23	862	3	1214
Cultural services	319	108837	299	2193	4203	2166	867	990	7	193
18. Aesthetic	0	11390	0	0	1292	0	0	0	0	167
19. Recreation	319	96302	256	2193	2211	2166	867	989	7	26
20. Inspiration	0	1145	43	0	700	0	0	0	0	0
Total economic value	490	352250	28916	193843	25681	4267	5263	3015	1588	2872

sustainably yield a certain amount of timber on an annual basis, the market price of timber can be used to determine the value of this provisional service.

Cost based methods, in this context, involve evaluating an ecosystem service by the cost of that service being damaged. These mostly apply to regulated services. Cost based methods can be applied in at least three different ways [4]:

1. **Avoided cost method** uses the cost of damage that would occur if the service was lost. For example, a mangrove wetland might provide flood protection from tsunamis to a village. Without the mangrove, the village might be destroyed every ten years. The avoided cost that wetland provides can be estimated by the cost of having to rebuild the village every ten years.
2. **Mitigation and restoration cost method** uses the cost of bringing back an ecosystem service. For example, if a forest was completely destroyed, the mitigation and restoration cost would include how much it would cost to replant the trees and carefully look after the area until the forest was returned to its previous state in terms of both intensity and biodiversity.
3. **Replacement cost method** uses the cost of replacing an ecosystem service with an alternative system. For example, a riparian wetland might be improving the water quality in a river through sediment retention and nutrient cycling. The value of this service can be estimated by determining the cost of an equivalent water treatment facility.

23.3.3 Lost Value by Ecosystem Conversion

Economic development often involves converting natural ecosystems to human-dominated ecosystems. For example: wetlands are drained to farm wheat and barley; forests are cleared to farm soya bean; mangroves are cleared and replaced by shrimp farms.

The monetary benefits captured from ecosystem services entering the market, referred to as the private benefits, generally favour conversion or unsustainable management. However, conversion often results in loss of ecosystem services leading to overall declines in human well-being and poverty being enhanced for some social groups [9].

Duraiappah et al. [8] reviewed four ecosystem conversion studies from around the world. In each case, it was found that the social benefit of managing the ecosystem more sustainably exceeded that of the converted human-dominated counterpart (see Table 23.4). Each of the four studies are summarised below.

23.3.3.1 Conversion of Freshwater Wetland to Agriculture

van Vuuren and Roy [10] studied the conversion of freshwater wetlands to intensive agriculture in Ontario, Canada. They looked at net present value (NPV) for a 50 year period with a 5% discount rate.

Table 23.4 Economic benefits under alternative management practices. NPV is net present value in USD per hectare. This data was extracted from [8]

Case study	Sustainably managed ecosystems		Converted ecosystems	
	Land use	NPV	Land use	NPV
Wetland (Canada)	Intact wetland	5800	Intensive farming	2300
Tropical forest (Cameroon)	Sustainable forestry	3500	Small-scale farming	2000
Mangrove (Thailand)	Intact mangroves	1000	Shrimp farming	190
Tropical forest (Cambodia)	Traditional forest use	1300	Unsustainable timber harvest	130

Inland wetlands are characterised by the presence of plants with special roots that can cope with waterlogged soils. They provide many important regulating services including flood retention, heavy metal stabilisation, pH regulation, nutrient cycling and carbon storage.

van Vuuren and Roy [10] found the NPV of maintaining an intact wetland was \$5800 per ha. In contrast, the NPV from draining the wetland and growing corn and soybean was \$2400 per ha. Intact wetland benefits, considered in the study, included small-scale agriculture, hunting, angling and trapping. The predicted NPV of intact wetlands would be substantially increased if additional regulating services were also accounted for.

23.3.3.2 Conversion of Tropical Forest to Plantation

Yaron [11] studied the conversion of tropical forest to small-scale agriculture and plantation in Cameroon. Specifically they looked at NPV for a 32 year period with a 10% discount rate. The NPV for sustainable forest management (i.e., low-impact logging) was \$3400 per ha. The NPV for small-scale agriculture was \$2000 per ha. The NPV for oil palm and rubber plantations was negative, at -\$1000 per ha, although positive NPV was realised in practice due to market distortions caused by taxes and subsidies. The sustainable forest management option yielded higher NPV due to additional local benefits (non timber forest products, sedimentation control, and flood prevention) and global benefits (carbon storage along with option, bequest, and existence values).

23.3.3.3 Conversion of Mangrove Wetland to Shrimp Farm

Sathirathai and Barbier [12] studied the conversion of mangrove wetland to shrimp farm in Thailand. They looked at NPV for a 20 year period with a 10% discount rate. They found the NPV of maintaining intact mangrove wetland to be between \$1000

and \$36,000 per ha. In contrast, the NPV from converting the land totally to shrimp farm was found to be \$200 per ha.

Shrimp farming typically involves excavating a pond in close proximity to the shoreline. Fresh seawater is pumped into the pond. Post-larvae shrimp are placed in the pond and fed until they reach a marketable size. Once all the shrimp are ready, the entire pond is drained and the shrimp are collected. The cycle then begins again. However, after around five years, shrimp diseases build up and the ponds are abandoned. Mangrove wetlands are frequently deforested to provide land for new shrimp farms.

Intact mangrove wetland yields high NPV due to small scale sustainable shrimp farming, timber, charcoal and non-timber forest products along with the additional social benefits provided by offshore fisheries and storm protection.

Mangrove trees grow in coastal wetlands. They possess a special salt filtration system and root system, which enables them to cope with salt water immersion and wave action. Mangrove trees reduce coastal erosion and provide flood protection. They also provide essential breeding grounds and nursery habitat for marine life. Furthermore, their root systems filter out sediment from terrestrial runoff providing a clean water source for surrounding coral reefs. Mangroves also provide important subsistence commodities for local communities such as food, medicines, fuel wood and wood products.

23.3.3.4 Timber Extraction from Tropical Forest

Bann [13] performed a cost benefit analysis comparing traditional forest practices with commercial timber extraction for a tropical forest in Cambodia. Their alternative sustainable and traditional scenario included swidden agriculture, extraction of non timber forest products (including fuelwood, rattan and bamboo, wildlife, malva nuts, and medicine) and ecological and environmental functions (including water regulation, biological control and carbon storage). They looked at NPV for a 90 year period with a 6% discount rate. The NPV for their sustainable and traditional scenario was between \$1,300 and \$4,500 per ha. The NPV for commercial timber extraction was between \$150 and \$1,100 per ha.

23.4 Pollution and Health

Another way of evaluating damage to the environment is to consider the cost of pollution on health. [14] defines pollution as “unwanted, often dangerous, material that is introduced into the Earth’s environment as the result of human activity, that threatens human health, and that harms ecosystems”. Pollution related diseases accounted for 9 million premature deaths in 2015, representing 16% of total global mortality [15].

In the context of health, environmental pollution is usefully placed into four categories [14]:

Table 23.5 Percent of deaths attributed to different pollution risk factors globally for different diseases (see [14, Table C.2])

	Air (%)	Water (%)	Lead (%)
Lower respiratory infections	20		
Tracheal, bronchus, and lung cancer	6		
Ischemic heart disease	30		49
Ischemic stroke	8		14
Hemorrhagic stroke	12		18
Chronic obstructive pulmonary disease	24		
Diarrheal diseases		88	
Typhoid fever		10	
Paratyphoid fever		2	
Hypertensive heart disease			10
Other cardiovascular and circulatory diseases			3
Chronic kidney disease			6

Table 23.6 Estimated millions of deaths by pollution risk factor and country income level for 2015 (data from [14])

Country income level	Low	Low middle	Upper middle	High
Air	0.63	3.11	2.23	0.49
Water	0.42	1.16	0.13	0.06
Occupation	0.02	0.27	0.38	0.17
Soil, chemicals & metals	0.04	0.22	0.16	0.08

1. Air (particulate matter, NO₂, O₃, etc.);
2. Water (unsafe sanitation and water sources);
3. Occupation (carcinogens, particulates, fumes, etc.);
4. Soil (including toxic organics and heavy metals).

Examples of diseases associated with air pollution, water pollution and lead exposure are provided in Table 23.5.

The relevance of different pollution categories is strongly dependent on the development status of the region of concern. Air pollution tends to dominate number

of deaths as compared to water, occupation and soil. The relevance of water and soil pollution decreases with increasing income level due to associated improvements in environmental regulations and technologies (see Table 23.6).

23.4.1 Health Costs of Pollution

A lower bound estimate of the cost of pollution can be obtained by studying resulting defensive expenditures [16, p. 174]. For example, we can consider the amount of money spent on air purifiers to mitigate the effects of air pollution or the amount of money spent on bottled water to mitigate the effects of water pollution.

Another approach involves studying health related costs due to pollution. These include [14]:

- Direct medical expenditures, such as hospital, physician, and medication costs, long-term rehabilitation or home care, and non-clinical services such as management, support services, and health insurance costs.
- Indirect health related expenditures, such as time lost from school or work, costs of special education, and the cost of investments in the health system (including health infrastructure, research and development, and medical training).
- Diminished economic productivity in persons whose brains, lungs, and other organ systems are permanently damaged by pollution.
- Losses in output resulting from premature death.
- Intangible costs, such as those of poor health in people made ill by pollution and/or disruption of family stability when a person of working age becomes disabled or dies prematurely as a result of pollution.

The cost of pollution on health is often assessed using cost based methods. The cost of a single case of illness is often measured as the sum of medical expenses incurred plus the loss in productivity due to premature death and/or disability. The associated cost of a pollution component is then determined by multiplying the cost of a single case of illness by the total number of cases that occur in a year and then by multiplying by the so-called “fractional contribution” of pollution to causation of a particular disease.

The issue with such an approach is that (1) it heavily relies on the availability of strong public health data systems (normally not present in low-income economies), and (2) it fails to consider the important intangible costs of death and illness.

23.4.2 Value of Statistical Life (VSL)

The value of statistical life approach (VSL) provides an appropriate alternative. [14] defines VSL as the “total of what many people would pay for small reductions in the probability of dying over the coming year that, together, add up to a single life”.

Table 23.7 Value of statistical life (VSL) and willingness to pay (WTP) (\$ per capita) to prevent deaths caused by different pollution risk factors by country income level for 2015 (based on purchasing power parity) (see [14, Tables B.1 and B.2])

World bank region	VSL	Air	Water	Lead
High income	\$3,830,000	\$1793	\$23	\$283
Upper middle income	\$1,351,932	\$1390	\$35	\$94
Lower middle income	\$342,554	\$503	\$196	\$32
Low income	\$80,473	\$93	\$67	\$3

For example, if 10,000 people are willing to annually pay £100 to reduce their risk of dying by 1 in 10,000, one statistical life would be saved and the VSL would equal $£100 \times 10,000 = £1,000,000$.

VSL can be determined from cost based methods, revealed preference methods and stated preference methods [3, p. 466]:

- Cost based methods look at people's WTP pay for products or services that reduce the risk of fatality (e.g., by studying the price of seat belts or cycling helmets, etc.).
- Stated preference methods typically involve soliciting answers from survey respondents using multiple choice questions about how much they would be WTP for different risk reduction scenarios.
- Revealed preference methods mostly include hedonic pricing analyses looking at how much more workers generally get paid for risky jobs, to compensate for the additional fatality risk they incur.

These methods lead to a wide range of estimated VSLs [3]. The UK government uses a value of 1.6 million GBP₂₀₁₀ [17]. The median value adopted by EU-27 countries is 3.6 million USD₂₀₀₅ [18, p. 127]. The US Department of Transportation uses a value of 9.6 million USD₂₀₁₆ [19].

It can be appreciated that VSL is likely to be dependent on income, with higher incomes leading to higher VSL. [14] determined separate VSL values for low, lower middle, upper middle and high income countries. These were used to estimate people's WTP to prevent deaths caused by pollution (see Table 23.7). It is of interest to note that WTP to reduce air pollution dominates for all income groups.

A problem with the above analysis is that it treats all lives as being equal regardless of age. Fig. 23.1a shows how global deaths due to pollution are distributed with age. There is a small peak for post neonatal and 1–4 year olds. But this seems less significant as compared to the number of deaths seen in the over 55s. However, it is unclear that it is useful to value the death of somebody with their whole life ahead of them as being the same as somebody who would have only lived a small number of years without the pollution.

23.4.3 Disability-Adjusted Life Year (DALY)

A more precise method of studying the cost of pollution on health can be achieved by considering disability-adjusted life years (DALY). The advantage about DALY is that it combines the effects of mortality (deaths) and morbidity (illness). The DALY caused by a specific event is found from [20, p. 4]

$$\text{DALY} = \text{YLL} + \text{YLD} \quad (23.2)$$

where YLL represents the years of life lost due to premature death and YLD represents the years of healthy life lost due to disability.

The YLL is determined by subtracting the age at which a subject dies (or is expected to die with their condition) from an average life expectancy (currently around 81 years in the UK).

The YLD is found from

$$\text{YLD} = \sum_{n=1}^{N_{LD}} \text{EDW}_n \quad (23.3)$$

where N_{LD} is the number of years lived with disability and EDW_n is an effective disability weighting factor that describes the condition of the subject during the n th year, found from [20]

$$\text{EDW}_n = 1 - \prod_{k=1}^{M_n} (1 - \text{DW}_{n,k}) \quad (23.4)$$

where M_n represents the number of different disabilities that affected the subject during the n th year and $\text{DW}_{n,k}$ is the disability weighting factor for the k th condition that occurred in the n th year.

Disability weighting factors range from zero, for perfect health, to one, for death. These weighting factors are derived from surveys asking people to rate and compare different health states. Some examples are provided in Table 23.8.

Figure 23.1b shows how global DALY due to pollution are distributed with age. Results using DALY show that the most vulnerable groups to pollution are post neonatal, 1-4 year olds and then 60-64 year olds. Interestingly, YLL (as opposed to YLD) represented around 93% of global DALYs attributed to pollution [14].

23.4.4 WTP to Eliminate a DALY

DALY (disability adjusted life year) can be used to estimate the cost of pollution by considering the WTP to eliminate a DALY, which in turn should be equal to the value of a life year (VLY). UK government policies currently assume a VLY of 60,000 GBP₂₀₁₀ [17].

The VLY represents the equivalent annual cost of the VSL (value of a statistical life), spread over the average number of remaining years of life for the population

Table 23.8 Examples of disability weights (after [20])

Condition	Disability weight
Amputation of toe	0.008
Impotence	0.019
Amputation of one leg: with treatment	0.021
Diarrhoea: mild	0.061
Alcohol problem use	0.115
Asthma: uncontrolled	0.132
Heart failure: severe	0.186
Infectious disease: post-acute consequences	0.254
Diarrhoea: severe	0.281
Hearing loss: complete	0.281
Distance vision blindness	0.338
Heroin and other opioid dependence	0.340
Major depressive disorder: moderate episode	0.406
Headache: migraine	0.433
Intellectual disability: profound	0.444
Terminal phase cancer: without medication	0.519
Dementia: severe	0.545
Stroke: severe long-term consequences	0.567
Schizophrenia: acute state	0.756

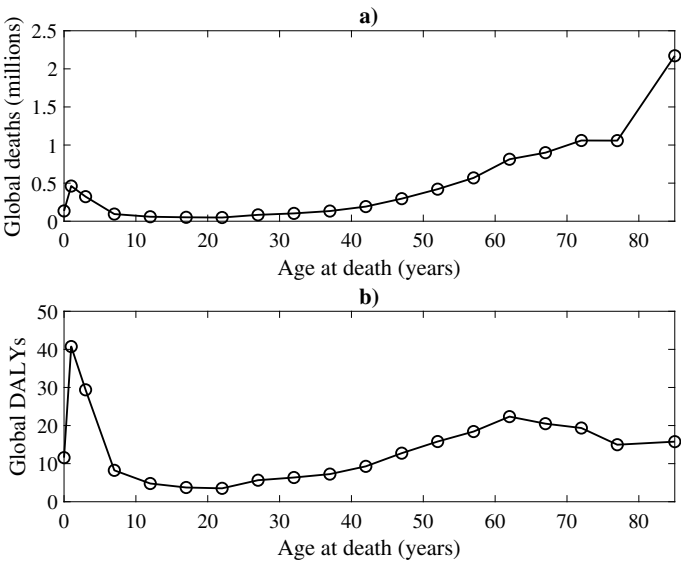


Fig. 23.1 a) Estimated global deaths due to pollution by age for 2015. b) Estimated global DALYs due to pollution by age for 2015. This data was extracted from [14]

the VSL was assessed for. Note that VSL represents a present value. Considering Eqs. (21.1) and (21.7) [3, p. 470]

$$VLY = \left[\frac{i}{1 - (1 + i)^{-N}} \right] VSL \quad (23.5)$$

where i is a discount rate and N is the average number of remaining years of life for the population.

23.4.5 Discounting YLL and YLD

Challenge 23.1 Determine expressions for values of YLL and YLD that compensate for the effects of a discount rate.

YLL and YLD can also be discounted using:

$$YLL = \sum_{n=1}^{N_{LL}} \frac{1}{(1 + i)^{n+N_{LD}}} = \frac{1 - (1 + i)^{-N_{LL}}}{i(1 + i)^{N_{LD}}} \quad (23.6)$$

and

$$YLD = \sum_{n=1}^{N_{LD}} \frac{EDW_n}{(1 + i)^n} \quad (23.7)$$

where N_{LD} is the number of years lived with disability and N_{LL} is the undiscounted YLL.

23.5 Problem Sheet

Problem 23.1 (see Worked Solution 23.1)

Study the data in Table 23.9 concerning house prices in London and their relation to green space. House prices are mean house prices for a given borough. Crime is the number of burglaries in a year as a percentage of the number of adults living in a borough. Travel time is the mean travel time from homes to Central London. Green space is the area of land, within each borough, designated open green space.

(a) Use multiple linear regression to develop a hedonic pricing function that relates the natural log of house prices to crime, travel time and percentage green space (i.e., the percentage area of each borough designated open green space).

(b) Determine:

(i) an average household's WTP for a one point increase in percentage green space within each borough;

(ii) an average household's WTP for the development of 1 km² of new green space

Table 23.9 Extract of data from the “Valuing Greenness” report published by the Greater London Authority in 2003 [21]

Borough	House price (£)	Area (km ²)	Number of homes	Crime (%)	Travel time (min)	Green space (km ²)
Westminster	411127	21.44	134796	15.08	9.98	5.21
Camden	342121	21.72	103599	17.99	17.52	4.47
Richmond	300115	57.18	109506	10.27	45.05	30.98
Merton	204522	37.50	93821	8.74	37.58	10.80
Hackney	179896	19.01	95221	24.37	22.36	3.36
Enfield	154170	81.88	165863	12.47	42.40	35.80
Croydon	144664	86.21	184112	12.33	40.86	27.65
Lewisham	134782	35.00	113867	15.43	33.65	5.23
Newham	115229	36.10	130620	14.63	29.65	7.17

Table 23.10 Survey data concerning recreational visits to Hamsterley forest

County	Mean travel distance (miles)	Population	Number of visits per year
Durham	17.1	867000	90300
Tyne and Wear	28.8	1140000	96400
North Yorkshire	32.9	1160000	83100
Northumberland	50.8	320000	16200

within each borough;

(iii) the value of 1 km² of green space within each borough.

(c) Attempt to explain the variation in results.

Problem 23.2 (see Worked Solution 23.2)

Hamsterley forest is a 2000 ha forest in County Durham, popular with cyclists, hikers and runners. Forestry England is considering a one-year closure to reduce safety costs associated with sustainable logging (this is complete fiction by the way). As part of a cost-benefit analysis, they are seeking to estimate the recreational value of the forest using the travel cost method. Relevant data concerning recreational visits to Hamsterley forest is provided in Table 23.10.

Transport to Hamsterley forest is predominately by car. Operating costs for cars in the UK are around £0.40 per mile. The average number of adult passengers in a car is 1.4. The average number of child passengers in a car is 1.6. Average wages in North East England are around £13.50 per hour. The opportunity cost to adults of travel time is around 40% of their wage rate. The average car speed for travelling to Ham-

Table 23.11 Data concerning cycle helmets for young children (5–9 years) living in the US in 1997 from [22]

Cost of a helmet in USD ₁₉₉₇	25.85
Number of years a helmet is used	4
Total number of young children	19670000
Number of associated deaths on bikes	93
Fraction of young children that ride bikes	0.727
Fraction of bike deaths caused by head injuries	0.641
Fraction of bike riders that own helmets	0.575
Fraction of helmet owners that regularly wear helmets	0.553
Fraction of deaths prevented with helmet use	0.790

sterley is around 40 miles per hour. The car park at Hamsterley Forest cost £6 per day.

(a) Determine the average cost per person of a visit to Hamsterley Forest and the number of visits per person per year from each county.

(b) Use linear regression to determine an empirical relationship between the number of visits per person per year and average cost per person.

(c) The total number of annual visits is currently 286,000. Use the linear regression relationship, developed in part (b), to estimate the number of visits that would be expected from each county with free parking and then sum these to estimate the resulting total number of visits.

(d) Use the linear regression relationship, developed in part (b), to estimate the number of visits that would be expected from each county with free parking but an entry tariff of £1 per person then sum these to estimate the resulting total number of visits.

(e) Use the linear regression relationship, developed in part (b), to determine the minimum entry tariff that leads to zero visitors, even with free parking.

(f) Repeat the steps in part (d) whilst sequentially increasing the hypothetical entry tariff by £1 until the total number of visitors drops down to zero and plot the resulting demand schedule.

(g) Estimate the consumer surplus from the demand schedule developed in part (f) assuming free entry and free parking. This represents the recreational value of Hamsterley Forest.

Problem 23.3 (see Worked Solution 23.3)

Study the data in Table 23.11 concerning cycle helmets for young children (5-9 years) living in the US in 1997.

(a) Determine the number of deaths caused by a head injury that would have occurred if:

(i) none of the children owned helmets;

(ii) all of the children owned a helmet.

(b) Determine the probability of a child dying from a head injury on a bike if:

(i) none of the children owned helmets;

(ii) all of the children owned a helmet.

(c) Determine the equivalent annual cost of one helmet assuming a discount factor of 0.3%.

(d) Jenkins et al. [22] assume that half the cost of a helmet represents parents' WTP to reduce the probability of a fatality and the other half, the WTP to reduce the probability of a non-fatal injury. Use this idea to estimate the VSL of a young child.

Problem 23.4 (see Worked Solution 23.4)

(a) UK government policy generally assumes a VSL of £1.6 million (2010 prices). Assuming that the VSL directly applies to a 40 year old person expecting to live to reach 81 years old (these are current average numbers for the UK) and that the discount rate is 2.235%, determine the associated VLY.

(b) A factory emits high levels of air pollution, which is attributed to 50 premature deaths per year. Estimate the annual health cost of this pollution using the UK government's VSL.

(c) Victims typically experienced four years of asthma and severe depression, combined with conditions associated with heart failure during their final year. The average age at death linked to this pollution was 65 years old. Refine your previous health cost estimate using DALYs.

23.6 Worked Solutions

Worked Solution 23.1 (see Problem 23.1)

(a) Our hedonic pricing function takes the form (Eq. (23.1))

$$\ln p = c_0 + \sum_{k=1}^M c_k q_k$$

where p is the house price, q_1 , q_2 and q_3 are crime, travel time and percentage green space, respectively, c_0 is a constant, and c_1 , c_2 and c_3 are the coefficients for crime, travel time and percentage green space, respectively.

Prior to applying multiple linear regression, the data, from Table 23.9, needs to be properly weighted to account for the variation in the number of homes in each borough. The hedonic function can be developed using the following MATLAB script:

```
%Data from table
dataA=[411127 21.44 134796 15.08 9.98 5.21
342121 21.72 103599 17.99 17.52 4.47
300115 57.18 109506 10.27 45.05 30.98
204522 37.50 93821 8.74 37.58 10.80
179896 19.01 95221 24.37 22.36 3.36
154170 81.88 165863 12.47 42.40 35.80
144664 86.21 184112 12.33 40.86 27.65
134782 35.00 113867 15.43 33.65 5.23
115229 36.1 130620 14.63 29.65 7.17];
%Reproduce data to appropriately weight dataA to
%account for variation in the number of homes
%in each borough and store in dataB
Homes=dataA(:,3);
dataB=[];
for n=1:size(dataA,1)
dataB=[dataB;repmat(dataA(n,:),Homes(n),1)];
end
%Define house price array
p=dataB(:,1);
%Define q array
q(:,1)=dataB(:,4); %Crime
q(:,2)=dataB(:,5); %Travel time
%Determine percentage green space
Area=dataB(:,2);
GreenSpace=dataB(:,6);
q(:,3)=100*GreenSpace./Area;
%Perform multiple linear regression
```

```
c=[ones(size(p)) q]\log(p);
```

The resulting coefficients are:

$$\begin{aligned}c_0 &= 13.07, & c_1 &= -0.02120, \\c_2 &= -0.04549, & c_3 &= 0.02939.\end{aligned}$$

Not surprisingly, this indicates that house price is negatively correlated with crime and travel time to central London and positively correlated with percentage green space.

(b) (i) The average households' WTP for a % point increase in green space for each borough is found from

$$\left. \frac{\partial p}{\partial q_3} \right|_{p_j} = c_3 p_j$$

where p_j is the average house-price of the j th borough.

(ii) Noting that the area associated with a percentage green space of 1% is found from $\text{Area} \div 100$, the average households's WTP for the development of 1 km² of new green space within each borough is found by multiplying the answer from part (i) by $100 \div \text{Area}$.

(iii) The total value of 1 km² of new green space within each borough can be found by multiplying the answer from part (ii) by the number of homes.

The results to parts (i), (ii) and (iii) can be obtained by appending the following additional MATLAB code to the script developed for part (a):

```
% (i) WTP for one percentage point
Price=dataA(:,1);
% Note that c(1)=c0 so c(4)=c3
WTPpercent=c(4)*Price;
% (ii) WTP for 1 km2
Area=dataA(:,2);
WTPkm2=WTPpercent*100./Area;
% (iii) Total value for 1 km2
TotalCost=WTPkm2.*Homes;
```

The results are presented in Table 23.12.

(c) The WTP for 1% point increase in green space is mostly dependent on house price. The WTP for 1 km² of new green space is dependent on the ratio of house price to area of borough (the larger the borough, the smaller a 1 km² of land will be in terms of percentage green space). The total value of 1 km² of new green space is dependent on the ratio of house price to area of borough multiplied by the number of households living in the borough (the more people there are, the more that can be paid for the land).

Table 23.12 Results for Problem 23.1b in 2003 money and assuming 2003 house prices

Borough	(i) WTP for 1% point (£)	(ii) WTP for 1 km ² (£)	(iii) Total value for 1 km ² (million £)
Westminster	12084	56361	7597
Camden	10056	46296	4796
Richmond	8821	15427	1689
Merton	6011	16030	1504
Hackney	5287	27814	2648
Enfield	4531	5534	918
Croydon	4252	4932	908
Lewisham	3961	11319	1289
Newham	3387	9382	1225

Worked Solution 23.2 (see Problem 23.2)

(a) The average cost per person, p_c , of a visit to Hamsterley Forest is found from the following equation

$$p_c = \frac{2 \left(C_{\text{car}} + \frac{N_{\text{adult}} C_{\text{opp}}}{v} \right) L + C_{\text{park}}}{N_{\text{adult}} + N_{\text{child}}}$$

where C_{car} is the operational cost for cars, N_{adult} is the average number of adults in a car, N_{child} is the number of children in a car, C_{opp} is the opportunity cost to adults for travel time, v is the average speed of the car, L is the mean travel distance from homes to the forest, C_{park} is the parking cost. Note that the factor of 2 is required to recognise the need to drive to and from the forest.

It is worth performing these calculations using MATLAB since there is a table of data. This can be achieved with the following code:

```
%Data from table
data=[17.1 867000 90300
28.8 1140000 96400
32.9 1160000 83100
50.8 320000 16200];
L=data(:,1); %Distance (miles)
Pop=data(:,2); %Population
CountyVisits=data(:,3); %Number of visits
%Other data from information given
Ccar=0.4; %Cost of car (GBP/mile)
Nadul=1.4; %Number of adults in car
Nchil=1.6; %Number of children in car
```

Table 23.13 Results for Problem 23.2a

County	Average cost per person, p_c	Number of visits per person per year, N_{visit}
Durham	£8.72	0.1042
Tyne and Wear	£13.31	0.08456
North Yorkshire	£14.92	0.07164
Northumberland	£21.95	0.05063

```

Copp=0.4*13.5; %Opportunity cost (GBP/hour)
v=40; %Car speed (miles/hour)
Cpark=6; %Car park tarif (GBP)
%Determine average cost per person (GBP/visit)
pc=(2*(Ccar+Nadul*Copp/v)*L+Cpark)/(Nadul+Nchil);
%Determine number of visits per person per year
Nvisits=CountyVisits./Pop;

```

The results are shown in Table 23.13.

(b) Let $N_{\text{visit}} = X_1 + X_2 p_c$ where X_1 is the zero intercept and X_2 is the slope of a linear regression function and N_{visits} is the number of visits per person per year. Values of X_1 and X_2 can be found using the following MATLAB code:

```

%Apply linear regression
X=[ones(size(pc)) pc]\Nvisits;

```

From which it is found that $X_1 = 0.1373$ and $X_2 = -0.004045$.

(c) The following code can be used to determine the total annual number of visitors that would be expected if the car park was made free.

```

%Determine cost of car park per person
ppark=Cpark/(Nadul+Nchil);
%Total number of visits with free parking
CountyVisitsFree=CountyVisits-Pop*X(2)*ppark;
TotalVisitsFree=sum(CountyVisitsFree,1);

```

The answer is 314,200 visitors.

(d) The following code can be used to determine the total annual number of visitors that would be expected with free parking but with a per person tariff, p_t , of £1.

```

%Total number of visits with free parking
%and 1 GBP per person tariff
pt=1; %Per person tariff
CountyVisitTariff=CountyVisits-Pop*X(2)*(ppark-pt);
TotalVisitsTariff=sum(CountyVisitTariff,1);

```

The answer is 300,100 visitors.

(e) The minimum entry tariff that leads to zero visitors (even with free parking) is found by solving the equation in the above code for p_t using the county that is closest (i.e., Durham) and setting the number of visitors from that county (when the tariff is applied) to zero. This is achieved with the following code:

```
%Determine tariff at which there will be no
%visits despite the free parking
ptZERO=ppark-Nvisits(1)/X(2);
```

Note that `Nvisits(1)` provides the value for Durham. This minimum entry tariff turns out to be £27.75 per person (that would require a dedicated mountain biker).

(f) The following code will calculate a set of visitor numbers that correspond to a range of different entry tariffs but with free parking. The code also generates a relevant plot that corresponds to the demand schedule for Hamsterley Forest.

```
%Determine total visits for a range of pt values
%but with free parking
pt=0:1:ceil(ptZERO);
CountyVisitTariff=CountyVisits+Pop*X(2).*(pt-ppark);
%Reset negative visits to zero visits
CountyVisitTariff(CountyVisitTariff<0)=0;
%Determine total number of visits
TotalVisitsTariff=sum(CountyVisitTariff,1);
figure(1); clf %Plot demand schedule
plot(TotalVisitsTariff/1000,pt,'ko-')
xlabel('Number of visits (1000s)')
ylabel('Entry tariff (GBP per visit)')
```

The resulting demand schedule is shown in Fig. 23.2.

(g) The consumer surplus can be found by trapezoidal integration using the following code:

```
%Determine consumer surplus
ConsumerSurplus=-trapez(TotalVisitsTariff,pt);
```

The minus sign is needed because we are integrating from 312,200 to zero. The answer is £3,608,500. So the recreational value of Hamsterley Forest is estimated to be £3,608,500 per year.

Worked Solution 23.3 (see Problem 23.3)

(a) The number of deaths caused by a head injury in 1997

$$= 0.641 \times 93 = 59.61$$

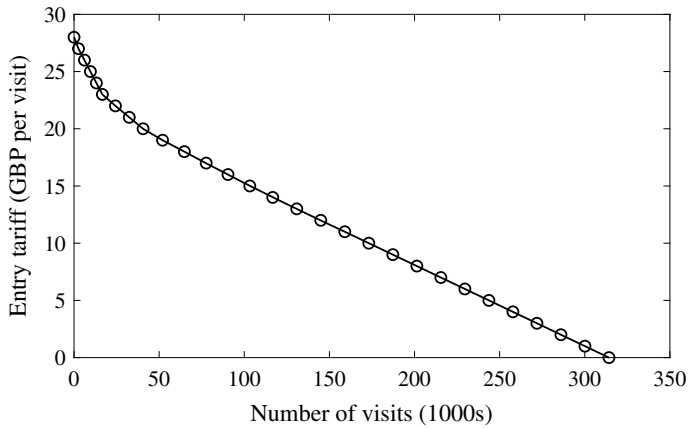


Fig. 23.2 Demand schedule for visiting Hamsterly forest as developed for Problem 23.2f

(i) The fraction of deaths that would have been prevented

$$= 0.575 \times 0.553 \times 0.790 = 0.2512$$

The number of deaths caused by a head injury that would have occurred if none of the children owned helmets

$$= 59.61 \div (1 - 0.2512) = 79.61$$

(ii) The fraction of deaths that would have been prevented if all the children owned a helmet (although not all of them might be regularly wearing the helmets) $= 0.553 \times 0.790 = 0.4369$

The number of deaths caused by a head injury that would have occurred if all of the children owned helmets

$$= 79.61 \times (1 - 0.4369) = 44.83$$

(b) The number of children riding bikes

$$= 19670000 \times 0.727 = 14300000$$

(i) The probability of a child dying from a head injury on a bike if none of the children own helmets

$$= 79.61 \div 14300000 = 5.567 \times 10^{-6}$$

(ii) The probability of a child dying from a head injury on a bike if all of the children own helmets

$$= 44.83 \div 14300000 = 3.135 \times 10^{-6}$$

(c) Consider Eq. (23.5), the equivalent annual cost of a helmet

$$= \left[\frac{0.003(1.003)^4}{1.003^4 - 1} \right] 25.85 = \$6.511$$

d) Parents spend \$6.511 per year on cycling helmets. Assuming 50% of this cost represents their WTP to reduce the probability of a fatality, they are WTP \$3.256 to reduce the probability of a child dying from a head injury on a bike.

The resulting reduction in probability

$$= 5.567 \times 10^{-6} - 3.135 \times 10^{-6} = 2.432 \times 10^{-6}$$

This implies that the VSL of a young child

$$= 3.256 \div (2.432 \times 10^{-6}) = 1.339 \times 10^6$$

So the VSL of a young child is 1.34 million USD₁₉₉₇.

Worked Solution 23.4 (see Problem 23.4)

(a) The VLY can be determined from Eq. (23.5). The discount rate, $i = 0.02235$, the number of years, $N = 81 - 40 = 41$, and $VSL = £1,600,000$ so

$$VLY = \left[\frac{i}{1 - (1 + i)^{-N}} \right] VSL = £60,000$$

(b) The UK government's VSL is £1.6 million. Given that there were 50 premature deaths, the cost of the pollution is estimated at £80 million.

(c) The first step is to determine the discounted YLL. The discount rate, $i = 0.02235$, the number of years lived with disability, $N_{LD} = 4$ years, the average undiscounted number of years lost due to premature death, $N_{LL} = 81 - 65 = 16$. From Eq. (23.6) we then have that

$$YLL = \frac{1 - (1 + i)^{-N_{LL}}}{i(1 + i)^{N_{LD}}} = 12.20 \text{ years}$$

The next step is to determine the effective disability weighting factors, EDW_n , found from Eq. (23.4). From Table 23.8, $DW_{n,k} = 0.132$ for asthma, 0.406 for depression and 0.186 for heart failure. It follows that

$$EDW_{1,2,3} = 1 - (1 - 0.132)(1 - 0.406) = 0.4844$$

and

$$EDW_4 = 1 - (1 - 0.4844)(1 - 0.186) = 0.5803$$

Now we can determine the discounted YLD from Eq. (23.7)

$$\begin{aligned} YLD &= \sum_{n=1}^{N_{LD}} \frac{EDW_n}{(1 + i)^n} \\ &= \left[\frac{1 - (1 + i)^{-3}}{i} \right] \times 0.4844 + \frac{0.5803}{(1 + i)^4} = 1.922 \text{ years} \end{aligned}$$

The discounted DALY is found from

$$\text{DALY} = \text{YLL} + \text{YLD} = 12.20 + 1.922 = 14.12 \text{ years}$$

There are 50 people affected each year therefore the total number of DALYs per year is 706. Multiplying this by the VLY, obtained for part (a), then leads to £42.36 million.

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Abstract

This chapter focuses on technologies for air quality control. Pollutants include particulate matter, ozone, nitrogen oxides and sulphur oxides. Technologies covered include settling chambers, cyclone separators, electrostatic precipitators, fabric filters, wet dust scrubbers, combustion control and flue gas treatment. Mathematical equations are derived for particle settling velocities in settling chambers and particle radial velocities in cyclone separators. These are used to derive removal efficiency equations based on waste gas particle size distributions. Practical applications for settling tanks and cyclone separators are presented through a problem sheet with worked solutions.

Notation

A	Plan area [L^2].
A_p	Projected area of a particle normal to the particle movement [L^2].
B	Breadth of rectangular settling chamber [L].
C_d	Drag coefficient [-].
D	Particle diameter [L].
D_{50}	Particle diameter that has a collection efficiency of 50% [L].
D_{c1}	Cyclone separator diameter [L].
D_{c2}	Cyclone separator outlet diameter [L].
E	Collection efficiency for a single size of particle [-].
E_T	Total collection efficiency [-].
$f(v)$	Probability density function for settling velocities [$L^{-1}T$].
$F(v)$	Cumulative distribution function for settling velocities [-].
F_b	Buoyancy force [MLT^{-2}].
F_c	Centrifugal force [MLT^{-2}].
F_d	Drag force [MLT^{-2}].

F_g	Gravitational force [MLT^{-2}].
g	Gravitational acceleration [LT^{-2}].
H	Thickness of rectangular settling chamber [L].
H_c	Cyclone separator inlet height [L].
K	Dimensionless settling regime number [-].
L	Length of rectangular settling chamber [L].
L_{c1}	Cyclone body length [L].
L_{c2}	Cyclone cone length [L].
N_e	Number of effective turns [-].
Q	Volumetric flow rate [L^3T^{-1}].
r	Radius of outer vortex [L].
Re	Reynolds number [-].
t_r	Residence time [T].
t_s	Settling time [T].
v	Settling velocity [LT^{-1}].
v_i	Settling velocity for particles of diameter, D_i [LT^{-1}].
v_r	Radial velocity [LT^{-1}].
v_t	Tangential velocity [LT^{-1}].
V_p	Volume of particle [L^3].
w_i	Mass fraction of particles in a mixture with an average settling velocity, v_i [-].
W_c	Cyclone separator inlet width [L].
α	Empirical exponent for Lapple's method [-].
β	Empirical parameter describing the number of velocity heads that have been lost [-].
γ	Another empirical parameter used to determine β [-].
μ	Dynamic viscosity of fluid [$ML^{-1}T^{-1}$].
ρ	Mass density of fluid [ML^{-3}].
ρ_p	Mass density of the suspended particles [ML^{-3}].

24.1 Introduction

In Chap. 23 we saw how air pollution causes the vast majority of pollution related deaths irrespective of country income level. In this chapter we look at the main causes of air pollution and the various technologies available to reduce air pollution at the source.

The World Health Organisation identifies four important types of air pollution: (1) particulate matter, (2) ozone, (3) nitrogen dioxide and (4) sulphur dioxide. First we look at particulate matter and discuss different reduction methods including settling chambers, cyclone separators, electrostatic precipitators, fabric filters and wet dust scrubbers. Next we discuss the causes and problems of ozone and how they can

be reduced by controlling nitrogen oxides and volatile organic carbon. Nitrogen oxides result from various combustion practices. A range of different nitrogen oxide reduction strategies are discussed including fuel switching, combustion control and flue gas treatment. We then look at sulphur oxide reduction strategies associated with sour gas treatment, ore smelting and combustion of coal.

Following on from this we develop necessary theory for understanding gravity settling of suspended particles. This leads to the development of collection efficiency equations for designing settling chambers and cyclone separators. The theory of settling of particles is also used in Chap. 28, to design facilities to remove suspended particles from water. The design of flue gas treatments for reducing nitrogen oxides and sulphur oxides involve an understanding of countercurrent absorption, which is developed in Chap. 25 in the context of carbon capture and storage.

24.2 Air Quality Guidelines and Standards

Governments around the world adopt air quality standards, which specify concentrations of different pollutants considered to be acceptable in terms of what is scientifically known about the effects of each pollutant on health and on the environment. Normally the concentrations are specified in terms of a mean over a particular time-period (annual mean, 24-h mean etc.). Many standards include an aspiration to meet the World Health Organisation (WHO) air quality guidelines given in Table 24.1. Below we will discuss each of the five pollutants identified in the WHO guidelines in terms of their source, environmental impact and treatment option.

Table 24.1 WHO air quality guidelines: global update 2005 [1]

Pollutant	Concentration	Time-scale
Fine particulate matter (PM _{2.5})	10 $\mu\text{g m}^{-3}$	Annual mean
	25 $\mu\text{g m}^{-3}$	24-h mean
Coarse particulate matter (PM ₁₀)	20 $\mu\text{g m}^{-3}$	Annual mean
	50 $\mu\text{g m}^{-3}$	24-h mean
Ozone (O ₃)	100 $\mu\text{g m}^{-3}$	8-h mean
Nitrogen dioxide (NO ₂)	40 $\mu\text{g m}^{-3}$	Annual mean
	200 $\mu\text{g m}^{-3}$	1-h mean
Sulphur dioxide (SO ₂)	20 $\mu\text{g m}^{-3}$	24-h mean
	500 $\mu\text{g m}^{-3}$	10-min mean

24.3 Particulate Matter

Particulate matter (PM) affects more people than any other pollutant [1]. PM includes suspensions of both solid particles (dust, fumes, smoke and soot) and liquid droplets (spray and mists) and both organic (carbon, condensible organics etc.) and inorganic (metal oxides, salts etc.) compounds [2].

Dust includes particles formed by grinding. Fumes are solid particles formed by condensation (e.g., lead or mercury fumes). Smoke is made up of small carbonaceous particles resulting from the burning of organic matter. Main sources of PM include material handling processes (crushing or grinding ores, loading dry materials in bulk), combustion processes, industrial processes, farming (ploughing, field burning etc.), unpaved roads and road construction [2].

Particles less than $10\text{ }\mu\text{m}$ in diameter (PM_{10}) can penetrate and lodge deep inside the lungs. Particles less than $2.5\text{ }\mu\text{m}$ in diameter ($\text{PM}_{2.5}$) can penetrate the lung barrier and enter the bloodstream [1]. Health risks include heart or lung disease, non-fatal heart attacks, irregular heartbeat, aggravated asthma, decreased lung function, increased respiratory problems and lung cancer [3].

A number of different methods can be used to reduce PM from point sources. These include settling chambers, cyclone separators, electrostatic precipitators, fabric filters and wet dust scrubbers [2].

24.3.1 Settling Chambers

Settling chambers involve passing a waste gas through a sufficiently large vessel whereby the residence time is sufficient to allow suspended particles to settle out by gravity [4, p. 420] (see Fig. 24.1). Settling chambers are particularly suitable for removing particles $>50\text{ }\mu\text{m}$ ($\text{PM}_{>50}$). See Table 24.2 for an associated list of advantages and disadvantages.

Fig. 24.1 Schematic diagram of a settling chamber

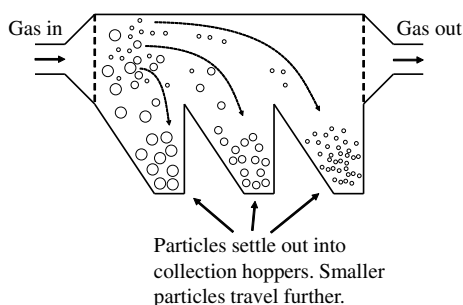


Table 24.2 Some advantages and disadvantages of settling chambers (adapted from [4, p. 422])

Advantages	Disadvantages
Simple installation and low investment cost	Poor removal efficiency for $PM_{<10}$
No moving parts hence low maintenance and operating cost	Unable to handle sticky materials
Low energy consumption	Large space requirement

24.3.2 Cyclone Separators

Cyclone separators operate by creating a double vortex inside a cyclone body [4, p. 423] (see Fig. 24.2). Incoming gas is forced into a circular motion. Suspended particles collide with the walls of the vessel due to centrifugal forces. Following collision, they fall to the bottom of the cyclone and are collected in a hopper. Efficiency can be improved by spraying water into the gas stream (this is done in wet cyclones) to increase the weight of the particulate material, hence giving it greater inertia and likelihood of collision with the vessel walls. Cyclone separators are particularly suitable for removing particles $>10\text{ }\mu\text{m}$ ($PM_{>10}$). See Table 24.4 for an associated list of advantages and disadvantages.

24.3.3 Electrostatic Precipitators

Electrostatic precipitators (ESP) uses electrical forces to move particles entrained within a waste gas stream onto collector plates [4, p. 428] (see Fig. 24.3). Entrained

Fig. 24.2 Schematic diagram of a cyclone separator. A list of standard design ratios is given in Table 24.3

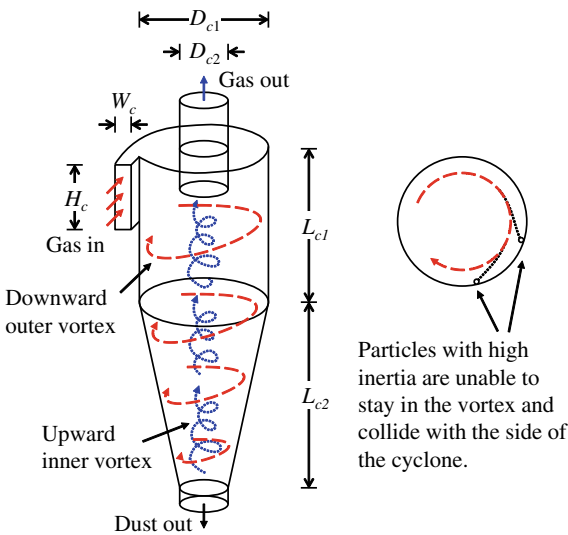


Table 24.3 Standard design ratios for the cyclone separator shown in Fig. 24.2 (after [5, p. 315])

Feature	Ratio	Value
Inlet height	H_c/D_{c1}	0.5
Inlet width	W_c/D_{c1}	0.25
Gas exit diameter	D_{c2}/D_{c1}	0.5
Body length	L_{c1}/D_{c1}	1.75
Cone length	L_{c2}/D_{c1}	2.0

Table 24.4 Some advantages and disadvantages of cyclone separators (adapted from [4, p. 427])

Advantages	Disadvantages
Simple installation and low investment cost.	Low removal efficiency for $PM_{<10}$
No moving parts hence low maintenance and operating cost	Relatively high pressure drop hence high energy requirements
PM can be removed dry, which is good for recycling	Unable to handle sticky materials
Low space requirements	Noise

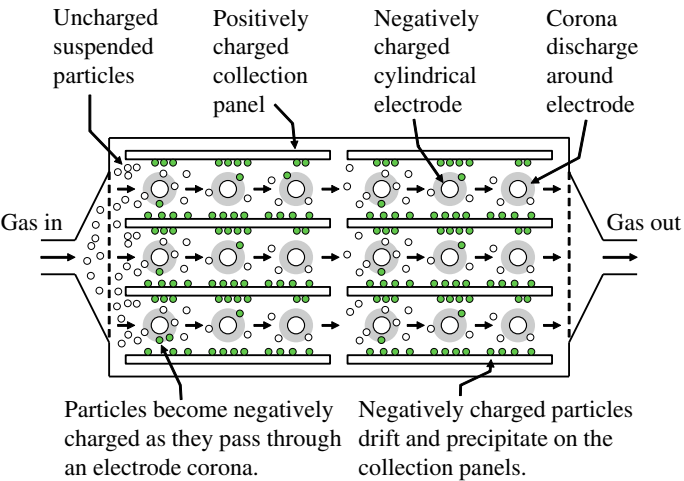


Fig. 24.3 Schematic diagram of an electrostatic precipitator

particles are given an electrical charge as they pass through a corona where gaseous ions flow. Electrodes in the centre of the flow lane are maintained at a high voltage and generate the electrical field that forces the particles to the collector walls. Particles are removed from the collector walls by periodic tapping or shaking such that they fall to the base of the vessel and are collected in a hopper. ESP can remove PM_5 with >99.9% efficiency and PM_1 with >97% efficiency [4]. See Table 24.5 for an associated list of advantages and disadvantages.

Table 24.5 Some advantages and disadvantages of electrostatic precipitators (adapted from [4, p. 435])

Advantages	Disadvantages
High efficiency with small particles	High voltage hazard requires specialist training
Low pressure drop and therefore low energy requirement	Relatively large space required
PM can be removed dry, which is good for recycling	Requires relatively consistent gas stream

24.3.4 Fabric Filters

Fabric filters involve forcing waste gas through tightly woven fabric, which filters out the PM [4, p. 446]. Typical configurations include baghouse filters where gas is forced upwards through vertically suspended cylindrical fabric bags (see Fig. 24.4). A dust cake forms inside the bag, which increases the removal efficiency of increasingly smaller particles. However, eventually the pressure loss across the dust cake becomes prohibitively high such that the cake must be removed by shaking the bags. The dust then falls to the base of the vessel where it can be removed by a collection hopper. See Table 24.6 for an associated list of advantages and disadvantages.

24.3.5 Wet Dust Scrubbers

Wet dust scrubbing involves extracting dust by intensively mixing waste gas with water. Aside from dust, other pollutants such as SO₂, NH₃, volatile organic carbon

Fig. 24.4 Schematic diagram of a baghouse fabric filter

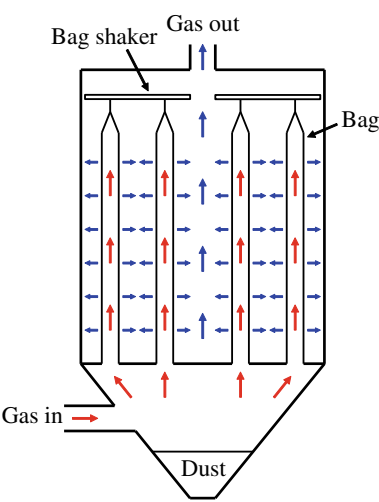


Table 24.6 Some advantages and disadvantages of fabric filters (adapted from [4, p. 456])

Advantages	Disadvantages
High removal efficiency for coarse and fine particles	Maximum operating temperature due to fire risk of fabric
Particles are removed dry and can be suitable for recycling	Not suitable for wet or sticky dusts
Reliable and simple operation	High space requirements

Table 24.7 Some advantages and disadvantages of wet dust scrubbers (adapted from [4, p. 445])

Advantages	Disadvantages
Can handle gas streams containing flammable and explosive chemicals with low risk	Significant water usage and wastewater generation
Provides cooling for hot gases	Waste gas may require reheating to reduce plume visibility
Simultaneous removal of dust and water soluble components	PM may be contaminated, which may prohibit recycling
Corrosive gases can be neutralised	Protection against freezing required

(VOC) and heavy metals, which may be attached to the dust, will also be removed [4]. See Table 24.7 for an associated list of advantages and disadvantages.

There are several different configurations including fibrous packing scrubbers, moving bed scrubbers, plate scrubbers, spray towers and venturi scrubbers [4, p. 437]. For brevity we will focus on spray towers since they are a good example to illustrate the key features (see Fig. 24.5).

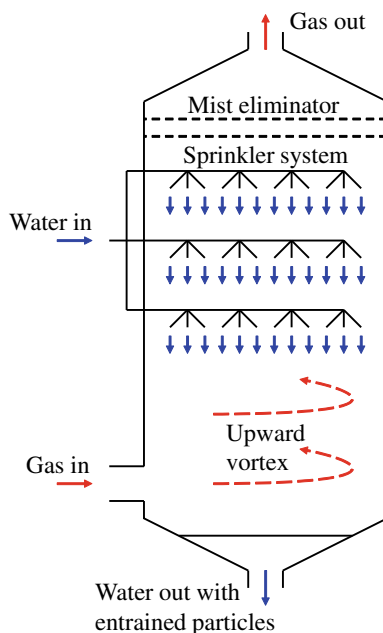
Waste gas enters the base of a spray tower through an inlet on the side and exits the tower through an outlet at the top. The gas flow pattern within the tower assumes an upward vortex. Water sprinklers are placed at multiple vertical intervals within the tower. The water increases the mass of the suspended particles whilst centrifugal forces cause particles to collide with the side of the vessel. Separated particles are collected in a hopper at the base of the dust scrubber.

24.4 Ozone

Ground level ozone (O_3) is the main component of photochemical smog. O_3 is formed when sunlight reacts with pollutants such as nitrogen oxides (NO_x) and volatile organic compounds (VOC) (i.e., a photochemical reaction) [1]. High levels of O_3 tend to occur where there are high levels of sunshine in the presence of high concentrations of NO_x and VOC (both emitted by vehicles for example).

Ozone causes muscles in the airways in the respiratory system to constrict, trapping air in the alveoli that leads to wheezing and shortness of breath [3]. Ozone can

Fig. 24.5 Schematic diagram of a sprinkler tower



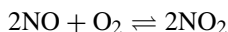
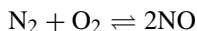
also have adverse effects on vegetation by reducing photosynthesis, slowing plant growth and increasing plant vulnerability to other sources of harm [3]. Control of ground level ozone is best achieved by reducing emissions of NO_x and VOC.

24.5 Nitrogen Oxides

Breathing air with high nitrogen dioxide, NO_2 , concentrations can irritate airways in the respiratory system [3]. It can also form an important fraction of $\text{PM}_{2.5}$ and lead to the development of O_3 [1].

Nitrogen oxides (NO_x) are formed when any fuel is burned in air (vehicles, power generation, boilers, wood burning etc.). Although there are seven oxides of nitrogen known to occur, NO and NO_2 are the most significant in the context of air pollution [6, p. 523]. Furthermore, once emitted to the atmosphere, NO will rapidly oxidise to form NO_2 [3], hence the WHO only specifically provides guidelines for NO_2 .

Relevant stoichiometric relationships include [6, p. 527]



24.5.1 Fuel, Thermal and Prompt NO_x

Engineers typically distinguish between (1) Fuel NO_x, (2) Thermal NO_x and (3) Prompt NO_x. An understanding about why this is the case is important to help explain current approaches to reducing NO_x in emissions.

Some fuels contain organically-bound nitrogen (primary coal or heavy oil). When such fuels are burned with sufficiently high oxygen concentrations, the nitrogen component will oxidise to form NO_x, referred to as fuel NO_x [6, p. 524].

Where fuels are burned in air, molecular nitrogen, N₂, will be present at high concentrations. High temperatures and high oxygen concentrations leads to oxidation of N₂ to form NO_x, referred to as thermal NO_x. The rate of oxidation is strongly dependent on temperature [6, p. 529].

The presence of hydrocarbon radicals within a combustion chamber will significantly increase the rate of NO_x formation. NO_x associated with hydrocarbon radicals is therefore referred to as prompt NO_x [6, p. 531]. Furthermore, prompt NO_x formation will persist at much lower temperatures and oxygen concentrations than required for thermal NO_x formation.

Three associated categories of NO_x reduction methods include fuel switching, combustion control and flue gas treatment.

24.5.2 Fuel Switching

Fuel NO_x formation can be minimised by avoiding fuels containing organically-bound nitrogen. In some cases, operators exchange high-N fuels for low-N fuels (e.g., natural gas) during periods of intensive sunshine so as to avoid emissions leading to O₃ generation [3].

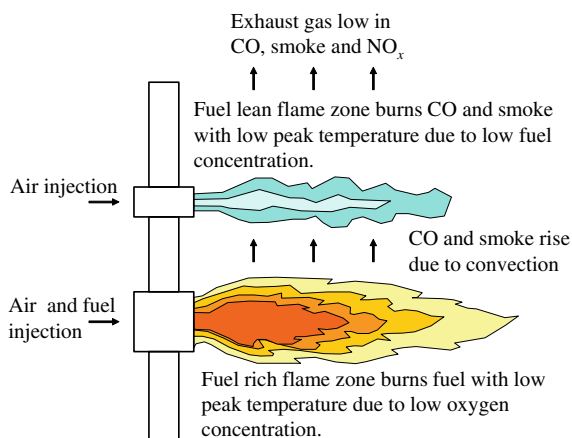
24.5.3 Combustion Control

Thermal NO_x formation can be reduced by minimising the residence time, peak temperature and/or oxygen concentration within the flame zone of a combustion chamber [6, p. 537]. There are a number of different combustion control measures that can be taken to achieve this.

Peak temperature within a combustion chamber occurs within the flame zone. Air-fuel equivalence ratio (AFER) is an important control factor. An AFER of one corresponds to when the minimum amount of oxygen is supplied to completely burn the associated fuel under ideal conditions. However, because oxygen, fuel and temperature are rarely uniformly distributed within a furnace, an AFER of one will generally lead to incomplete combustion of fuel, giving rise to CO and smoke formation. Therefore excess air is often provided to ensure CO and smoke production are sufficiently low.

When AFER is less than one, a burner is said to be fuel rich. When AFER is greater than one, excess air is present and a burner is said to be fuel lean. Whilst fuel

Fig. 24.6 Schematic diagram of a dual flame zone for off-stoichiometric combustion



lean burners benefit from low CO and smoke formation, the excess oxygen leads to high temperatures within the flame zone and excessive thermal NO_x formation. Careful combustion control measures are therefore required to collectively minimise CO, smoke and NO_x formation.

One such method is off-stoichiometric combustion (OSC). The approach is to provide two or more flame zones within the combustion chamber [6, p. 538] (see Fig. 24.6). Fuel is injected into a fuel rich primary flame zone (i.e. with low AFER) at the base of the burner. The advantage is that the peak temperature is reduced and oxygen concentrations remain low such that thermal NO_x formation is minimised. A secondary lean flame zone (i.e. with high AFER) is developed above by injecting an additional air stream without injecting additional fuel. Combustion of the remaining fuel, CO and smoke is completed within the secondary flame zone.

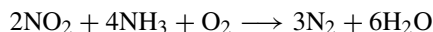
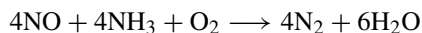
Although this latter flame zone is oxygen rich, the peak temperature is low due to the lack of fuel, hence low levels of thermal NO_x formation are maintained without producing a CO and smoke rich exhaust gas. Note that reducing the peak temperature in the flame zone does not necessarily lead to reduced total heat flux from the furnace.

Other combustion control measures include low-excess-air firing, flue gas recirculation, gas reburning, reduced air preheat and water injection [6, pp. 538–540]. Which ever method is adopted, accurate temperature and oxygen concentration monitoring systems throughout the furnace are critical for ensuring successful operation.

24.5.4 Flue Gas Treatment

Combustion measures can lead to significant reduction in thermal NO_x formation but are unlikely to have a large impact on fuel or prompt NO_x formation. Therefore flue gas treatment techniques are also required. A common approach is to perform a selective reduction by mixing flue gas with ammonia (NH_3). NO and NO_2 will react

with NH_3 in the presence of O_2 to form N_2 and H_2O . The relevant stoichiometric relationships are [6, p. 544]



Non-catalytic selective reduction requires temperatures between 900°C and 1000°C [6, p. 548]. However, the same reactions will occur at between 300°C and 400°C in the presence of an appropriate catalyst [6, p. 544]. Relevant catalyst materials include vanadium pentoxide, titanium dioxide and tungsten trioxide [6, p. 546].

24.6 Sulphur Oxides (SO_x)

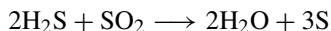
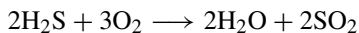
The term sulphur oxides (SO_x) accounts for sulphur dioxide (SO_2), sulphur trioxide (SO_3) and sometimes sulphuric acid (H_2SO_4). Anthropogenic SO_x mostly results from the burning of fossil fuels and the smelting of sulphur containing mineral ores [1].

Health issues associated with SO_x include irritation of the eyes, inflammation of the respiratory tract, coughing, mucus secretion, aggravation of asthma and chronic bronchitis [1]. SO_x emissions are also a major contributor to acid rain, which is damaging to both buildings and vegetation.

SO_x emissions can be reduced by either removing sulphur from fuel/ore before it is burned/smelted or removing SO_x from the waste gas stream.

24.6.1 Recovering Sulphur from Sour Gas

Natural gas often includes a hydrogen sulphide component (H_2S). Gases with high and low H_2S content are referred to as sour and sweet gases, respectively. The Claus process can be used to recover the sulphur from H_2S in element form. This involves partially burning the H_2S to form SO_2 , which is then mixed with the remainder of the H_2S to form water and element sulphur. The net reactions are [6, p. 488]:

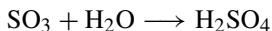
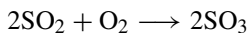
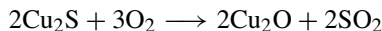


Element sulphur is a valuable commodity used in many different industrial processes.

24.6.2 Recovering Sulphuric Acid from Sulphide Ores

Sulphur can be removed from sulphide ores of copper, zinc, lead and nickel prior to smelting by pre-heating in air (roasting), which produces a concentrated stream of SO_2 . The SO_2 is then oxidised in air again to form SO_3 , which is then absorbed in

water to make sulphuric acid (H_2SO_4) [6, p. 489]. An example set of reactions for extracting H_2SO_4 by roasting chalcocite are:

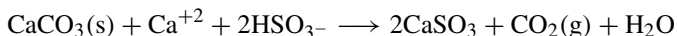
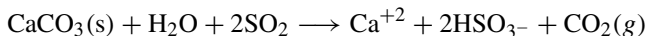


Absorption typically takes place within an absorption tower (very similar to the wet dust scrubbing spray tower described above), which typically involves spraying water on the gas stream such that the SO_3 reacts with the water to form the H_2SO_4 . The sulphuric acid is collected at the base and can be sold on as a valuable commodity.

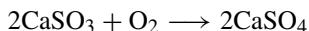
Commonly, absorption towers are packed with inert solid materials of various geometric shapes, designed to maximise interfacial area between the gas and absorbent whilst minimising pressure loss within the tower [6, p. 418].

24.6.3 Forming Gypsum From Sulphur Dioxide in Flue Gas

Burning of coal represents a significant source of SO_2 . Limestone scrubbing is a commonly applied removal process. The main benefit of limestone scrubbing compared to alternative methods is that limestone is often available in large quantities and at low cost. The flue gas mixture from a combustion chamber is typically driven upwards through an absorption tower (again very similar to the wet dust scrubbing spray tower described above) where it is sprayed with a limestone slurry. The slurry reacts with the SO_2 to produce calcium sulphite (CaSO_3). The reaction sequence is as follows [6, p. 491]:



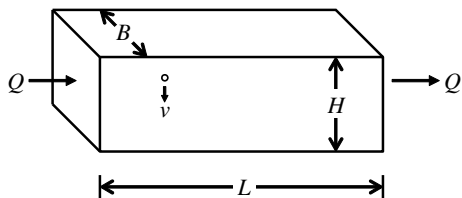
The calcium sulphite can then be oxidized in air to form gypsum (CaSO_4), which is an important building material used in plaster and cement.



24.7 Particle Settling Theory

In this section we develop the necessary equations to design and analyse settling chambers (Sect. 24.3.1) and cyclone separators (Sect. 24.3.2). Theory developed here is also subsequently used when we look at the removal of suspended solids from water using clarifiers (Sect. 28.2.3) and the cleansing of water filters by back-washing (Sect. 28.3.4). First we derive expressions for collection efficiency in terms of particle settling velocity. We then derive expressions for calculating the settling velocity of spherical particles in terms of Reynolds number. A problem with the

Fig. 24.7 Schematic diagram of a rectangular settling chamber



Reynolds number is that it requires a priori knowledge about settling velocity. However, it is possible to derive a dimensionless settling regime number which enables the elimination of the Reynolds number and explicit calculation of settling velocity. We subsequently show how the centrifugal acceleration in a cyclone separator is analogous to gravitational acceleration in a settling chamber. Finally we derive an additional collection efficiency equation for a cyclone separator.

24.7.1 Collection Efficiency

24.7.1.1 Collection Efficiency for Single Particle Size

Consider a rectangular settling chamber of breadth, B [L], thickness, H [L], and length, L [L] (see Fig. 24.7). A mixture of fluid and suspended particles moves through the chamber at a steady volumetric flow rate, Q [L³T⁻¹]. The suspended particles are identical in nature and settle at a steady velocity, v [LT⁻¹].

The residence time of fluid in the settlement chamber, t_r [T], is found from

$$t_r = \frac{BHL}{Q}$$

The time it takes for suspended particles to travel from the top of the chamber to bottom of the chamber, t_s [T], is found from

$$t_s = \frac{H}{v}$$

If $t_r > t_s$ then all the suspended particles will be retained. It follows that for a settling chamber that retains all suspended particles

$$\frac{BHL}{Q} > \frac{H}{v}$$

The plan area, $A \equiv BL$ [L²], of the settling chamber required to ensure all suspended particles are retained is therefore found from

$$A = \frac{Q}{v} \quad (24.1)$$

Suppose that $A < \frac{Q}{v}$. In that case not all of the particles will be retained. An estimate for the collection efficiency, E [-], of a settling chamber can be obtained from [7, p. 289]

$$E(v) = \begin{cases} 1, & v > \frac{Q}{A} \\ \frac{Av}{Q}, & v \leq \frac{Q}{A} \end{cases} \quad (24.2)$$

The collection efficiency represents the fraction of particles entering a settling chamber that will be retained due to gravitational settling.

24.7.1.2 Collection Efficiency for a Distribution of Particle Sizes

Suppose that the suspended particles possess a random distribution of settling velocities. Let $F(v)$ [-] be the mass fraction of suspended particles that have a settling velocity less than v . The term $F(v)$ represents a cumulative distribution function (CDF), defined by

$$F(v) = \int_{-\infty}^v f(v) dv$$

where $f(v)$ [$L^{-1}T$] is the underlying probability density function (PDF).

The total collection efficiency of a settling chamber for such a particle mixture, E_T [-], is found from

$$E_T = \int_{-\infty}^{\infty} E(v) f(v) dv$$

where $E(v)$ is found from Eq. (24.2).

The CDF is often characterised by a discrete set of data describing an experimentally obtained particle size distribution. In this case

$$F(v_k) = \sum_{i=1}^k w_i$$

where w_i [-] is the mass fraction of particles in a mixture with an average settling velocity of v_i [LT^{-1}]. The corresponding total collection efficiency is obtained from

$$E_T = \sum_{i=1}^N E(v_i) w_i \quad (24.3)$$

where N is the total number of discrete data points.

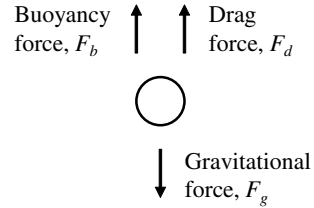
24.7.2 Settling Velocity

Consider a particle of volume, V_p [L^3], and density, ρ_p [ML^{-3}], falling through an otherwise static body of fluid of density, ρ [ML^{-3}], at a steady settling velocity, v [LT^{-1}]. A frictional resistance develops as the particle moves through the fluid. The resulting drag force, F_d [MLT^{-2}], is found from [8, p. 325]

$$F_d = \frac{\rho v^2 C_d A_p}{2} \quad (24.4)$$

where A_p [L^2] is the projected area of the particle normal to the particle movement and C_d [-] is known as the drag coefficient.

Fig. 24.8 Force balance on a settling particle



Challenge 24.1 Use a force balance to derive an expression for the settling velocity of the particle in terms of the dimensions of the particle, the difference between the two mass densities and the drag coefficient.

The presence of a steady vertical velocity implies a force balance in the vertical direction. Three forces are acting on the particle including, a downward gravitational force, F_g [MLT^{-2}], due to the self-weight of the particle, an upward buoyancy force, F_b [MLT^{-2}], due to the weight of fluid displaced by the particle and the drag force (see Sect. 1.2.4.1), F_d , which is upward acting (see Fig. 24.8).

It follows that

$$F_g = F_b + F_d \quad (24.5)$$

where

$$F_g = V_p \rho_p g \quad \text{and} \quad F_b = V_p \rho g \quad (24.6)$$

Substituting Eqs. (24.4) and (24.6) into Eq. (24.5) gives us

$$V_p \rho_p g = V_p \rho g + \frac{\rho v^2 C_d A_p}{2} \quad (24.7)$$

and solving Eq. (24.7) for v^2 leads to

$$v^2 = \frac{2V_p(\rho_p - \rho)g}{\rho C_d A_p} \quad (24.8)$$

Now consider a spherical particle of diameter, D [L]. In this case, $V_p = \frac{\pi D^3}{6}$ and $A_p = \frac{\pi D^2}{4}$ so

$$v^2 = \frac{4D(\rho_p - \rho)g}{3\rho C_d} \quad (24.9)$$

24.7.2.1 Spherical Particles with Laminar Flow

The drag force due to laminar flow around a spherical particle of diameter, D [L], is found from Stokes' Law [8, p. 331]

$$F_d = 3\pi D\mu v \quad (24.10)$$

where μ [$\text{ML}^{-1}\text{T}^{-2}$] is the dynamic viscosity of the fluid.

The Reynolds number, Re [-], for flow around a sphere is found from

$$Re = \frac{\rho v D}{\mu} \quad (24.11)$$

Challenge 24.2 Determine an expression for the drag coefficient in terms of Reynolds number, which describes laminar flow around a sphere. Then derive an associated concise expression for the settling velocity of a spherical particle.

Noting that $A_p = \frac{\pi D^2}{4}$, equating Eqs. (24.4) and (24.10) leads to

$$\frac{\pi \rho v^2 C_d D^2}{8} = 3\pi D \mu v \quad (24.12)$$

Solving Eq. (24.12) for C_d and substituting Eq. (24.11) gives us [8, p. 331]

$$C_d = \frac{24}{Re}, \quad Re < 0.1 \quad (24.13)$$

Substituting Eqs. (24.11) and (24.13) into Eq. (24.9) leads to [8, p. 335]

$$v = \frac{D^2(\rho_p - \rho)g}{18\mu}, \quad Re < 0.1 \quad (24.14)$$

24.7.2.2 Spherical Particles with General Flow

Under turbulent flow conditions [9, p. 187]

$$C_d = 0.44, \quad 500 < Re < 10^5$$

In the context of settling spherical particles, the following general expression is often adopted [10, p. 792]

$$C_d = \begin{cases} \frac{24}{Re}, & Re < 2 \\ \frac{18.17}{Re^{0.5987}}, & 2 \leq Re \leq 500 \\ 0.44, & 500 < Re < 2 \times 10^5 \end{cases} \quad (24.15)$$

Note that the equation for the transition region, $Re \in [2, 500]$, has been obtained by fitting a power law to link the end points of the laminar flow and turbulent flow models.

We need to know the Reynolds number to calculate the drag coefficient, which we need in order to calculate the settling velocity (recall Eq. (24.9)). A problem with the above set of equations is that we need to know the settling velocity to calculate the Reynolds number.

Challenge 24.3 Develop a criterion, alternative to Reynolds number, for determining which drag coefficient expression should be used to calculate settling velocity, without prior knowledge of the settling velocity.

Substituting Eq. (24.9) into Eq. (24.11) gives us

$$\text{Re} = \frac{\rho D}{\mu} \sqrt{\frac{4D(\rho_p - \rho)g}{3\rho C_d}} \quad (24.16)$$

Transferring all the dimensionless terms in Eq. (24.16) to the left-hand-side leads to [10, p. 793]

$$K \equiv \left(\frac{3C_d \text{Re}^2}{4} \right)^{1/3} = \left[\frac{D^3 \rho (\rho_p - \rho) g}{\mu^2} \right]^{1/3} \quad (24.17)$$

where K represents a dimensionless settling regime number.

From Eq. (24.15) we know the values of C_d at the critical values of Re and can therefore determine corresponding values of K . At $\text{Re} = 2$, $C_d = 12$ and $K = 3.302$. At $\text{Re} = 500$, $C_d = 0.44$ and $K = 43.53$. At $\text{Re} = 2 \times 10^5$, $C_d = 0.44$ and $K = 2363$. It follows that

$$C_d = \begin{cases} \frac{24}{\text{Re}}, & K < 3.302 \\ \frac{18.17}{\text{Re}^{0.5987}}, & 3.302 \leq K \leq 43.53 \\ 0.44, & 43.53 < K < 2363 \end{cases} \quad (24.18)$$

Challenge 24.4 Use Eq. (24.17) to completely eliminate Reynolds number from Eq. (24.18).

Solving Eq. (24.17) for Re^2 gives us

$$\text{Re}^2 = \frac{4K^3}{3C_d} \quad (24.19)$$

Substituting Eq. (24.19) into Eq. (24.18) leads to [7, p. 273]

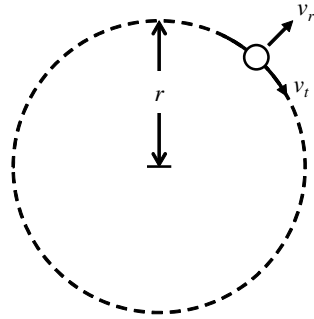
$$C_d = \begin{cases} \frac{432}{K^3}, & K < 3.302 \\ \frac{55.46}{K^{1.282}}, & 3.302 \leq K \leq 43.53 \\ 0.44, & 43.53 < K < 2363 \end{cases} \quad (24.20)$$

The advantage of the Eq. (24.20) over Eq. (24.15) is that it enables the determination of C_d without prior knowledge of v .

24.7.3 Cyclonic Separation

Cyclone separators involve passing fluid into a funnel shaped device. The funnel geometry causes the fluid to form a downward outer vortex, which is reflected from the base as an upward inner vortex, which is directed to a fluid outlet at the top of the device (see Fig. 24.2). Fluid rotates around the vertical axis of the separator and the centrifugal forces in the outer vortex drive suspended particles to the outer casing.

Fig. 24.9 Schematic diagram illustrating the directions of the tangential velocity, v_t , and radial velocity, v_r , of a particle within the downward outer vortex of a cyclonic separator



Following collision, these particles lose their suspension and slide down the walls to a collection hopper at the base.

Let v_t [LT^{-1}] be the average tangential velocity within the outer vortex and r [L] be the average radius of the outer vortex (see Fig. 24.9). The resulting centrifugal force on a suspended particle is found from [5, p. 311]

$$F_c = \frac{V_p \rho_p v_t^2}{r} \quad (24.21)$$

An associated buoyancy force and drag force are also developed:

$$F_b = \frac{V_p \rho v_t^2}{r} \quad (24.22)$$

$$F_d = \frac{\rho v_r^2 C_d A_p}{2} \quad (24.23)$$

where v_r [LT^{-1}] is the radial velocity of the suspended particle travelling away from the centre of the vortex (see Fig. 24.9).

The tangential velocity can be related back to the volumetric flow rate of gas through the separator, Q [L^3T^{-1}], through

$$v_t = \frac{Q}{W_c H_c} \quad (24.24)$$

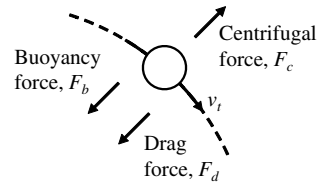
where W_c [L] and H_c [L] are the width and height of the inlet, respectively, as indicated in Fig. 24.2.

Challenge 24.5 Assume steady-state laminar flow conditions and derive a concise expression for the radial velocity, v_r , of a suspended spherical particle of diameter, D .

Under steady-state conditions, a suspended particle will travel, within the downward outer vortex, at a constant velocity and the following force balance will apply (see Fig. 24.10)

$$F_c = F_b + F_d \quad (24.25)$$

Fig. 24.10 Force balance on a particle within the downward outer vortex of a cyclonic separator



Substituting Eqs. (24.21), (24.22) and (24.23) into Eq. (24.25) and solving for v_r^2 gives us

$$v_r^2 = \frac{2V_p(\rho_p - \rho)v_t^2}{\rho C_d A_p r} \quad (24.26)$$

Note that Eq. (24.26) becomes identical to Eq. (24.8) when $v_t^2/r = g$. It follows that for a spherical particle of diameter, D , travelling under laminar flow conditions (consider Eq. (24.14))

$$v_r = \frac{D^2(\rho_p - \rho)v_t^2}{18\mu r}, \quad \text{Re} < 0.1 \quad (24.27)$$

24.7.3.1 Collection Efficiency

The residence time within the outer vortex, t_r [T], is found from

$$t_r = \frac{2\pi N_e r}{v_t} \quad (24.28)$$

where N_e [-] is the number of “effective turns” within the vortex, typically found from [6, p. 140]

$$N_e = \frac{1}{H_c} \left(L_{c1} + \frac{L_{c2}}{2} \right) \quad (24.29)$$

where H_c [L] is the inlet, L_{c1} [L] is the length of cyclone body and L_{c2} [L] is the length of cyclone lower cone, as indicated in Fig. 24.2.

The time it takes for a particle starting at the inner boundary of the outer vortex to collide with the outer casing, t_c [T], is found from

$$t_c = \frac{W_c}{v_r} \quad (24.30)$$

where W_c [L] is the inlet width, as indicated in Fig. 24.2.

Providing $t_c < t_r$, all suspended particles of radial velocity, v_r , will be retained by the cyclone separator. Suppose that $t_c > t_r$. In that case not all of the particles will be retained. Similar, to Eq. (24.2), the collection efficiency, E [-], of the cyclone separator can be estimated from

$$E = \begin{cases} 1, & t_c < t_r \\ \frac{t_r}{t_c}, & t_c \geq t_r \end{cases}$$

Substituting Eqs. (24.27), (24.28) and (24.30) then leads to

$$E(D) = \begin{cases} 1, & t_c < t_r \\ \frac{\pi N_e D^2 (\rho_p - \rho) v_t}{9\mu W_c}, & t_c \geq t_r \end{cases} \quad (24.31)$$

24.7.3.2 Lapple's Method

It is generally found that Eq. (24.31) is quite accurate at determining the diameter of particles that have a 50% collection efficiency. However, above and below 50% efficiency, Eq. (24.31) tends not to be sufficiently accurate. Instead, collection efficiency for cyclone separators is often determined from the following empirical equation [3,5,6]

$$E(D) = \left[1 + \left(\frac{D_{50}}{D} \right)^\alpha \right]^{-1} \quad (24.32)$$

where D_{50} [L] is the particle diameter that has a collection efficiency, according to Eq. (24.31), of 50%, and α is an empirical exponent that ranges from 2 to 6.

Substituting $E = 0.5$ and $D = D_{50}$ in Eq. (24.31) and solving for D_{50} leads to

$$D_{50} = \sqrt{\frac{9\mu W_c}{2\pi N_e (\rho_p - \rho) v_t}} \quad (24.33)$$

The use of Eqs. (24.32) and (24.33) is widely referred to as Lapple's method and attributed to [11].

24.7.3.3 Pressure Loss

Generally it is found that the smaller the diameter of the cyclone, D_{c1} , the higher the collection efficiency. However, with reducing diameter comes increasing pressure loss across the cyclone separator. Therefore a reduction in the size of the separator leads to benefits in collection efficiency but at the expense of increased energy requirements to push the waste gas through the system.

The pressure loss across a cyclone separator, ΔP [$\text{ML}^{-1}\text{T}^{-2}$], is typically a linear function of the velocity head associated with the tangential velocity, v_t [6, p. 146]:

$$\Delta P = \frac{\beta \rho v_t^2}{2} \quad (24.34)$$

where β [-] is an empirical parameter describing the number of velocity heads that have been lost, which can be estimated from

$$\beta = \frac{\gamma H_c W_c}{D_{c2}^2}$$

where H_c , W_c and D_{c2} are cyclone dimensions, as shown in Fig. 24.2, and γ is an empirical coefficient commonly taken to be 16. For the standard design ratios shown in Table 24.3, $\beta = 8$.

24.8 Problem Sheet

Problem 24.1 (see Worked Solution 24.1)

A dust-laden gas stream is discharged at $3.68 \text{ m}^3 \text{ s}^{-1}$. The density and dynamic viscosity of the gas are 1.24 kg m^{-3} and $18.3 \text{ } \mu\text{Pa s}$, respectively. The density of the particles is 7620 kg m^{-3} .

- Determine the area of a settling chamber required to remove all particles greater than $35 \text{ } \mu\text{m}$ diameter.
- Determine the collection efficiency of the same settling chamber for removing particles of $20 \text{ } \mu\text{m}$ diameter from the same gas stream.

Problem 24.2 (see Worked Solution 24.2)

A settling chamber, of plan area 15.1 m^2 , is used to remove particulate matter from waste gas, which exits a furnace at a rate of $3.68 \text{ m}^3 \text{ s}^{-1}$. The density of the particles is 2650 kg m^{-3} . The density and viscosity of the gas are 1.01 kg m^{-3} and $26.0 \text{ } \mu\text{Pa s}$, respectively. The particle size distribution data for the waste gas entering the settling chamber is given in Table 24.8. Determine the total collection efficiency of the settling chamber and the total exiting mass concentration of particulate matter leaving the settling chamber.

Problem 24.3 (see Worked Solution 24.3)

Standard design cyclone separators (i.e., ones that use the design ratios given in Table 24.3) are used to remove particulate matter from waste gas, which is produced

Table 24.8 Particle size distribution for the waste gas in Problem 24.2

Particle size range (μm)	Median particle diameter (μm)	Mass concentration (mg m^{-3})
0–20	10	219
20–30	25	562
30–40	35	763
40–50	45	855
50–60	55	855
60–70	65	770
70–80	75	569
80–94	87	770
>94	>94	2760

Table 24.9 Particle size distribution for the waste gas in Problem 24.3

Median particle diameter (μm)	Mass fraction (%)
1	3
5	20
10	15
20	20
30	16
40	10
50	6
60	3
100	7

at a rate of $20 \text{ m}^3 \text{ s}^{-1}$. The density of the particles is 2900 kg m^{-3} . The density and viscosity of the gas are 1.29 kg m^{-3} and $20.0 \mu\text{Pa s}$, respectively. The particle size distribution data for particles suspended within the waste gas entering the settling chamber is given in Table 24.9. Determine the total collection efficiency and the energy requirement using:

- (a) One cyclone separator of diameter, $D_{c1} = 3 \text{ m}$.
- (b) One cyclone separator of diameter, $D_{c1} = 1 \text{ m}$.
- (c) Two parallel cyclone separators of diameter, $D_{c1} = 1 \text{ m}$.
- (d) Nine parallel cyclone separators of diameter, $D_{c1} = 1 \text{ m}$.

Assume $\alpha = 2$ in Lapple's equation (Eq. (24.32)).

24.9 Worked Solutions

Worked Solution 24.1 (see Problem 24.1)

(a) The plan area of the settling chamber can be determined from Eq. (24.1) where the discharge rate, $Q = 3.68 \text{ m}^3 \text{ s}^{-1}$. Assuming the particles are spherical, the settling velocity, v , can be determined from Eq. (24.9). Let $D = 35 \times 10^{-6} \text{ m}$, $\rho_p = 7620 \text{ kg m}^{-3}$ and $\rho = 1.24 \text{ kg m}^{-3}$. The remaining term to be calculated is the drag coefficient, C_d , which can be determined from Eq. (24.20). This in turn, requires a value for the dimensionless settling regime number, K , which is found from Eq. (24.17). Letting $\mu = 18.3 \times 10^{-6} \text{ Pa s}$, it is found that $K = 2.281$. It follows that

$C_d = 36.41$ and $v = 0.2779 \text{ m s}^{-1}$. The required plan area of the settling chamber is therefore $3.68 \div 0.2779 = 13.24 \text{ m}^2$.

(b) The efficiency of the chamber at removing particles of $20 \text{ }\mu\text{m}$ diameter can be found from Eq. (24.2). From part (a) we have that $A = 13.24 \text{ m}^2$ and $Q = 3.68 \text{ m}^3 \text{ s}^{-1}$. However, in this case $D = 20 \times 10^{-6} \text{ m}$ so $K = 1.303$, $C_d = 195.1$ and $v = 0.09076 \text{ m s}^{-1}$. The efficiency of the settling chamber at removing $20 \text{ }\mu\text{m}$ particles is therefore $13.24 \times 0.09076 \div 3.68 = 0.3265$. This means that the chamber would only remove 32.7% of particles, which have a diameter of $20 \text{ }\mu\text{m}$.

Worked Solution 24.2 (see Problem 24.2)

This involves using Eq. (24.3). The following MATLAB code can be used:

```
A=15.1; %Area of chamber (m2)
Q=3.68; %Flow rate (m3/s)
rho_p=2650; %Density of particles (kg/m3)
rho=1.01; %Density of air (kg/m3)
mu=26e-6; %Viscosity of air (Pa s)
g=9.81; %Gravitational acceleration (m/s2)
%Median diameter of particles (m)
D=[10 25 35 45 55 65 75 87 94]*1e-6;
%Mass concentration (mg/m3)
C=[219 562 763 855 855 770 569 770 2760];
%Determine settling regime number
K=D*(rho*(rho_p-rho)*g/mu^2)^(1/3);
%Determine drag coefficient
Cd=432./K.^3;
Cd(K>3.302)=55.46./K(K>3.302).^1.282;
Cd(K>43.53)=0.44;
%Determine settling velocities
vi=sqrt(4*D*(rho_p-rho)*g/3/rho./Cd);
%Determine efficiency factor for each diameter
Ei=A*vi/Q;
Ei(vi>Q/A)=1;
%Determine mass fractions
wi=C/sum(C);
%Determine total efficiency
Et=sum(Ei.*wi);
Cin=sum(C); %Inlet concentration (mg/m3)
Cout=Cin*(1-Et); %Outlet concentration (mg/m3)
num2str([Cin Et Cout]',3) %Print results
```

The total particulate matter mass concentration in the gas entering the chamber is 8120 mg m^{-3} . The total collection efficiency of the chamber is 0.754. The total

particulate matter mass concentration in the gas exiting the chamber is 2000 mg m^{-3} .

Worked Solution 24.3 (see Problem 24.3)

Given that the cyclones are of a standard design, the dimensions of the cyclones can be determined from the specified diameter using the design ratios given in Table 24.3. The next step is to determine the tangential velocity, v_t , by dividing the flow rate, Q , by the total area of the inlets, NH_cW_c , where N is the number of parallel cyclones, H_c is the height of the inlet and W_c is the width of the inlet.

Following on from this it is necessary to calculate the number of effective turns within the cyclone, N_e , from Eq. (24.29), the D_{50} parameter, from Eq. (24.33), and the incremental collection efficiencies for each particle size, E_i , using Eq. (24.32). Equation (24.3) can then be used to estimate the total collection efficiency of the cyclone set.

The power required can be determined by multiplying the flow rate by the pressure loss within the cyclone. The pressure loss can be calculated using Eq. (24.34) and because the cyclone is a standard design we can set the number of velocity heads, $\beta = 8$.

A MATLAB code to perform the analysis is presented below:

```
Q=20; %Flow rate (m3/s)
rho_p=2900; %Density of particles (kg/m3)
rho=1.29; %Density of air (kg/m3)
mu=20e-6; %Viscosity of air (Pa s)
N=[1 1 2 9]'; %Number of parallel cyclones
Dc1=[3 1 1 1]'; %Cyclone diameter (m)
alpha=2; %Lapple's empirical factor
beta=8; %Number of velocity heads
%Median diameter of particles (m)
D=[1 5 10 20 30 40 50 60 100]*1e-6;
%Mass fraction (-)
wi=[3 20 15 20 16 10 6 3 7]/100;
%Use standard ratios to get cyclone dimensions
Hc=0.5*Dc1; Wc=0.25*Dc1; Lc1=1.75*Dc1; Lc2=2*Dc1;
vt=Q./N./Hc./Wc; %Tangential velocity (m/s)
Ne=(Lc1+Lc2/2)./Hc; %Number of effective turns
%Determine 50% efficiency diameter
D50=sqrt(9*mu*Wc/2/pi./Ne./(rho_p-rho)./vt);
%Determine incremental efficiency (-)
Ei=1./(1+(D50./D).^alpha);
E=sum(Ei.*wi,2); %Total efficiency (-)
dP=beta*rho*vt.^2/2; %Pressure loss (Pa)
```

Table 24.10 Results for Problem 24.3

	Number of cyclones	Diameter of cyclones (m)	Power (kW)	Collection efficiency (%)
(a)	1	3	32.6	70.4
(b)	1	1	2640	95.1
(c)	2	1	660	92.6
(d)	9	1	32.6	82.2

```
Power=dP*Q; %Determine energy requirement (W)
num2str([Power*1e-3 E*100],3) %Print results
```

The results from the above analysis are given in Table 24.10. Note that the larger cyclone has a low energy requirement but only provides a collection efficiency of 70.4%. The efficiency is substantially increased by reducing the diameter of the cyclone because this leads to a reduction in the particle collision time. However, the increased tangential velocity gives rise to a significantly greater energy requirement. The energy requirement can be reduced by distributing multiple cyclones in parallel. However, this leads to a reduced tangential velocity, which in turn causes a reduction in the centrifugal force acting on the particles and a consequential reduction in collection efficiency.

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Abstract

This chapter explores key concepts associated with carbon capture and storage (CCS). A focus is made on the particular significance of CCS for industrial emissions associated with the production of cement, iron, steel, hydrogen and ammonia. A range of different CO₂ capture technologies are described, including absorption, adsorption, membrane separation and oxy-fuel combustion. Various trapping mechanisms, associated with long term storage of CO₂ in geological formations are explained, including structural, residual, solubility and mineral trapping. Simple equations are presented for CO₂ storage capacity estimation in confined and unconfined brine aquifers. Henry's law and the two film model are used to derive mathematical equations for designing countercurrent absorption towers associated with CO₂ separation by amine absorption. Practical applications are presented through a problem sheet with worked solutions.

Notation

A	Cross-sectional area of absorption tower [L^2].
b_G	Gas film thickness [L].
b_L	Liquid film thickness [L].
c_R	Rock compressibility [$M^{-1}LT^2$].
c_W	Water compressibility [$M^{-1}LT^2$].
C_G	Mass concentration of a chemical component in the gas phase [ML^{-3}].
$\hat{C}_G$	Mass concentration of a chemical component in the gas phase outside the diffusive film [ML^{-3}].
C_{GA}	Mass concentration for the inlet gas [ML^{-3}].
C_{GB}	Mass concentration for the outlet gas [ML^{-3}].
C_{GI}	Mass concentration for the gas phase at the gas-liquid interface [ML^{-3}].
C_L	Mass concentration of a chemical component in the liquid phase [ML^{-3}].

$\hat{C}_L$	Mass concentration of a chemical component in the liquid phase outside the diffusive film [ML^{-3}].
C_{LA}	Mass concentration for the outlet liquid [ML^{-3}].
C_{LB}	Mass concentration for the inlet liquid [ML^{-3}].
C_{LI}	Mass concentration for the liquid phase at the gas-liquid interface [ML^{-3}].
D_G	Molecular diffusion coefficient for the gas phase [L^2T^{-1}].
D_L	Molecular diffusion coefficient for the liquid phase [L^2T^{-1}].
E	Dimensionless efficiency factor [-].
g	Gravitational acceleration [LT^{-2}].
H	Absorption tower height [L].
J_G	Gaseous diffusive mass flux [$\text{ML}^{-2}\text{T}^{-1}$].
J_I	Net mass flux of a chemical component from the gas phase to the liquid phase [$\text{ML}^{-2}\text{T}^{-1}$].
J_L	Liquid diffusive mass flux [$\text{ML}^{-2}\text{T}^{-1}$].
K	Henry's law coefficient ($C_L = K C_G$) [-].
k_a	Effective mass transfer coefficient [T^{-1}].
M_{CO_2}	CO_2 storage capacity [M].
p	Pressure [$\text{ML}^{-1}\text{T}^{-2}$].
p_f	Fracture pressure [$\text{ML}^{-1}\text{T}^{-2}$].
p_{max}	Maximum allowable pressure [$\text{ML}^{-1}\text{T}^{-2}$].
p_0	Initial pressure [$\text{ML}^{-1}\text{T}^{-2}$].
Q_G	Volumetric gas flow rate [L^3T^{-1}].
Q_L	Volumetric liquid flow rate [L^3T^{-1}].
r_a	The rate at which mass of chemical component dissolves into the liquid phase per unit volume of absorption tower [$\text{ML}^{-3}\text{T}^{-1}$].
s	Distance normal to the gas-liquid interface [L].
V	Volume of brine aquifer or volume of absorption tower [L^3].
z	Depth below land surface (or seabed) or elevation within an absorption tower [L].
β	Gas-liquid interfacial area per unit volume of absorption tower [L^{-1}].
λ	Auxiliary parameter (see Eq. (25.21)) [L^{-1}].
ρ_W	Mass density of water [ML^{-3}].
ρ_{CO_2}	Mass density of CO_2 [ML^{-3}].
ϕ	Porosity [-].
CCS	Carbon capture and storage.
MEA	Mono ethanol amine.
SMR	Steam methane reforming.
WGSR	Water gas shift reaction.

25.1 Introduction

Combustion of fossil fuels leads to the production of CO₂, which is one of a suite of greenhouse gases, attributed to anthropogenic driven global climate change. Much effort is currently under way to reduce CO₂ emissions to net zero by 2050, so as to minimise the most acute environmental impacts (e.g. [1]).

Renewable energy from solar, wind and geothermal are a critical component of this effort and are continuing to become more cost effective with time [2]. However, large-scale anthropogenic CO₂ emissions are likely to continue for the following reasons:

- Many important industrial processes, such as the production of steel, cement and ammonia (for fertilizer), produce CO₂ by their very nature.
- Much of the hydrogen required for non-CO₂ emitting heating will likely be derived from coal and natural gas, leading to co-production of CO₂.
- It will likely remain necessary to buffer electricity, from renewable energy, with coal and gas fired power stations.

Carbon capture and storage (CCS) represents an important approach to preventing these emissions from entering the atmosphere. The concept of CCS typically includes capturing CO₂ at source, transporting it to a suitable storage location and then injecting it deep underground, where it will be stored indefinitely within the pore-space of underlying geological formations.

CCS can mitigate CO₂ emissions from combustion of fossil fuels and other industrial processes. Furthermore, CCS can be applied to processes involving combustion of biofuels, leading to net negative CO₂ emissions. CCS can also be used to take CO₂ directly out from the atmosphere.

In this chapter we will explore some key aspects of CCS. Various carbon capture processes of interest will be explained. We will look at the types of geological formation that are likely to be suitable for CO₂ storage. Theory will be developed for estimating the CO₂ storage capacity of a given geological formation. Some necessary equations used to design absorption facilities commonly applied for existing CO₂ capture enterprises are then derived.

25.2 Carbon Capture

25.2.1 Separation Processes

Three important CO₂ separation processes include absorption, adsorption and membrane separation.

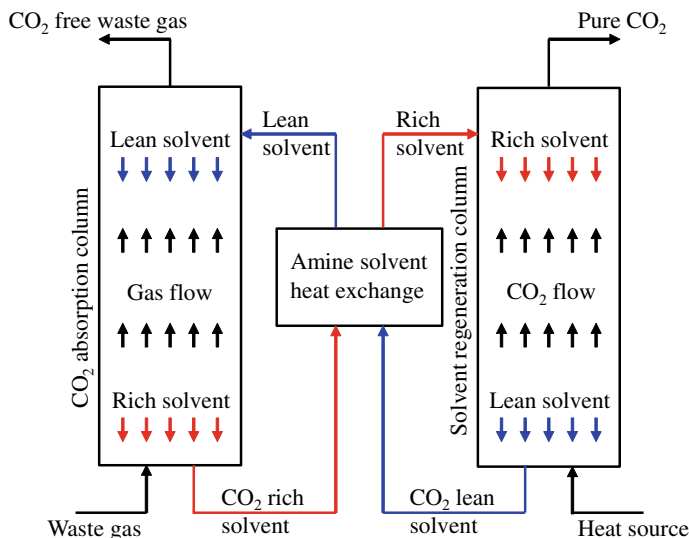


Fig. 25.1 Schematic diagram of a CO₂ absorption column with an associated solvent regeneration column

25.2.1.1 Absorption

Absorption is the most established technique for CO₂ separation. Absorption typically takes place within a packed absorption tower where liquid solvents, with high CO₂ affinity, flow downwards, countercurrent to a rising waste gas stream (Fig. 25.1). The CO₂ is stripped out of the gas stream as it is absorbed by the solvent. The CO₂ rich solvent is then transported to a solvent regeneration column. Here the solvent is heated up such that the CO₂ comes out of solution as a close to pure gas stream. The regenerated lean solvent is then sent back to the absorption tower and the process repeats. Relevant solvents typically need to be around 40–60°C for CO₂ absorption and around 120–160°C for CO₂ desorption [3].

The most commonly applied solvent is mono ethanol amine (MEA) [3]. Amines are organic compounds with molecular structures that resemble ammonia [4]. The main issues around the use of solvents for removing CO₂ are high costs associated with heating (for solvent regeneration) and solvent losses due to thermal and chemical degradation [3].

Commonly absorption towers are packed with inert solid materials of various geometric shapes, designed to maximise interfacial area between the gas and absorbent (see Fig. 25.2) whilst minimising pressure loss within the tower [4, p. 418].

25.2.1.2 Adsorption

Adsorption involves passing waste gas through a packed bed of solid adsorbent. As the gas moves through the material, the CO₂ adsorbs (becomes attached) to the surface of the adsorbent (Fig. 25.3).

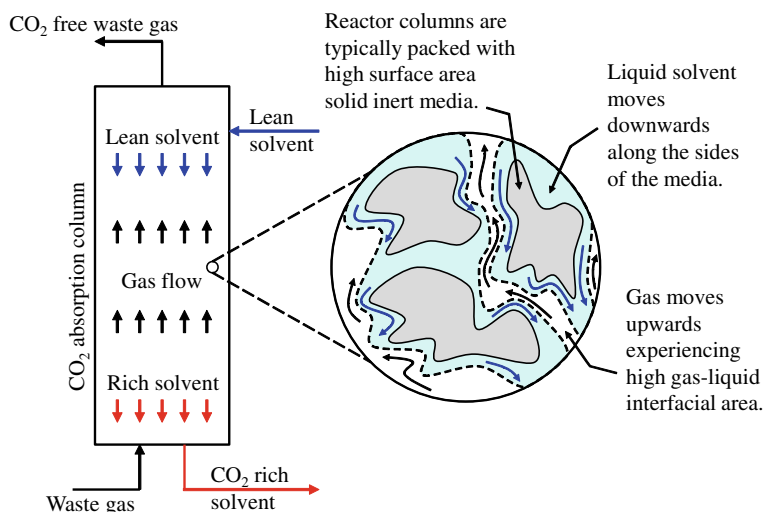


Fig. 25.2 Schematic diagram illustrating the gas-liquid interfacial area that develops along the surface of packed media within a CO_2 absorption tower

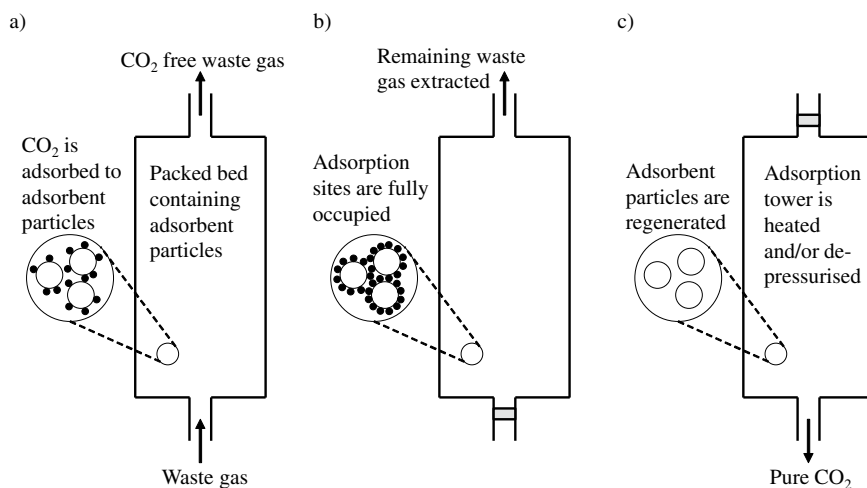
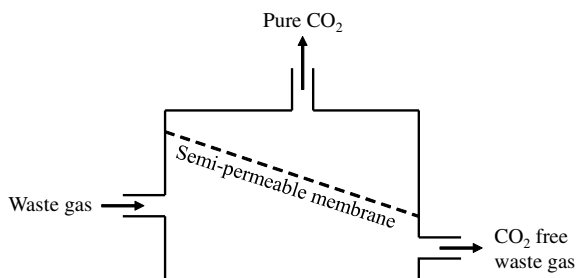


Fig. 25.3 Schematic diagram of a packed bed adsorption column. **a** CO_2 is stripped out of the waste gas by adsorption. **b** All the adsorption sites are occupied so the waste gas inlet is closed and the remaining waste gas is removed. **c** The adsorbent is either heated or de-pressurised to release the CO_2 as a pure stream. The adsorbent is now regenerated so the cycle can repeat

Fig. 25.4 Schematic diagram for a CO₂ membrane separation process



Once all the adsorption sites are occupied, the waste gas is sent to an alternative adsorption tower, and the spent adsorption tower is regenerated either by increasing the temperature or reducing the pressure. The CO₂ then leaves the surface of the adsorbent and forms a relatively pure stream which is collected and transported away. The adsorbent can then be cooled and/or re-pressurised and used again for stripping CO₂ out of the waste gas stream.

Many different materials can be used as adsorbents including zeolites, activated carbon and alkali-metal based oxides. See [3] for a detailed discussion concerning advantages and disadvantages.

25.2.1.3 Membrane Separation

Membrane separation involves pressurising waste gas in the presence of a semi-permeable membrane (Fig. 25.4). A membrane is required such that CO₂ molecules permeate through the membrane more readily than other molecules present.

Membrane separation works best with high gas pressures and high CO₂ content. However, for CO₂ gas streams with less than 10% CO₂ content, amine absorption is significantly more energy efficient [3]. Another problem, is that commercial membranes cannot be applied at high temperatures and therefore require the waste gas to be pre-cooled [3].

Membrane materials include organic polymer options, inorganic options (including alumina, carbon, silica or glass) and mixed matrix options where inorganic particles are combined within a polymer matrix [3].

25.2.1.4 Cost of CO₂ Separation from Different Sources

The cost of CO₂ separation, on a USD per tonne of CO₂ basis, increases with decreasing concentration in the gas stream. This is because [5]:

1. Reduced concentrations imply that a larger volume of waste gas must be handled for a given mass of CO₂, which leads to an increase in capital cost for the separation equipment.
2. The more dilute the source, the more energy is required to overcome the entropy of mixing, to separate out a pure stream of CO₂.

Table 25.1 CO₂ content [6] and levelised cost of CO₂ capture [7] by sector

Sector	CO ₂ content (%)	USD ₂₀₁₉ per tonne CO ₂
Direct air capture	0.04	134–342
Power generation	3–15	50–100
Cement	14–33	60–120
Iron and steel	16–42	40–100
Hydrogen	30–100	50–80
Ammonia	98–100	25–35

Table 25.1 shows levelised cost of CO₂ capture for different industrial sectors. Direct capture from air is the most expensive option because the natural concentration in air is very low. CO₂ capture from high concentration industrial sources is much cheaper. Hence CCS for industrial emissions often represents a significant component of national CO₂ reduction strategies (e.g. [1]).

25.2.2 Industrial Sources

As mentioned earlier, many industrial processes produce high levels of CO₂ emissions in addition to those associated with combustion for heating requirements [6]. Some representative sectors are compared alongside CO₂ emissions from power generation in Table 25.2.

Below we will look in more detail at the causes of process emissions from the production of cement, iron, steel, hydrogen and ammonia.

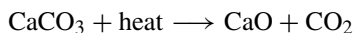
25.2.2.1 Cement Production

Cement production involves sintering (fusing without melting) calcium carbonate (CaCO₃) with silica, alumina and iron oxide. This requires the CaCO₃ to go through

Table 25.2 Importance of CO₂ emissions from different sectors alongside a breakdown into the percentage of emissions from process and combustion [6]

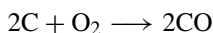
Sector	2014 US emissions (%)	Process (%)	Combustion (%)
Power generation	36.7	0	100
Cement	1.16	93.2	6.8
Iron and steel	1.00	45.3	54.7
Hydrogen	0.77	92.8	7.2
Ammonia	0.26	62.6	37.4

an intermediate process of calcination, whereby calcium oxide (CaO) and CO₂ are formed [6]

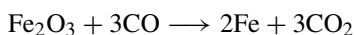


25.2.2.2 Iron and Steel Production

Iron and steel production involves mixing iron ore with coke (a high carbon content fuel) in the presence of preheated air within a blast furnace. The coke reacts with O₂ in the air to form carbon monoxide (CO) [6]



The CO is then used to reduce the iron ore to form elemental iron and CO₂ [6]

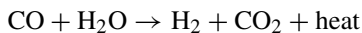


25.2.2.3 Hydrogen Production

Hydrogen (H₂) is commonly formed from methane (CH₄) using a process known as steam methane reforming (SMR). This involves mixing preheated steam with CH₄ to form CO and H₂ [6]

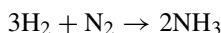


The CO is then mixed with water, in a process known as a water-gas shift reaction (WGSR), to produce additional H₂ and CO₂ [6]



25.2.2.4 Ammonia Production

Ammonia (NH₃) production involves the Haber-Bosch process, whereby NH₃ is formed from H₂ and atmospheric nitrogen (N₂).



The H₂ is often made on site using SMR, hence ammonia production is also associated with high levels of CO₂ emissions.

25.2.3 Alternative Combustion Options

As we saw in Table 25.1, the cost of CO₂ capture is strongly dependent on the concentration of CO₂ in the waste gas. Conventional power generation leads to a low CO₂ content gas stream and hence a high cost of CO₂ capture. However, the cost of CO₂ capture can be reduced by modifying the combustion process to produce waste gas with a higher CO₂ content. In this context it is useful to distinguish between post-combustion, pre-combustion and oxy-fuel combustion [4].

25.2.3.1 Post-combustion

Post-combustion simply involves separating the CO_2 from the gas stream following conventional combustion of a fuel. The disadvantage is that the waste gas typically contains large quantities of N_2 , and therefore the CO_2 capture cost will be very high.

25.2.3.2 Pre-combustion

Pre-combustion involves producing H_2 and CO_2 from a fuel and then separating out the CO_2 prior to the combustion of H_2 . The advantage is that the pre-combustion gas stream has a higher CO_2 content (as compared to conventional post-combustion) and therefore a lower CO_2 capture cost.

25.2.3.3 Oxy-Fuel Combustion

Oxy-fuel combustion involves burning a fuel in pure oxygen [4]. The advantage here is that the waste gas stream mostly only contains H_2O and CO_2 . The CO_2 can then be easily separated by condensing the H_2O . Pure oxygen is mixed with waste gas (CO_2 and H_2O) to reduce the flame temperature where necessary. The disadvantage of oxy-fuel is the added cost of producing pure oxygen from air by cryogenic separation.

Oxy-fuel combustion can also be achieved by chemical looping [8]. In this case, metal oxides are added to a combustion chamber to provide the oxygen. Following fuel combustion, the reduced metal oxides are removed and re-oxidised by heating. The metal oxides are then fed back to the combustion chamber and re-used, hence the process is referred to as chemical looping. The advantage is that it does not require cryogenic separation of oxygen from air.

25.3 Carbon Storage

25.3.1 Storage Options

A range of different geological formations have been considered for CO_2 storage including depleted oil and gas reservoirs, brine aquifers and coal seams [9]. Suitable storage formations should satisfy the following criteria:

1. The formation should be greater than 800 m depth such that the CO_2 is in a dense phase.
2. The rocks should have sufficient porosity to store the CO_2 .
3. The rocks should have sufficient permeability to enable the CO_2 to be easily injected.
4. The storage formation should be overlain by an impermeable formation, known as a cap rock, to ensure the CO_2 does not migrate back to the surface.

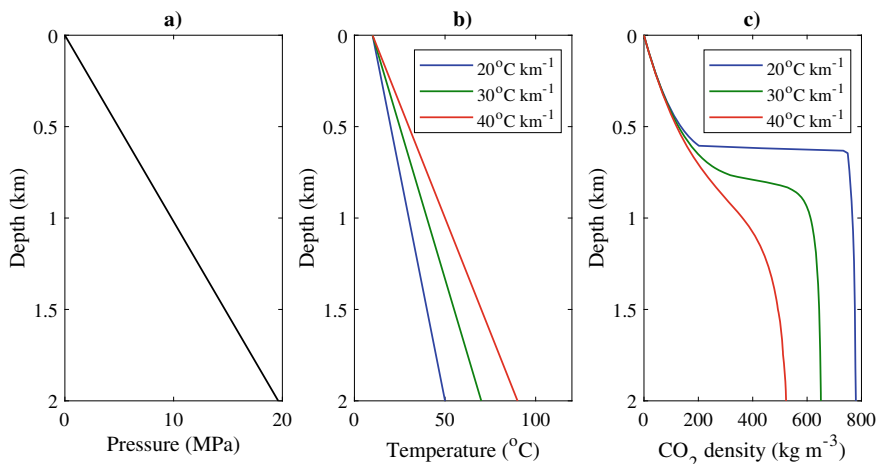


Fig.25.5 Plots of pressure, temperature and CO₂ density with depth assuming hydrostatic pressure and different geothermal gradients. CO₂ density data was acquired from [10]

25.3.1.1 The Importance of CO₂ Density

The density of CO₂ at standard conditions is 1.98 kg m⁻³. However, the density dramatically increases with pressure. It is therefore advantageous to store the CO₂ in a high pressure environment, such that the volume requirement is reduced.

A common objective with CCS is to store the CO₂ within the pore-space of sedimentary rocks. Ordinarily, this pore-space is filled with water and sometimes with oil or gas.

The pressure of fluids stored within a pore-space, p [ML⁻¹T⁻²], is strongly dependent on depth, z [L]. A lower bound estimate for pore-pressure can be obtained by assuming a hydrostatic pressure profile, i.e.,

$$p = \rho_w g z \quad (25.1)$$

where ρ_w [ML⁻³] is the density of water and g [LT⁻²] is gravitational acceleration. Assuming a water density of 1000 kg m⁻³, it can be understood that the hydrostatic pressure gradient would be 9.81 MPa km⁻¹.

However, temperature also increases with depth, due to the heat flux from the Earth's interior, and the density of CO₂ decreases with increasing temperature. Typical geothermal gradients range between 20 and 40 °C km⁻¹. Nevertheless, the over-riding effect of depth on CO₂ density is due to pressure.

Figure 25.5 shows a plot of CO₂ density against depth assuming a hydrostatic pressure profile along with various geothermal gradients. It can be seen that below 800m, the density of CO₂ is between 240 and 800 kg m⁻³. Consequently, greater than 800m depth is often specified as a requirement for CO₂ storage reservoirs [9]. However, CO₂ density will likely remain less than that of water and therefore it will be buoyant and rise back to the land surface unless a suitable barrier is in place.

25.3.1.2 Depleted Oil and Gas Reservoirs

Oil and gas is formed in low permeability, organic rich, source rocks. Following formation, oil and gas migrates upwards to the land surface due to it being buoyant in water. However, in some cases, oil and gas becomes trapped underneath impermeable cap rocks such as shale or salt. The underlying permeable geological formations containing the oil and/or gas are referred to as reservoir formations. Typical reservoir rocks include sandstones and limestones.

There are many advantages associated with storing CO₂ in depleted oil and gas reservoirs:

- Reservoir formations have a proven cap rock that has retained oil and/or gas for many millions of years.
- There will be existing datasets describing the formations, which will be useful when designing a new CO₂ storage facility.
- Existing infrastructure such as off-shore platforms, wells, and pipelines, can potentially be reused for CO₂ storage.

Associated disadvantages include:

- They might be far away from relevant CO₂ sources.
- Many nations do not have access to oil and gas reservoirs.
- Although the reservoirs might be classified as depleted, CO₂ injection might affect the rights of neighbouring oil and gas asset holders.
- Abandoned oil and gas wells might present a CO₂ leakage hazard.
- Reuse of existing infrastructure might not be suitable due to the corrosive properties of CO₂.

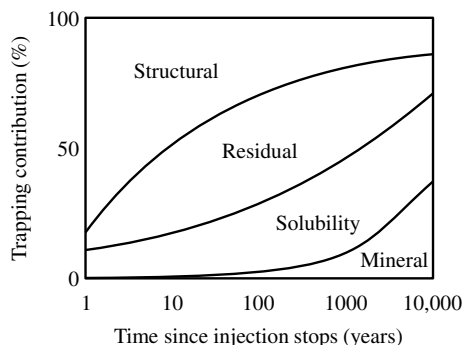
25.3.1.3 Brine Aquifers

Brine aquifers are commonly sandstone or limestone rock formations, which contain water that is too saline to be considered of value from a potable water resource perspective. The good thing about brine aquifers is that they are almost everywhere in the world. The disadvantage is that not all brine aquifers have a suitable cap rock to prevent CO₂ rising back to the surface. Furthermore, such assets have rarely been exploited previously, therefore significant expenditure is required to develop a good understanding of a potential prospect. Nevertheless, brine aquifers are likely to be the most common formations used for CCS in the future, simply due to their prevalence worldwide.

25.3.1.4 Coal Seams

Coal seams are highly fractured and therefore have significant permeability. An attractive aspect of storing CO₂ in coal seams is that CO₂ adsorbs to the surface of coal particles rendering it immobile. However, the adsorption of CO₂ leads to the swelling of coal particles, which in turn leads to a closing up of the fractures and a loss

Fig. 25.6 Approximate times at which different CO₂ trapping mechanisms become important (inspired by [9])



in permeability. Whilst there have been many theoretical studies related to storing CO₂ in coal seams, coal seams have received much less attention for full-scale pilot projects as compared to oil and gas reservoirs and brine aquifers.

25.3.2 Trapping Mechanisms

When considering CO₂ storage in brine aquifers or oil and gas reservoirs, four trapping mechanisms are often invoked to assure that the CO₂ will remain within a storage formation. These include structural trapping, residual trapping, solubility trapping and mineral trapping [9, 11]. The relative time-scales at which these different mechanisms become important are indicated in Fig. 25.6.

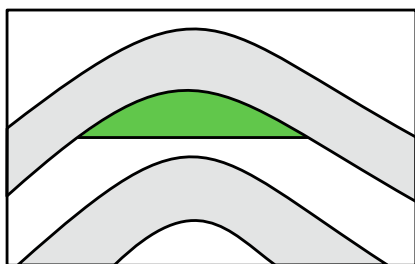
25.3.2.1 Structural Trapping

Structural trapping is the most important trapping mechanism because this provides the bulk of storage integrity at the beginning of a project. The idea is simply that the geological structure of a CO₂ storage formation prevents stored CO₂ rising back to the land surface due to its buoyancy. Three important geological structures that will achieve this are illustrated in Fig. 25.7. The presence and nature of a structural trap in deep geological formations can be determined from a combination of drilling exploratory wells and performing a three-dimensional seismic survey.

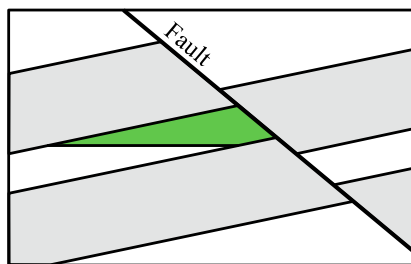
Before we discuss these further, it is important to understand some basic aspects of sedimentary geology. Sedimentary formations include sandstones, limestones, shales and evaporites. These rocks are formed where particles have settled out from either water or air. The size of the particles that settle out is a function of the speed at which they were originally transported by water or air.

Permeable sandstone formations have a relatively large grain size suggesting that the particles were transported in a high energy environment such as a fast flowing river. Impermeable shales have much smaller grain size suggesting that the particles were transported in a low energy environment such as a lake or a wide estuary. Limestones are comprised of calcium carbonate, represented as a mixture of fossils,

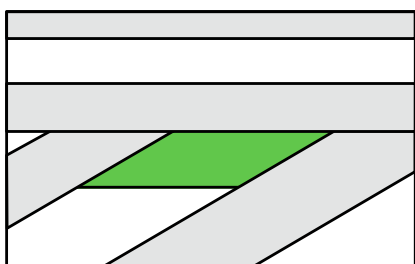
a) Anticline trap



b) Fault trap



c) Unconformity trap



-  Permeable formation
-  Impermeable formation
-  Stored CO₂

Fig. 25.7 Schematic diagrams showing different types of geological structural traps for underground storage of CO₂

carbonate sediment particles and cements; porosity exists a combination of primary porosity, plus secondary porosity arising from later dissolution processes and fracturing. Low permeability evaporites are formed of particles of various salts that settled out in shallow evaporating seas.

Environments change with time. Consequently, horizontal layers of varying properties (permeable and impermeable) overlay each other with time. As burial depth increases, pressure increases, leading to dissolution and remineralisation of various constituents and the formation of consolidated rocks. Subsequently, these horizontal sedimentary beds are deformed by regional tectonic movements.

Figure 25.7a shows a schematic diagram of an anticline trap. Here alternating horizontal layers of impermeable (e.g. shale) and permeable (e.g. sandstone) rocks have been folded. If CO₂ is injected into a permeable layer, it will rise up to the top of the fold and then remain trapped underneath the overlying folded impermeable layer.

Figure 25.7b shows a schematic diagram of a fault trap. Alternating layers of rock have been tilted and then displaced along a fault. This results in a permeable layer being offset by an impermeable layer. If CO₂ is injected into the interior permeable formation, it will rise up and remain trapped against both the overlying and offset impermeable layers.

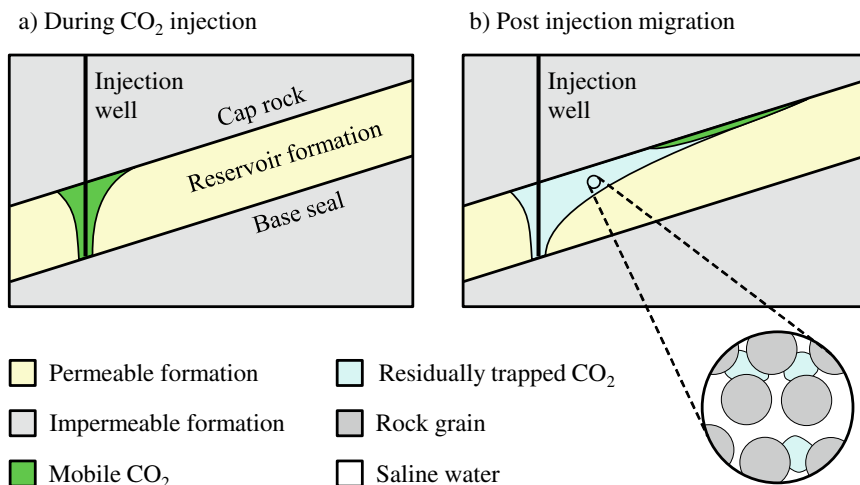


Fig. 25.8 Schematic diagrams illustrating the process of residual trapping of CO₂

Figure 25.7c shows a schematic diagram of an unconformity trap. Alternating layers of rock have been tilted and then eroded to form a flat horizontal surface. A subsequent round of deposition has led to the development of a new set of overlying horizontal sedimentary beds. If CO₂ is injected into the underlying permeable unit, it will rise up and remain trapped in-between the surrounding impermeable layers.

25.3.2.2 Residual Trapping

The presence of a structural trap is important for ensuring the long term effectiveness of a CO₂ storage project. However, in many locations, such a feature may not be available. Nevertheless, stored CO₂ can be expected to stay underground, even in an open tilted reservoir formation. This is due to a process referred to as residual trapping.

Figure 25.8a shows CO₂ being injected into a tilted reservoir formation underneath an impermeable cap rock. Whilst the plume is being injected, inertia from the injection well will cause CO₂ to spread out in all directions, displacing any previously residing brine. However, buoyancy forces will lead to the CO₂ moving preferential upwards against the inclined cap rock surface.

Once injection ceases, the resulting CO₂ plume will migrate upwards along the base of the inclined cap rock (Fig. 25.8b). This displacement is driven by brine re-invading the pore-space. Furthermore, most reservoir rocks are hydrophilic, which means that brine will have a tendency to run along the surface of the rock grains, leading to the isolation of microscopic bubbles of CO₂. These bubbles are expected to be held in place, despite gravitational forces, by a phenomenon known as surface tension. This overall process is commonly referred to as residual trapping.

25.3.2.3 Solubility and Mineral Trapping

Solubility trapping refers to the transformation of CO_2 from a free phase to a dissolved phase in the co-residing brine. The density of water increases with increasing CO_2 concentration. Therefore, dissolution takes out the buoyancy risk of CO_2 causing it to sink deeper into the Earth's crust.

The solubility limit of CO_2 decreases with increasing temperature and increasing salinity. Brine co-residing in the same pore-space as free phase CO_2 reaches chemical equilibrium very fast. Once this has occurred, dissolution of the remaining CO_2 plume is controlled by the much slower processes of convection and diffusion [9].

With further time, the dissolution of CO_2 gives rise to a weak acid that will react with metallic components of host rocks to form new solid minerals, which is a process referred to as mineral trapping [9].

25.3.3 Environmental Impacts

The environmental impacts associated with storing CO_2 in geological formations include [9]:

- CO_2 leaking to the surface and causing asphyxiation.
- CO_2 leaking into lakes, seas or oceans, causing local reductions in pH, which leads to ecosystem disruption or destruction.
- Excessive changes in underground fluid pressure, leading to induced seismicity.
- Displacement of brine into freshwater aquifers leading to contamination of freshwater resources.

Such impacts can be minimised by good quality site characterisation, performance assessment with numerical simulation, environmental impact assessment and environmental monitoring during and after the CO_2 injection period.

25.3.4 Storage Capacity Estimation

An important question commonly asked concerns how much CO_2 can be safely stored within a specified geological formation. Obtaining an answer to this question typically involves extensive site characterisation followed by numerical simulation of the CO_2 storage exercise using expensive reservoir simulation software. However, a rough estimate for CO_2 storage capacity estimation can be obtained using some relatively simple equations. Here we will develop some simple storage capacity equations commonly used for looking at CO_2 storage in brine aquifers.

An important distinction often made concerns whether an aquifer is fully confined or not. Fully confined aquifers are completely sealed on all sides such that when CO_2 is injected, it is accommodated within the pore-space by compression of the brine and formation rock. In contrast, open aquifers have a hydraulic connection with neigh-

bouring aquifers. When CO₂ is injected into an open aquifer, it is accommodated within the pore-space by displacing brine into neighbouring formations.

25.3.4.1 Fully Confined Aquifers

A consequence of injecting CO₂ into a fully confined aquifer is that the fluid pressure within the pores will increase. Excessive increases in fluid pressure can lead to the development of hydraulic fractures or re-shearing of existing fractures, which in turn can compromise the overlying cap rock (which is important because it is the cap rock that stops the CO₂ migrating back to the atmosphere). Consequently, a maximum allowable pressure should be specified to ensure that the cap rock remains adequate for long-term CO₂ storage.

An upper bound for the mass of CO₂, M_{CO_2} [M], that can be safely stored within a fully confined aquifer can therefore be found from [12]

$$M_{\text{CO}_2} = \rho_{\text{CO}_2} V (\phi c_W + c_R) (p_{\text{max}} - p_0) \quad (25.2)$$

where ρ_{CO_2} [ML⁻³] is the density of the CO₂, V [L³] is the volume of the aquifer, ϕ [-] is the porosity of the aquifer, c_W [M⁻¹LT²] is the compressibility of the water, c_R [M⁻¹LT²] is the compressibility of the rock, p_{max} [ML⁻¹T⁻²] is the maximum allowable pressure within the aquifer and p_0 [ML⁻¹T⁻²] is the pore-pressure within the aquifer prior to CO₂ injection.

Note that the CO₂ density should be determined using the temperature within the aquifer and the maximum allowable pressure, p_{max} . An estimate of the initial pressure, p_0 , can be obtained by assuming hydrostatic conditions (see Eq. (25.1)).

The maximum allowable pressure, p_{max} , is commonly taken to be 90% of the so-called fracture pressure, p_f [ML⁻¹T⁻²], which represents the pressure at which hydraulic fractures are expected to take place. An estimate of fracture pressure can be obtained from the following empirical equation [13]

$$p_f = 0.71 p_0 + 8500z \quad (25.3)$$

where p_0 is in Pa and z is depth below the land surface or sea-bed in m.

25.3.4.2 Open Aquifers

Pressure buildup due to CO₂ injection in open aquifers is considerably less than in fully confined aquifers. This is because injected CO₂ is accommodated by the displacement of brine out of the aquifer. The maximum capacity of CO₂ in an open aquifer is instead dictated by how much CO₂ can be injected before it starts to leak into neighbouring formations.

An upper bound for the mass of CO₂, M_{CO_2} [M], that can be safely stored within an open aquifer is commonly found from [12]

$$M_{\text{CO}_2} = \rho_{\text{CO}_2} V \phi E \quad (25.4)$$

where E [-] is a dimensionless efficiency factor.

This efficiency factor will vary from one aquifer to the next and is commonly estimated using numerical models that simulate the migration of CO₂ within an

aquifer formation. However, in the absence of such studies, E is commonly taken to be about 0.02 [12].

25.3.4.3 Cost of Storing CO₂

The cost of storing CO₂ is strongly dependent on the number of injection wells required to get the CO₂ into the target formation. The life-time cost of one offshore injection well with platform and facilities is around 128 million USD₂₀₁₉ (based on [13]).

The rate at which CO₂ can be safely injected into a single well is dependent on a number of physical properties including the permeability and porosity of the aquifer, the connectivity of the aquifer and the density and viscosity of the CO₂ [14]. Nevertheless, statistical studies based on previous experience with oil and gas production suggest that a typical injection well can be expected to accommodate around 0.35 Mt CO₂ per year [15].

A typical injection well can be expected to operate for around 20 years [13]. This would suggest that the cost of storing CO₂ in a brine aquifer can be expected to be around 18 USD₂₀₁₉ per tonne of CO₂, which is just below the low end of cost associated with CO₂ capture (see Table 25.1).

25.4 Absorption Theory

In this section we develop some fundamental equations used to design packed absorption towers. The first step involves the development of a two film model, which describes the diffusion of chemicals across a gas-liquid interface. A set of coupled mass conservation equations are developed to describe chemical transport within gas and liquid phases co-existing within a packed absorption tower. These are then combined using the two-film model to form a single linear second-order ordinary differential equation, which is solved to obtain an analytical solution describing the chemical distribution within the absorption tower.

25.4.1 Two Film Model

Here we will describe the conceptual model associated with the two film theory for mass transfer across a gas-liquid interface attributed to [16]. Consider a gas-liquid interface (Fig. 25.9). The mass concentration profile for different chemical components in the gaseous phase are assumed uniform due to turbulent mixing except for within a thin gas film of thickness, b_G [L], adjacent to the gas-liquid interface, where transport is controlled by molecular diffusion. Similarly, the mass concentration profiles for different chemical components in the liquid phase are assumed to be uniform due to turbulent mixing except for within a thin liquid film

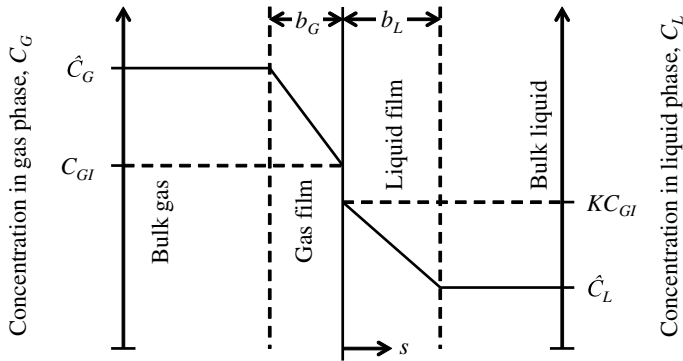


Fig. 25.9 Schematic diagram of the two film model used to describe mass transfer across a gas-liquid interface

of thickness, b_L [L], adjacent to the gas-liquid interface, where transport is also controlled by molecular diffusion.

Fick's first law gives that the gaseous diffusive mass flux for a given chemical component, J_G [$\text{ML}^{-2}\text{T}^{-1}$], is found from

$$J_G = -D_G \frac{\partial C_G}{\partial s} \quad (25.5)$$

where D_G [L^2T^{-1}] is the molecular diffusion coefficient for the gas phase, C_G [ML^{-3}] is the mass concentration of a chemical component in the gas phase and s [L] is a distance normal to the gas-liquid interface, pointing into the liquid mass.

In the same way, the liquid diffusive mass flux for the same chemical component, J_L [$\text{ML}^{-2}\text{T}^{-1}$], is found from

$$J_L = -D_L \frac{\partial C_L}{\partial s} \quad (25.6)$$

where D_L [L^2T^{-1}] is the molecular diffusion coefficient for the liquid phase, C_L [ML^{-3}] is the mass concentration, for the component of concern, in the liquid phase.

Providing the films are sufficiently thin, the concentration profiles can be treated as being in a quasi-steady-state such that

$$J_G = J_I, \quad -b_G \leq s \leq 0$$

and

$$J_L = J_I, \quad 0 \leq s \leq b_L$$

where J_I [$\text{ML}^{-2}\text{T}^{-1}$] is the net mass flux of a chemical component from the gas phase to the liquid phase.

Let $\hat{C}_G$ [ML^{-3}] and $\hat{C}_L$ [ML^{-3}] be the uniform mass concentrations, for the component of concern, in the bulk mass of gas and liquid, outside of the diffusive films, respectively. Also let C_{GI} be the mass concentration of a chemical component in the gas phase, at the gas-liquid interface.

Henry's law gives that, for a liquid solution in equilibrium with an interfacing gas mixture, the mass concentration of a component in the liquid phase is linearly proportional to its mass concentration in the gas phase, i.e. [17]

$$C_L = K C_G \quad (25.7)$$

where K [-] is the Henry's law coefficient for a component.

Challenge 25.1 Invoke two film theory, Fick's first law and Henry's law to derive an expression for the net mass flux of a chemical component from a gas phase to a liquid phase at a gas-liquid interface, J_I . The final answer should be in terms of the difference between the product of Henry's law coefficient and the bulk gaseous mass concentration, $K \hat{C}_G$, and the bulk liquid mass concentration, $\hat{C}_L$.

From Fick's first law for the gas film (Eq. (25.5)), we have that

$$J_I = J_G = \frac{D_G}{b_G} (\hat{C}_G - C_{GI}) \quad (25.8)$$

From Fick's first law for the liquid film (Eq. (25.6)), combined with Henry's law (Eq. (25.7)), we have that

$$J_I = J_L = \frac{D_L}{b_L} (K C_{GI} - \hat{C}_L) \quad (25.9)$$

Equating Eqs. (25.8) and (25.9) and solving for C_{GI} leads to

$$C_{GI} = \frac{b_L D_G \hat{C}_G + b_G D_L \hat{C}_L}{b_L D_G + b_G D_L K} \quad (25.10)$$

Substituting Eq. (25.10) into Eq. (25.9) gives us [18, p. 124]

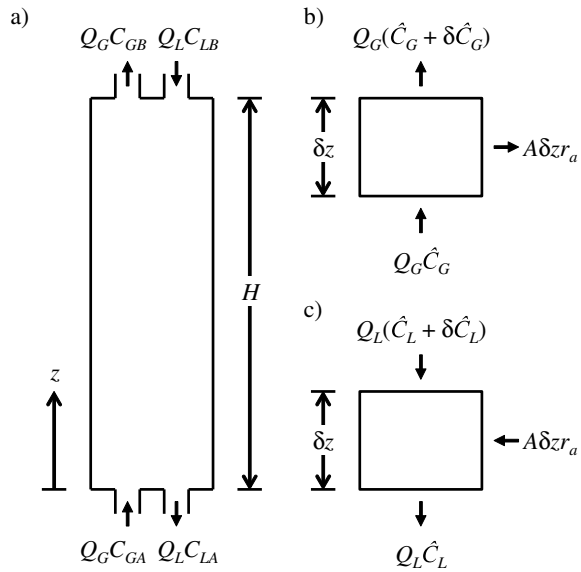
$$J_I = \left(\frac{b_L}{D_L} + \frac{K b_G}{D_G} \right)^{-1} (K \hat{C}_G - \hat{C}_L) \quad (25.11)$$

Equation (25.11) is commonly referred to as the two-film model and is attributed to [16]. The important point about Eq. (25.11) is that it tells us that the flux of a component across a gas-liquid interface can be approximated as a linear function of $(K \hat{C}_G - \hat{C}_L)$.

25.4.2 Countercurrent Absorption Model

Consider the countercurrent gas absorption tower shown in Fig. 25.10a. A gas mixture flows upwards at a volumetric flow rate of Q_G [L^3T^{-1}]. A liquid solvent flows downwards at a volumetric flow rate of Q_L [L^3T^{-1}]. Both the gas mixture and the liquid solution contain a mass concentration of a given chemical component. The mass concentration of the gas at the gas inlet is C_{GA} [ML^{-3}]. The mass concentration

Fig. 25.10 **a** Schematic diagram of a countercurrent gas absorption tower. **b** Control-volume for mass conservation in the gas phase. **c** Control-volume for mass conservation in the liquid phase



of the liquid at the liquid inlet is C_{LB} [ML^{-3}]. The height and cross-sectional area of the tower are H [L] and A [L^2], respectively.

A gas-liquid interface persists throughout the tower. Let r_a [$\text{ML}^{-3}\text{T}^{-1}$] be the mass of gaseous component of a given chemical that dissolves into the liquid per unit volume of tower and per unit time. Let β [L^{-1}] be the gas-liquid interfacial area per unit volume of tower. It follows from Eq. (25.11) that

$$r_a = k_a \cdot (K \hat{C}_G - \hat{C}_L) \quad (25.12)$$

where k_a [T^{-1}] is the effective mass transfer coefficient found from

$$k_a = \beta \left(\frac{b_L}{D_L} + \frac{K b_G}{D_G} \right)^{-1} \quad (25.13)$$

In practice, it is very difficult to determine values for β , b_L and b_G . Instead, values of k_a are obtained directly using empirical equations.

Considering the two control volume diagrams shown in Fig. 25.10b and c, mass conservation dictates that

$$Q_G \hat{C}_G = Q_G(\hat{C}_G + \delta \hat{C}_G) + A \delta z r_a$$

and

$$Q_L(\hat{C}_L + \delta \hat{C}_L) + A \delta z r_a = Q_L \hat{C}_L$$

It follows that

$$Q_G \frac{d\hat{C}_G}{dz} = -A r_a \quad (25.14)$$

and

$$Q_L \frac{d\hat{C}_L}{dz} = -A r_a \quad (25.15)$$

The relevant boundary conditions are:

$$\begin{aligned}\hat{C}_G &= C_{GA}, \quad z = 0 \\ \hat{C}_L &= C_{LB}, \quad z = H\end{aligned}\quad (25.16)$$

The above set of equations can be solved to derive expressions for the gaseous and liquid concentrations at the outlets, C_{GB} and C_{LA} , respectively.

25.4.2.1 General Solution

Challenge 25.2 Derive general solutions for $\hat{C}_G$ and $\hat{C}_L$.

Substituting Eq. (25.12) into Eqs. (25.14) and (25.15) leads to:

$$Q_G \frac{d\hat{C}_G}{dz} = -Ak_a(K\hat{C}_G - \hat{C}_L) \quad (25.17)$$

$$Q_L \frac{d\hat{C}_L}{dz} = -Ak_a(K\hat{C}_G - \hat{C}_L) \quad (25.18)$$

From Eq. (25.17) we have

$$\hat{C}_L = \frac{Q_G}{Ak_a} \frac{d\hat{C}_G}{dz} + K\hat{C}_G \quad (25.19)$$

which on substitution into Eq. (25.18) leads to

$$\frac{Q_L Q_G}{Ak_a} \frac{d^2 \hat{C}_G}{dz^2} + Q_L K \frac{d\hat{C}_G}{dz} = -Ak_a K \hat{C}_G + Q_G \frac{d\hat{C}_G}{dz} + Ak_a K \hat{C}_G$$

which, after some rearranging, reduces to

$$\frac{d^2 \hat{C}_G}{dz^2} + \lambda \frac{d\hat{C}_G}{dz} = 0 \quad (25.20)$$

where

$$\lambda = Ak_a \left(\frac{K}{Q_G} - \frac{1}{Q_L} \right) \quad (25.21)$$

The general solution of an ordinary differential equation of the form

$$a \frac{d^2 y}{dx^2} + b \frac{dy}{dx} + cy = 0$$

is [19, p. 1093]

$$y(x) = A_1 \exp \left[\left(\frac{-b + \sqrt{b^2 - 4ac}}{2a} \right) x \right] + A_2 \exp \left[\left(\frac{-b - \sqrt{b^2 - 4ac}}{2a} \right) x \right]$$

where A_1 and A_2 are unknown constants defined by any associated boundary conditions.

For Eq. (25.20), $a = 1$, $b = \lambda$ and $c = 0$, so the general solution is

$$\hat{C}_G = A_1 + A_2 e^{-\lambda z} \quad (25.22)$$

Substituting Eq. (25.22) into Eq. (25.19) then leads to

$$\hat{C}_L = K A_1 + \frac{Q_G}{Q_L} A_2 e^{-\lambda z} \quad (25.23)$$

25.4.2.2 Application of Boundary Conditions

Challenge 25.3 Apply the boundary conditions to find expressions for the two integration constants.

From the lower boundary condition we have that $\hat{C}_G = C_{GA}$ at $z = 0$. Equation (25.22) therefore tells us that

$$A_1 + A_2 = C_{GA} \quad (25.24)$$

From the upper boundary condition we have that $\hat{C}_L = C_{LB}$ at $z = H$. Equation (25.23) therefore tells us that

$$K A_1 + \frac{Q_G}{Q_L} A_2 e^{-\lambda H} = C_{LB} \quad (25.25)$$

Solving Eqs. (25.24) and (25.25) for A_1 and A_2 leads to

$$A_1 = \frac{Q_L C_{LB} - Q_G e^{-\lambda H} C_{GA}}{Q_L K - Q_G e^{-\lambda H}} \quad (25.26)$$

and

$$A_2 = \frac{Q_L (K C_{GA} - C_{LB})}{Q_L K - Q_G e^{-\lambda H}} \quad (25.27)$$

Substituting Eqs. (25.26) and (25.27) into Eqs. (25.22) and (25.23) gives us

$$\hat{C}_G = \frac{Q_L C_{LB} - Q_G e^{-\lambda H} C_{GA} + Q_L (K C_{GA} - C_{LB}) e^{-\lambda z}}{Q_L K - Q_G e^{-\lambda H}} \quad (25.28)$$

and

$$\hat{C}_L = \frac{K Q_L C_{LB} - K Q_G e^{-\lambda H} C_{GA} + Q_G (K C_{GA} - C_{LB}) e^{-\lambda z}}{Q_L K - Q_G e^{-\lambda H}} \quad (25.29)$$

25.4.2.3 Design Formulae

Challenge 25.4 Derive an expression for the minimum height of absorption tower required to achieve a specified outlet gas concentration.

An expression for the outlet gas concentration, C_{GB} , can be obtained by setting $z = H$ in Eq. (25.28) to get

$$C_{GB} = \frac{(Q_L K - Q_G) e^{-\lambda H} C_{GA} + Q_L C_{LB} (1 - e^{-\lambda H})}{Q_L K - Q_G e^{-\lambda H}} \quad (25.30)$$

The minimum length of absorption tower required to achieve an outlet gas concentration, C_{GB} , is found by solving Eq. (25.30) for H to get [18, p. 234]:

$$H = \frac{1}{\lambda} \ln \left[\frac{Q_L (K C_{GA} - C_{LB}) - Q_G (C_{GA} - C_{GB})}{Q_L (K C_{GB} - C_{LB})} \right] \quad (25.31)$$

Challenge 25.5 Derive an expression for the minimum length of absorption tower required to achieve a specified outlet liquid concentration.

An expression for the outlet liquid concentration, C_{LA} , can be obtained by setting $z = 0$ in Eq. (25.29) to get

$$C_{LA} = \frac{(Q_L K - Q_G)C_{LB} + Q_G K C_{GA}(1 - e^{-\lambda H})}{Q_L K - Q_G e^{-\lambda H}} \quad (25.32)$$

The minimum length of absorption tower required to achieve an outlet liquid concentration, C_{GA} , is found by solving Eq. (25.32) for H to get

$$H = \frac{1}{\lambda} \ln \left[\frac{Q_G (K C_{GA} - C_{LA})}{Q_G (K C_{GA} - C_{LB}) - Q_L K (C_{LA} - C_{LB})} \right]. \quad (25.33)$$

25.5 Problem Sheet

Problem 25.1 (see Worked Solution 25.1)

A structural trap within an offshore deep brine aquifer has been identified to store CO_2 captured from a nearby coal power station. The power station produces 3 Mt CO_2 per year. The sea-bed is 50m below sea-level. The base of the overlying cap-rock is 1100m below seabed. The thickness of the underlying aquifer formation is 70m. The plan area of the targeted aquifer is 800 km^2 . The rock compressibility and porosity of the aquifer are $1.6 \times 10^{-10} \text{ Pa}^{-1}$ and 0.25, respectively. The compressibility and density of the brine are $4.4 \times 10^{-10} \text{ Pa}^{-1}$ and 1000 kg m^{-3} , respectively. The density of CO_2 at this depth is 650 kg m^{-3} . The pressure regime within the aquifer is hydrostatic.

- Determine the storage capacity of the aquifer assuming it behaves as an open aquifer.
- Determine the storage capacity of the aquifer assuming it behaves as a fully confined aquifer.
- Determine the number of years of emissions from the power station that can be stored within the aquifer assuming fully confined aquifer conditions.
- Estimate the number of injection wells required to store these emissions.
- Estimate the cost per tonne of CO_2 stored.

Problem 25.2 (see Worked Solution 25.2)

It is planned to use a cylindrical packed absorption tower to separate CO_2 from combustion waste gas provided at a rate of $5.48 \text{ m}^3 \text{ min}^{-1}$. A solvent, containing 30% MEA, is to be supplied at a rate of $0.04 \text{ m}^3 \text{ min}^{-1}$. The solvent has an initial CO_2 concentration (C_{LB}) of 55.1 kg m^{-3} . The Henry's law coefficient for CO_2 in the solvent (K) is 19,100. The effective mass transfer coefficient (k_a) for the packed tower is assumed to be 0.00102 min^{-1} . The diameter of the packed tower is 0.43 m.

- (a) Determine the height of packed tower required if the CO_2 concentration in the waste gas is to be reduced from 0.0481 to 0.0153 kg m^{-3} .
- (b) Determine the outlet gas CO_2 concentration expected from the column designed in part (a) if the inlet gas CO_2 concentration is 0.281 kg m^{-3} .
- (c) Determine the height of packed tower required if the CO_2 concentration in the waste gas is to be reduced from 0.281 to 0.0153 kg m^{-3} (this latter scenario is based on Case 32 in Table 4 of [20]).
- (d) Determine the mass rate of CO_2 absorbed per unit volume of absorption tower for each of the scenarios described in parts (a), (b) and (c).

Problem 25.3 (see Worked Solution 25.3)

Waste gas from a power plant has an SO_2 concentration of $173 \text{ } \mu\text{g m}^{-3}$. A packed absorption tower has been installed to scrub the SO_2 with pure water. The cross-sectional area and height of the tower are 1.5 m^2 and 3.55 m, respectively. The waste gas is produced at a rate of $1.49 \text{ m}^3 \text{ s}^{-1}$. Pure water is supplied at a rate of $0.0396 \text{ m}^3 \text{ s}^{-1}$. The SO_2 concentration of the waste gas exiting the absorption tower is $43.3 \text{ } \mu\text{g m}^{-3}$.

- (a) Determine the effective mass transfer coefficient (k_a) of the absorption tower, assuming the Henry's law coefficient for SO_2 in water (K) is 33.4 (this is based on Example 6.10 of [18, p. 235]).
- (b) Determine the volume of packed absorption tower that is required to reduce the SO_2 concentration to $20 \text{ } \mu\text{g m}^{-3}$.

Problem 25.4 (see Worked Solution 25.4)

A factory needs to reduce the trichloroethylene concentration in its wastewater before it can be discharged to a municipal sewer. Wastewater is produced at a rate of $80 \text{ m}^3 \text{ h}^{-1}$. The mass concentration of trichloroethylene in the wastewater is $131 \text{ } \mu\text{g l}^{-1}$. The plan is to strip the trichloroethylene from the wastewater using countercurrent air flow in a packed absorption tower. The absorption tower has a volume of 4.4 m^3 and an effective mass transfer coefficient (k_a) of 44 h^{-1} . The Henry's law coefficient (K) for trichloroethylene in water is 2.43. Determine the volumetric air flow rate required to reduce the trichloroethylene concentration in the water to $13.1 \text{ } \mu\text{g l}^{-1}$ (this problem is based on Example 3 of [21, p. 1.350]).

25.6 Worked Solutions**Worked Solution 25.1** (see Problem 25.1)

(a) The storage capacity for open aquifers can be determined from Eq. (25.4). Let $\rho_{\text{CO}_2} = 650 \text{ kg m}^{-3}$, $\phi = 0.25$ and $V = 70 \times 800 \times 10^6 = 5.600 \times 10^{10} \text{ m}^3$. Given that there is no further information, let us assume that the efficiency factor, $E = 0.02$. It follows that the CO_2 storage capacity of the aquifer assuming open conditions is 182.0 Mt.

(b) The storage capacity for fully confined aquifers can be determined from Eq. (25.2). Let $c_R = 1.6 \times 10^{-10} \text{ Pa}^{-1}$ and $c_W = 4.4 \times 10^{-10} \text{ Pa}^{-1}$.

Because the system is hydrostatic, the initial pore-pressure can be determined from Eq. (25.1). Let us take the depth below sea-bed to be at the centroid of the aquifer, i.e., $z = 1100 + 70/2 = 1135 \text{ m}$ and $\rho_W = 1000 \text{ kg m}^{-3}$. Noting that the sea depth is 50 m, the initial pressure,

$$p_0 = 1000 \times 9.81 \times (1135 + 50) = 1.162 \times 10^7 \text{ Pa}$$

The maximum pressure, p_{max} , can be taken to be 90% of the fracture pressure, p_f . From Eq. (25.3), it follows that $p_f = 1.790 \times 10^7 \text{ Pa}$ and therefore $p_{\text{max}} = 1.611 \times 10^7 \text{ Pa}$.

Equation (25.2) then yields a CO_2 storage capacity of 44.09 Mt.

(c) The power station emits at a rate of 3 Mt per year so the number of years of emissions that can be stored is $44.09 \div 3 = 14.70$ years.

(d) A typical injection well can take around 0.35 Mt CO₂ per year. Therefore the number of injection wells required will be around $3 \div 0.35 = 8.571 = 9$.

(e) The typical lifetime-cost of an offshore injection well with platform and facilities is 128 million USD₂₀₁₉. It follows that the total cost will be around $9 \times 128 = 1152$ million USD₂₀₁₉. But given that this will store 44.09 Mt, the cost of storing the CO₂ will be around 26.13 USD₂₀₁₉ per tonne.

Worked Solution 25.2 (see Problem 25.2)

(a) In this case, the required height of packed absorption tower can be found from Eq. (25.31). Let $Q_G = 5.48 \text{ m}^3 \text{ min}^{-1}$, $Q_L = 0.04 \text{ m}^3 \text{ min}^{-1}$, $C_{LB} = 55.1 \text{ kg m}^{-3}$, $K = 19$, 100, $k_a = 0.00102 \text{ min}^{-1}$, $A = \pi \times 0.43^2/4$, $C_{GA} = 0.0481 \text{ kg m}^{-3}$ and $C_{GB} = 0.0153 \text{ kg m}^{-3}$. It follows that the packed tower height, H , will need to be at least 2.511 m.

(b) In this case, the outlet gas concentration can be found from Eq. (25.30). Letting $H = 2.511 \text{ m}$, $C_{GA} = 0.281 \text{ kg m}^{-3}$ and everything else staying the same as in part (a), it follows that the outlet gas CO₂ concentration, C_{GB} , will be 0.07925 kg m⁻³.

(c) The required height of packed absorption tower can again be found from Eq. (25.31). Letting $C_{GA} = 0.281 \text{ kg m}^{-3}$, $C_{GB} = 0.0153 \text{ kg m}^{-3}$ and everything else staying the same as in part (a), it follows that the packed tower height, H , will need to be at least 6.052 m.

(d) The mass rate of CO₂ absorbed per unit volume of absorption tower, $\hat{r}_a$ [ML⁻³T⁻¹], is found from

$$\hat{r}_a = \frac{Q_G \cdot (C_{GA} - C_{GB})}{AH}$$

It follows that:

$C_{GA} \text{ (kg m}^{-3}\text{)}$	$C_{GB} \text{ (kg m}^{-3}\text{)}$	$\hat{r}_a \text{ (kg m}^{-3} \text{ min}^{-1}\text{)}$
(a) 0.0481	0.0153	0.493
(b) 0.281	0.07925	3.03
(c) 0.281	0.0153	1.66

Note that $\hat{r}_a$ can be thought of as being inversely proportional to the cost rate of capturing CO₂. Scenario (a) is the most expensive scenario because the CO₂ content of the inlet is smallest. Scenario (b) is the least expensive scenario because both the inlet and outlet CO₂ concentrations are relatively large. The table above provides an interesting quantifiable demonstration about why it is economically preferable to increase the CO₂ content of a waste gas stream prior to separation.

Worked Solution 25.3 (see Problem 25.3)

(a) Substituting Eq. (25.21) into Eq. (25.31) and solving for k_a leads to

$$k_a = \frac{\ln \left[\frac{Q_L(KC_{GA} - C_{LB}) - Q_G(C_{GA} - C_{GB})}{Q_L(KC_{GB} - C_{LB})} \right]}{AH \left(\frac{K}{Q_G} - \frac{1}{Q_L} \right)} \quad (25.34)$$

Let $C_{GA} = 173 \mu\text{g m}^{-3}$, $C_{LB} = 0 \mu\text{g m}^{-3}$, $A = 1.5 \text{ m}^2$, $H = 3.55 \text{ m}$, $Q_G = 1.49 \text{ m}^3 \text{ s}^{-1}$, $Q_L = 0.0396 \text{ m}^3 \text{ s}^{-1}$, $C_{GB} = 43.3 \mu\text{g m}^{-3}$ and $K = 33.4$. It follows that $k_a = 0.03155 \text{ s}^{-1}$.

(b) The volume of absorption tower, $V = AH$, which can be obtained by rearranging Eq. (25.34)

$$V = \frac{\ln \left[\frac{Q_L(KC_{GA} - C_{LB}) - Q_G(C_{GA} - C_{GB})}{Q_L(KC_{GB} - C_{LB})} \right]}{k_a \left(\frac{K}{Q_G} - \frac{1}{Q_L} \right)}$$

Setting $k_a = 0.03155 \text{ s}^{-1}$ and $C_{GB} = 20 \mu\text{g m}^{-3}$ it follows that $V = 38.47 \text{ m}^3$. So the volume of an absorption tank would need to be at least 38.5 m^3 .

Worked Solution 25.4 (see Problem 25.4)

In this case, the outlet and inlet concentrations of the liquid stream, C_{LA} and C_{LB} , respectively, are defined so we should use Eq. (25.32). Unfortunately it is not possible to solve directly for the air-flow rate, Q_G , because Q_G is also featured in the expression for λ (Eq. (25.21)). However, we can use an iterative method to find the value of Q_G such that the C_{LA} from Eq. (25.32) is equal to the specified value. Below is a MATLAB script that minimises the error between the calculated and target values of C_{LA} by iteratively changing Q_G using MATLAB's optimisation function, `fminsearch`.

```
function DetermineAirFlowRate
QgGUESS = 80; %Guess air flow rate (m3/h)
%Use fminsearch to minimise objective function
Qg = fminsearch(@ObjFun, QgGUESS)
function Err = ObjFun(Qg)
%Objective function which when minimised
%determines an air flow rate required to
%obtain a desired water outlet concentration.
Ql = 80; %Water flow rate (m3/h)
V = 4.4; %Volume of absorption tower (m3)
ka = 44; %Mass transfer coefficient (1/h)
K = 2.43; %Henry's law coefficient (-)
```



```

Cla = 13.1; %Water outlet concentration (mug/l)
Clb = 131; %Water inlet concentration (mug/l)
Cga = 0; %Air inlet concentration (mug/l)
%Determine value of water outlet concentration
%for the given value of Qg
G = exp(-V*ka*(K/Qg-1/Q1));
ClaEST = ((Q1*K-Qg)*Clb+Qg*K*Cga*(1-G))/(Q1*K-Qg*G);
%Determine error between current and target values
Err = abs(Cla-ClaEST);

```

It is found that Q_G needs to be at least $2460 \text{ m}^3 \text{ h}^{-1}$.

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Abstract

This chapter develops some of the common mathematical methods used to design heights of chimney stacks for ensuring safe dispersion of atmospheric pollutants. The advection dispersion equation is derived using mass conservation and Reynolds decomposition. A steady-state analytical solution for plume dispersion is obtained using a Gaussian bivariate distribution function. The significance of the dry adiabatic lapse rate for defining atmospheric stability is explained. Empirical equations are presented to estimate plume dispersion coefficients using atmospheric stability classes. An analytical solution is derived to provide a theoretical basis for Briggs's plume rise equations. Practical applications are presented through a problem sheet with worked solutions.

Notation

A	Cross-sectional area [L^2].
c_p	Specific heat capacity [$L^2T^{-2}\Theta^{-1}$].
C	Mass concentration [ML^{-3}].
g	Gravitational acceleration [LT^{-2}].
F_0	Buoyancy flux parameter [L^4T^{-3}].
h_p	Enthalpy per unit mass within the plume [L^2T^{-2}].
h_e	Enthalpy per unit mass within environmental air surrounding the plume [L^2T^{-2}].
H	Enthalpy [ML^2T^{-2}].
H_0	Plume rise [L].
H_e	Effective stack height [L].
H_s	Actual stack height [L].
K_{ij}	Dispersion coefficient scalar [L^2T^{-1}].
$\mathbf{K}$	Dispersion coefficient tensor [L^2T^{-1}].
L	Characteristic length [L].

M_0	Mass flux of air through the plume [MT^{-1}].
M_d	Molecular mass of dry air (g mol^{-1}).
M_{i0}	Emission rate for component i [MT^{-1}].
N	Stability parameter [T^{-1}].
p	Pressure [$\text{ML}^{-1}\text{T}^{-2}$].
Q	Volumetric flow rate [L^3T^{-1}].
Q_h	Heat energy [ML^2T^{-2}].
R_u	Universal ideal gas constant ($\text{J mol}^{-1}\text{K}^{-1}$).
R	Radius of plume [L].
R_0	Radius of chimney stack [L].
s	Lagrangian distance from the plume's origin [L].
t	Time [T].
T	Temperature [Θ].
T_{e0}	Environmental temperature at the elevation of the chimney outlet [Θ].
T_{p0}	Temperature of the plume at the chimney outlet [Θ].
u	Velocity in the x direction or wind speed [LT^{-1}].
$\mathbf{u}$	Velocity vector [LT^{-1}].
U	Internal energy [ML^2T^{-2}].
v	Velocity in the y direction [LT^{-1}].
v_e	Velocity at which entrained air enters the plume [LT^{-1}].
v_s	Lagrangian velocity along the plume [LT^{-1}].
V	Volume [L^3].
w	Velocity in the z direction [LT^{-1}].
w_0	Vertical velocity of gas as it leaves a chimney stack [LT^{-1}].
W	Work done [ML^2T^{-2}].
x	Horizontal distance along the x -axis [L].
x_f	Distance at which the maximum plume rise is thought to occur [L].
X_i	Mass fraction for component i [-].
y	Horizontal distance along the y -axis [L].
z	Elevation [L].
α	Empirical factor describing air entrainment [-].
γ	Dimensionless stability parameter [-].
ζ	Dimensionless elevation [-].
μ	Dynamic viscosity of fluid [$\text{ML}^{-1}\text{T}^{-1}$].
ρ	Mass density of gas [ML^{-3}].
ρ_p	Mass density of gas within the plume [ML^{-3}].
ρ_e	Mass density of gas within environmental air surrounding the plume [ML^{-3}].
σ	Dimensionless Lagrangian distance [-].
σ_y	Standard deviation in the y direction [L].
σ_z	Standard deviation in the z direction [L].

26.1 Introduction

Waste gases are often discharged from high chimneys, referred to as stacks. The intention is that winds will blow away the gas and mix it with air, leading to a reduction in the concentration of pollutants. The aim is to reduce pollutant concentrations to an acceptably low level so as to avoid adverse impacts on downwind receptors (households, forests and other sensitive areas). In this chapter we develop some simple mathematical models to describe the atmospheric dispersion of pollutants around discharging chimney stacks.

First we develop an important governing equation known as the advection dispersion equation (ADE). This equation is used to describe how pollutants are transported within a moving turbulent fluid mass. It is then shown how a bivariate Gaussian distribution function can be used, as an analytical solution to the ADE, for a steady state point source in a semi-infinite domain. This latter function is extended to account for a land surface below the source, using a technique known as the method of images.

Following on from this, we discuss the role of meteorological conditions on atmospheric dispersion. Negative vertical temperature gradients give rise to unstable atmospheric conditions leading to greater vertical dispersion of pollution plumes. A critical temperature gradient, known as the dry adiabatic lapse rate, is derived using a combination of hydrostatics and the first law of thermodynamics. A set of empirical relationships are then provided, describing how the standard deviations of a Gaussian plume are affected by different levels of atmospheric stability.

The origin of a Gaussian plume associated with gas exiting a chimney stack is normally taken to be a finite vertical distance above the chimney outlet, referred to as the plume rise. The extent of plume rise is controlled by the buoyancy of the exiting gas, the exiting velocity, the wind speed and the level of atmospheric stability. Some simple empirical equations are provided to predict plume rise under different meteorological conditions. It is then shown how aspects of these empirical equations can be derived by combining statements of mass conservation, vertical momentum and heat conservation. Finally some practical exercises are provided to explore how these various equations can be used to support the design and analysis of chimney stacks.

26.2 The Advection Dispersion Equation

26.2.1 Mass Concentration of Waste Gases

The density of waste gas, ρ (g m^{-3}), is typically assumed to be approximately equal to that predicted by an ideal gas law for dry air:

$$\rho = \frac{pM_d}{R_u T} \quad (26.1)$$

where p (Pa) is pressure, $M_d = 28.96 \text{ g mol}^{-1}$ [1, p. 6] is the molecular mass of dry air, $R_u = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$ is the universal ideal gas constant and T (K) is temperature.

The quantity of a given component within a waste gas (e.g., CO, NO₂) can be specified as a mass fraction, X_i [-] (often specified in parts per million (ppm)) or as a mass concentration, C [ML⁻³] (often specified in $\mu\text{g m}^{-3}$).

Suppose a chimney emits waste gas at a volumetric rate, Q [L³T⁻¹], with a pollutant mass fraction, X_i . The emission rate of that pollutant, M_{i0} [MT⁻¹], is found from

$$M_{i0} = \rho Q X_i \quad (26.2)$$

or

$$M_{i0} = Q C. \quad (26.3)$$

26.2.2 Mass Conservation in a Control-Volume

Here we will develop a mass conservation statement for a pollutant moving through a control-volume (CV) of air. The CV has dimensions of δx , δy and δz (Fig. 26.1). The mass of pollutant stored in the CV is found from $\delta x \delta y \delta z C$.

Challenge 26.1 Use the expressions describing the inputs and outputs of the CV shown in Fig. 26.1 to derive a partial differential equation describing mass conservation for a pollutant moving through air.

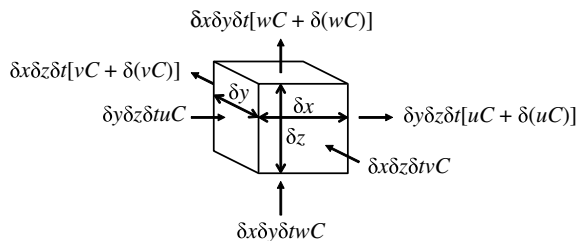
Under transient conditions, mass conservation dictates that, over a designated time-period, any mass of a substance entering a CV equals the mass of that substance leaving the CV plus an associated change in mass of the substance stored within the control-volume.

The mass of the pollutant entering the CV is

$$\delta y \delta z \delta t u C + \delta x \delta z \delta t v C + \delta x \delta y \delta t w C$$

where u [LT⁻¹], v [LT⁻¹] and w [LT⁻¹] are velocities of the air in the x , y and z directions, respectively.

Fig. 26.1 Mass conservation of a pollutant moving through a control-volume of air



The mass of the pollutant leaving the CV is

$$\delta y \delta z \delta t [uC + \delta(uC)] + \delta x \delta z \delta t [vC + \delta(vC)] + \delta x \delta y \delta t [wC + \delta(wC)]$$

The resulting change in the mass of the pollutant stored within the CV is

$$\delta x \delta y \delta z \delta C$$

Mass conservation therefore dictates that

$$\begin{aligned} \delta x \delta y \delta z \delta C &= \delta y \delta z \delta t uC + \delta x \delta z \delta t vC + \delta x \delta y \delta t wC \\ &\quad - \delta y \delta z \delta t [uC + \delta(uC)] - \delta x \delta z \delta t [vC + \delta(vC)] \\ &\quad - \delta x \delta y \delta t [wC + \delta(wC)] \end{aligned}$$

which can be simplified to get

$$\frac{\delta C}{\delta t} = -\frac{\delta(uC)}{\delta x} - \frac{\delta(vC)}{\delta y} - \frac{\delta(wC)}{\delta z}$$

If we now consider an infinitesimal time-period and an infinitesimal CV, this reduces further to the following partial differential equation

$$\frac{\partial C}{\partial t} = -\frac{\partial(uC)}{\partial x} - \frac{\partial(vC)}{\partial y} - \frac{\partial(wC)}{\partial z}$$

or in vector-calculus notation

$$\frac{\partial C}{\partial t} = -\nabla \cdot (\mathbf{u}C) \quad (26.4)$$

where

$$\mathbf{u} = \begin{bmatrix} u \\ v \\ w \end{bmatrix}$$

26.2.3 Reynolds Decomposition

Air flow is turbulent and fluid velocities fluctuate in a chaotic fashion. It is therefore helpful to adopt Reynolds decomposition such that it can be said that [2, p. 156]

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}' \quad (26.5)$$

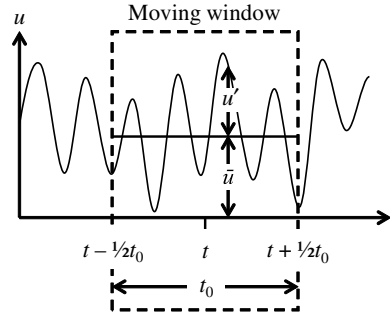
where $\bar{\mathbf{u}}$ is a vector containing moving temporal averages found from

$$\bar{\mathbf{u}} = \frac{1}{t_0} \int_{t-\frac{1}{2}t_0}^{t+\frac{1}{2}t_0} \mathbf{u}(\tau) d\tau$$

and $\mathbf{u}'$ is a vector containing the associated residuals and t_0 [T] is the duration of the moving average window (see Fig. 26.2), which needs to be significantly larger than the duration of the fluctuations. Important characteristics include that

$$\overline{\bar{\mathbf{u}}} = \bar{\mathbf{u}} \quad \text{and} \quad \overline{\mathbf{u}'} = 0 \quad (26.6)$$

Fig. 26.2 Schematic diagram illustrating the principle of Reynolds decomposition



Pollutant concentrations will also fluctuate chaotically and a similar Reynolds decomposition can be applied [2, p. 657]

$$C = \bar{C} + C' \quad (26.7)$$

where

$$\bar{\bar{C}} = \bar{C} \quad \text{and} \quad \bar{C'} = 0 \quad (26.8)$$

Also note that

$$\overline{\bar{u} C} = \bar{u} \bar{C}, \quad \overline{u' C} = 0 \quad \text{and} \quad \overline{\bar{u} C'} = 0 \quad (26.9)$$

The $\overline{u' C'}$ [$\text{ML}^{-2}\text{T}^{-1}$] terms are often referred to as turbulent diffusion fluxes. Analogous to Fick's first law of diffusion, an important additional assumption often made is that [2, p. 659]

$$\overline{u' C'} = -\mathbf{K} \nabla \bar{C} \quad (26.10)$$

where $\mathbf{K}$ [L^2T^{-1}] is known as the dispersion coefficient tensor found from

$$\mathbf{K} = \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix}$$

The K_{ij} coefficients are referred to as eddy diffusivities and are often treated as empirical properties.

Challenge 26.2 Use Reynolds decomposition to write an equation describing the transport of a pollutant in terms of time-averaged concentration, time-averaged velocity and the dispersion coefficient tensor.

Substituting Eqs. (26.5) and (26.7) into Eq. (26.4) leads to

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial C'}{\partial t} = -\nabla \cdot (\bar{u} \bar{C} + \mathbf{u}' \bar{C} + \bar{u} C' + \mathbf{u}' C') \quad (26.11)$$

Taking a temporal average of both sides of Eq. (26.11) gives us

$$\frac{\partial \bar{\bar{C}}}{\partial t} + \frac{\partial \bar{C'}}{\partial t} = -\nabla \cdot (\bar{\bar{u}} \bar{\bar{C}} + \overline{\mathbf{u}' \bar{C}} + \overline{\bar{u} C'} + \overline{\mathbf{u}' C'}) \quad (26.12)$$

Substituting Eqs. (26.8), (26.9) and (26.10) into Eq. (26.12) leads to ([3], p. 5)

$$\frac{\partial \bar{C}}{\partial t} = -\nabla \cdot (\bar{\mathbf{u}} \bar{C} - \mathbf{K} \nabla \bar{C}) \quad (26.13)$$

which is known as the advection dispersion equation.

The first term on the right-hand-side of Eq. (26.13) describes the advection of the pollutant. Advection is the transport of a substance or quantity by bulk motion of a fluid. The second term on the right-hand-side of Eq. (26.13) describes the dispersion of the pollutant from the mean bulk flow path of the air. This dispersion comes about due to the chaotic fluctuations associated with turbulent flow systems.

26.2.4 Gaussian Plume Modelling

A common set of assumptions for modelling atmospheric dispersion of pollutants include:

1. The stack can be treated as a point source, continuously emitting a pollutant at a constant mass rate, M_{i0} [MT^{-1}], located at $x = x_0$, $y = y_0$ and $z = z_0$.
2. The concentration field is steady-state.
3. The velocity field is steady-state, spatially uniform and zero in the y and z directions.
4. The dispersion coefficient tensor is steady-state, spatially uniform and only non-zero in the y and z directions.

Under these conditions, Eq. (26.13) reduces to

$$u \frac{\partial C}{\partial x} = K_{yy} \frac{\partial^2 C}{\partial y^2} + K_{zz} \frac{\partial^2 C}{\partial z^2} \quad (26.14)$$

Also note that under steady-state conditions, the mass flow rate of pollutant through any vertical plane downwind from the source, will be equal to the emission rate from the source, M_{i0} [MT^{-1}]. It follows that

$$M_{i0} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u C dy dz \quad (26.15)$$

Consider a Gaussian bivariate distribution function for two uncorrelated variables [4, p. 707]

$$f(y, z) = \frac{F_0}{2\pi\sigma_y\sigma_z} \exp \left[-\frac{(y - y_0)^2}{2\sigma_y^2} - \frac{(z - z_0)^2}{2\sigma_z^2} \right] \quad (26.16)$$

where σ_y [L] and σ_z [L] are the standard deviations of y and z , respectively, and

$$F_0 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(y, z) dy dz \quad (26.17)$$

It can be shown that Eq. (26.16) is a particular solution of Eq. (26.14).

Challenge 26.3 Obtain expressions for the second-order partial derivative of Eq. (26.16) with respect to y and z .

Let us make the substitution

$$\lambda = \frac{(y - y_0)^2}{2\sigma_y^2} + \frac{(z - z_0)^2}{2\sigma_z^2} \quad (26.18)$$

Partially differentiating Eq. (26.16) with respect to y and z (using the chain rule) leads to:

$$\frac{\partial f}{\partial y} = \frac{\partial \lambda}{\partial y} \frac{\partial f}{\partial \lambda} = \frac{(y - y_0)}{\sigma_y^2} \left[-\frac{F_0 e^{-\lambda}}{2\pi\sigma_y\sigma_z} \right] = -\frac{(y - y_0)}{\sigma_y^2} f(y, z) \quad (26.19)$$

$$\frac{\partial f}{\partial z} = \frac{\partial \lambda}{\partial z} \frac{\partial f}{\partial \lambda} = \frac{(z - z_0)}{\sigma_z^2} \left[-\frac{F_0 e^{-\lambda}}{2\pi\sigma_y\sigma_z} \right] = -\frac{(z - z_0)}{\sigma_z^2} f(y, z) \quad (26.20)$$

Partially differentiating Eq. (26.19) with respect to y and Eq. (26.20) with respect to z (using the product rule) gives us:

$$\frac{\partial^2 f}{\partial y^2} = -\frac{(y - y_0)}{\sigma_y^2} \frac{\partial f}{\partial y} - \frac{1}{\sigma_y^2} f(y, z) = \left(\frac{(y - y_0)^2}{\sigma_y^4} - \frac{1}{\sigma_y^2} \right) f(y, z) \quad (26.21)$$

$$\frac{\partial^2 f}{\partial z^2} = -\frac{(z - z_0)}{\sigma_z^2} \frac{\partial f}{\partial z} - \frac{1}{\sigma_z^2} f(y, z) = \left(\frac{(z - z_0)^2}{\sigma_z^4} - \frac{1}{\sigma_z^2} \right) f(y, z) \quad (26.22)$$

Assuming $C = f$ and substituting Eqs. (26.21) and (26.22) into Eq. (26.14) then leads to

$$u \frac{\partial f}{\partial x} = \left[\frac{K_{yy}(y - y_0)^2}{\sigma_y^4} + \frac{K_{zz}(z - z_0)^2}{\sigma_z^4} - \left(\frac{K_{yy}}{\sigma_y^2} + \frac{K_{zz}}{\sigma_z^2} \right) \right] f(y, z) \quad (26.23)$$

But note that f is not apparently a function of x . However, the definitions of σ_y and σ_z have not yet been specified and therefore are free to form appropriate functions of x .

Challenge 26.4 Substitute the trial functions, $\sigma_y = \hat{\sigma}_y(x - x_0)^{1/2}$ and $\sigma_z = \hat{\sigma}_z(x - x_0)^{1/2}$, into Eq. (26.16) and derive expressions for $\hat{\sigma}_y$ and $\hat{\sigma}_z$ such that Eq. (26.23) is satisfied.

Let us try

$$\sigma_y = \hat{\sigma}_y(x - x_0)^{1/2} \quad \text{and} \quad \sigma_z = \hat{\sigma}_z(x - x_0)^{1/2} \quad (26.24)$$

such that Eqs. (26.16) and (26.18) become

$$f(x, y, z) = \frac{F_0 e^{-\lambda}}{2\pi \hat{\sigma}_y \hat{\sigma}_z (x - x_0)} \quad (26.25)$$

and

$$\lambda = \left(\frac{(y - y_0)^2}{2\hat{\sigma}_y^2} + \frac{(z - z_0)^2}{2\hat{\sigma}_z^2} \right) \frac{1}{x - x_0} \quad (26.26)$$

respectively.

Partially differentiating Eq. (26.25) with respect to x gives us (using the product rule and then the chain rule)

$$\begin{aligned} \frac{\partial f}{\partial x} &= \frac{1}{x - x_0} \frac{\partial \lambda}{\partial x} \frac{\partial}{\partial \lambda} [(x - x_0)f] - \frac{F_0 e^{-\lambda}}{2\pi \hat{\sigma}_y \hat{\sigma}_z (x - x_0)^2} \\ &= \left(\frac{(y - y_0)^2}{2\hat{\sigma}_y^2 (x - x_0)^2} + \frac{(z - z_0)^2}{2\hat{\sigma}_z^2 (x - x_0)^2} - \frac{1}{x - x_0} \right) f \end{aligned} \quad (26.27)$$

Substituting Eq. (26.27) into Eq. (26.23) leads to

$$\frac{u(y - y_0)^2}{2\hat{\sigma}_y^2 (x - x_0)} + \frac{u(z - z_0)^2}{2\hat{\sigma}_z^2 (x - x_0)} - u = \frac{K_{yy}(y - y_0)^2}{\hat{\sigma}_y^4 (x - x_0)} + \frac{K_{zz}(z - z_0)^2}{\hat{\sigma}_z^4 (x - x_0)} - \left(\frac{K_{yy}}{\hat{\sigma}_y^2} + \frac{K_{zz}}{\hat{\sigma}_z^2} \right) \quad (26.28)$$

Equating coefficients of $\frac{(y - y_0)^2}{x - x_0}$ and $\frac{(z - z_0)^2}{x - x_0}$ in Eq. (26.28) gives us

$$\hat{\sigma}_y = \left(\frac{2K_{yy}}{u} \right)^{1/2} \quad \text{and} \quad \hat{\sigma}_z = \left(\frac{2K_{zz}}{u} \right)^{1/2} \quad (26.29)$$

Substituting Eq. (26.29) into Eq. (26.24) leads to

$$\sigma_y = \left(\frac{2K_{yy}(x - x_0)}{u} \right)^{1/2} \quad \text{and} \quad \sigma_z = \left(\frac{2K_{zz}(x - x_0)}{u} \right)^{1/2} \quad (26.30)$$

So providing Eq. (26.30) is adopted, $C = f$ and (considering Eq. (26.16))

$$C(x, y, z) = \frac{F_0}{2\pi \sigma_y \sigma_z} \exp \left(-\frac{(y - y_0)^2}{2\sigma_y^2} - \frac{(z - z_0)^2}{2\sigma_z^2} \right) \quad (26.31)$$

Challenge 26.5 Determine an expression for F_0 in terms of the mass injection rate, M_{i0} .

Considering that $C = f$, multiplying Eq. (26.17) by u leads to Eq. (26.15). It follows that

$$F_0 = \frac{M_{i0}}{u} \quad (26.32)$$

Substituting Eq. (26.32) into Eq. (26.31) gives us

$$C(x, y, z) = \frac{M_{i0}}{2\pi \sigma_y \sigma_z u} \exp \left(-\frac{(y - y_0)^2}{2\sigma_y^2} - \frac{(z - z_0)^2}{2\sigma_z^2} \right) \quad (26.33)$$

26.2.5 Reflection From the Land Surface

Suppose that the source of the plume exists at an elevation, H_e , from the land surface, hereafter referred to as the effective stack height. The plume will not be able to disperse into the land surface. Therefore it is necessary to represent the land surface as a zero gradient boundary. Because Eq. (26.33) is linear in M_{i0} , we can use the so-called method of images (see Sect. 14.4). The idea is as follows:

Let C_1 be the mass concentration of a plume due to a source at $x_0 = 0$, $y_0 = 0$ and $z_0 = H_e$. From Eq. (26.33)

$$C_1 = \frac{M_{i0}}{2\pi\sigma_y\sigma_z u} \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{(z - H_e)^2}{2\sigma_z^2}\right) \quad (26.34)$$

Let C_2 be the mass concentration of a plume due to an imaginary source at $x_0 = 0$, $y_0 = 0$ and $z_0 = -H_e$. From Eq. (26.33)

$$C_2 = \frac{M_{i0}}{2\pi\sigma_y\sigma_z u} \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{(z + H_e)^2}{2\sigma_z^2}\right) \quad (26.35)$$

Note that C_2 is a mirror image of C_1 in the plane of $z = 0$. If we superimpose these two concentration distributions on one another, we end up with a zero gradient boundary at $z = 0$. Let $C = C_1 + C_2$ such that [3, p. 25]

$$C = \frac{M_{i0}}{2\pi\sigma_y\sigma_z u} e^{-\frac{y^2}{2\sigma_y^2}} \left[e^{-\frac{(z-H_e)^2}{2\sigma_z^2}} + e^{-\frac{(z+H_e)^2}{2\sigma_z^2}} \right] \quad (26.36)$$

Challenge 26.6 Confirm that Eq. (26.36) satisfies the boundary condition, $\left. \frac{\partial C}{\partial z} \right|_{z=0} = 0$.

Partially differentiating Eq. (26.36) with respect to z gives us

$$\frac{\partial C}{\partial z} = \frac{M_{i0}}{2\pi\sigma_y\sigma_z u} e^{-\frac{y^2}{2\sigma_y^2}} \left[-\frac{(z - H_e)}{\sigma_z^2} e^{-\frac{(z-H_e)^2}{2\sigma_z^2}} - \frac{(z + H_e)}{\sigma_z^2} e^{-\frac{(z+H_e)^2}{2\sigma_z^2}} \right]$$

from which it can be seen that $\left. \frac{\partial C}{\partial z} \right|_{z=0} = 0$.

Challenge 26.7 Confirm that Eq. (26.36) satisfies the constraint, $\int_0^\infty \int_{-\infty}^\infty u C(y, z) dy dz = M_{i0}$.

Let us confirm that the total mass flow rate in a given $y - z$ plane, described by Eq. (26.36), is indeed M_{i0} .

Consider the integral of Eq. (26.36) with respect to z

$$\begin{aligned}
 \int_0^{\infty} C dz &= \frac{M_{i0}}{2\pi\sigma_y\sigma_z u} e^{-\frac{y^2}{2\sigma_y^2}} \int_0^{\infty} \left[e^{-\frac{(z-H_e)^2}{2\sigma_z^2}} + e^{-\frac{(z+H_e)^2}{2\sigma_z^2}} \right] dz \\
 &= \frac{M_{i0}}{2\pi\sigma_y\sigma_z u} e^{-\frac{y^2}{2\sigma_y^2}} \left[\int_0^{\infty} e^{-\frac{(z-H_e)^2}{2\sigma_z^2}} dz + \int_{-\infty}^0 e^{-\frac{(z-H_e)^2}{2\sigma_z^2}} dz \right] \\
 &= \frac{M_{i0}}{2\pi\sigma_y\sigma_z u} e^{-\frac{y^2}{2\sigma_y^2}} \int_{-\infty}^{\infty} e^{-\frac{(z-H_e)^2}{2\sigma_z^2}} dz \quad (26.37)
 \end{aligned}$$

Substituting Eq. (26.34) into Eq. (26.37) and integrating both sides with respect to y leads to

$$\int_0^{\infty} \int_{-\infty}^{\infty} C(y, z) dy dz = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} C_1(y, z) dy dz \quad (26.38)$$

Given Eq. (26.15), it can be said that

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u C_1(y, z) dy dz = M_{i0} \quad (26.39)$$

Multiplying both sides of Eq. (26.38) by u and substituting Eq. (26.39) gives us

$$\int_0^{\infty} \int_{-\infty}^{\infty} u C(y, z) dy dz = M_{i0} \quad (26.40)$$

26.3 Atmospheric Stability

26.3.1 Dry Adiabatic Lapse Rate

Vertical air movement is largely controlled by buoyancy driven natural convection. The buoyancy comes about due to changes in air density associated with changes in temperature. A parcel of air that is warmer than its surroundings will rise. In contrast, a parcel of air that is cooler than its surroundings will sink.

Consider a local environment characterised by a negative temperature gradient such that the air gets cooler with increasing elevation. Now imagine a parcel of air released from a stack that is warmer than its surroundings. The parcel of air will rise due to buoyancy. However, the parcel of air will cool as it moves upwards, independently of the local environmental temperature gradient, due to expansion caused by the fact that air pressure reduces with elevation. The rate at which such a parcel of air will cool with elevation is referred to as the dry adiabatic lapse rate (DALR).

If the local temperature gradient is steeper than the DALR, the air parcel will always be warmer than the environmental air and will continue to rise indefinitely. This corresponds to an unstable condition. If the local temperature gradient is less steep than the DALR, the air parcel will eventually reach the same temperature as the environmental air and will stop rising. This corresponds to a stable condition. An expression to calculate the value of the DALR can be derived using hydrostatics and thermodynamics.

Challenge 26.8 Apply a vertical force balance on a control volume of static air to determine an expression for the vertical pressure gradient in a static body of air.

Consider a control volume (CV) of static air of density, ρ [ML^{-3}], vertical thickness, δz [L], and cross-sectional area, A [L^2]. Let p [$\text{ML}^{-1}\text{T}^{-2}$] and $p + \delta p$ [$\text{ML}^{-1}\text{T}^{-2}$] be the pressures at the base and top of the CV, respectively. A vertical force balance for the CV takes the form

$$pA = (p + \delta p)A + \rho g A \delta z$$

where g [LT^{-2}] is gravitational acceleration. It follows that

$$\frac{\partial p}{\partial z} = -\rho g \quad (26.41)$$

which is often referred to as a hydrostatic pressure gradient (see Sect. 1.2.1).

Although air is rarely static, the vertical pressure gradient in the atmosphere is often approximated as a hydrostatic pressure gradient.

A parcel of air moves vertically upwards. Because of the low thermal conductivity of the air, heat exchange between this parcel and the surrounding air can be ignored. In this way, the parcel of air can be said to be moving adiabatically.

Challenge 26.9 Assume a hydrostatic pressure distribution and use the first law of thermodynamics to determine an expression for the rate at which the temperature of the air parcel changes with elevation in terms of the specific heat capacity of air, c_p [$\text{L}^2\text{T}^{-2}\Theta^{-1}$], and gravitational acceleration, g [LT^{-2}].

The first law of thermodynamics gives that [5, p. 174]

$$Q_h - W = dU \quad (26.42)$$

where, in our context, Q_h [ML^2T^{-2}] is heat energy provided from the surrounding air, W [ML^2T^{-2}] is the work done by the parcel of air and dU [ML^2T^{-2}] is the resulting change in its internal energy as a consequence.

As stated earlier, heat exchange between the parcel of air and its surroundings can be ignored so $Q_h = 0$. Furthermore, the work done by the parcel of air is found

from $W = pdV$ [5, p. 166] where $V [\text{L}^3]$ is the volume of the parcel. It follows that Eq. (26.42) reduces to

$$dU = -pdV \quad (26.43)$$

The specific heat capacity, $c_p [\text{L}^2\text{T}^{-2}\Theta^{-1}]$, can be used to relate changes in enthalpy, $H [\text{ML}^2\text{T}^{-2}]$, with changes in temperature, $T [\Theta]$, through the relation [5, p. 179]

$$dH = \rho V c_p dT \quad (26.44)$$

Noting that $H = U + pV$ [5, p. 127] it can also be said that

$$dH = dU + pdV + Vdp \quad (26.45)$$

Substituting Eqs. (26.43) and (26.44) into Eq. (26.45) leads to

$$\rho V c_p dT = V dp \quad (26.46)$$

Partially differentiating Eq. (26.46) with respect to z and substituting Eq. (26.41) gives us the rate at which the parcel of air cools with elevation

$$\frac{\partial T}{\partial z} = -\frac{g}{c_p} \quad (26.47)$$

which is referred to as the dry adiabatic lapse rate (DALR).

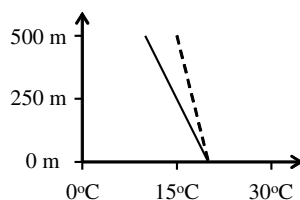
The specific heat capacity of air is $1005 \text{ J kg}^{-1} \text{ K}^{-1}$. It follows that the DALR is -9.76 K km^{-1} .

26.3.2 Impact on Plume Behaviour

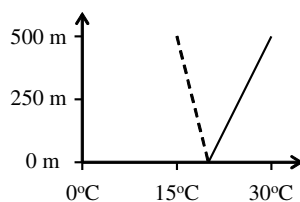
The behaviour of a plume leaving a chimney stack is strongly controlled by the stability of the surrounding air.

- When the environmental temperature gradient is steeper than the DALR, there will be significant upward convection giving rise to turbulent unstable conditions and a looping plume (see Fig. 26.3a).
- When the environmental temperature decreases at a slower rate as compared to the DALR, the air will be stable with little vertical flow. Therefore the plume will mostly only disperse in the horizontal direction, giving rise to a fanning plume (see Fig. 26.3b).
- When the environmental temperature gradient is equal to the DALR, the air is neutrally buoyant and the plume is expected to disperse equally in all directions, giving rise to a coning plume (see Fig. 26.3c).
- Locations of sign changes in temperature gradients are referred to as inversions. Where there is an inversion below the stack exit with stable air below and unstable air above, the plume will be trapped above the inversion forming a lofting plume (see Fig. 26.3d).
- Where there is an inversion above the stack exit with unstable air below and stable air above, the plume will be trapped below the inversion forming a fumigation plume (see Fig. 26.3e). This represents the worst-case scenario for people living in close proximity to the stack.

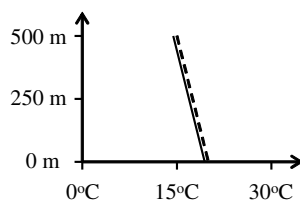
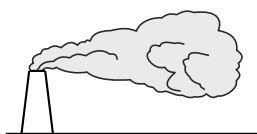
(a) Unstable conditions leads to a looping plume.



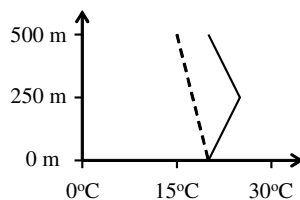
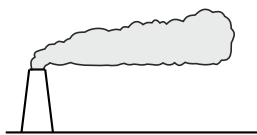
(b) Stable conditions leads to a fanning plume.



(c) Neutral conditions leads to a coning plume.



(d) Underlying inversion leads to a lofting plume.



(e) Overlying inversion leads to a fumigation plume.

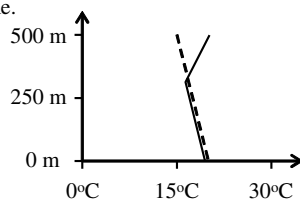


Fig. 26.3 Effect of temperature gradient on plume behaviour (inspired by [6]). The solid and dashed lines in the elevation temperature plots represent environmental temperature gradients and dry adiabatic lapse rate, respectively

26.3.3 Impact on Dispersion

Unfortunately, Eq. (26.30) is not found to be that accurate in practice. Instead, σ_y and σ_z are strongly controlled by atmospheric stability and have a more complicated relationship with distance, x . Atmospheric stability is a measure of the atmosphere's tendency to discourage vertical movement. Plume dispersion is much greater in unstable atmospheres. Seven stability classes, referred to as the Pasquill atmospheric stability classes, are often considered (see Table 26.1).

Empirical data relating σ_y and σ_z with stability class and distance from source were obtained from a set of field experiments carried out in the 1950 and 1960s as a part of a project known as Project Prairie Grass [3]. Many empirical equations have since been fitted to this data. A particularly effective set of equations was provided by [8], the details of which are given in Table 26.2.

In the past, stability class was commonly determined using the criteria provided in Table 26.3, which includes information about wind speed, incoming solar radiation and cloudiness. During the daytime, low wind speeds and/or high incoming solar radiation lead to more unstable conditions. During the night-time, low wind speeds and/or clear sky lead to more stable conditions. More recently, the US Nuclear

Table 26.1 Pasquill atmospheric stability classes in terms of vertical temperature gradient [7]

Stability class	Temperature gradient (K km^{-1})
(A) Extremely unstable	$\frac{\partial T}{\partial z} \leq -19$
(B) Moderately unstable	$-19 < \frac{\partial T}{\partial z} \leq -17$
(C) Slightly unstable	$-17 < \frac{\partial T}{\partial z} \leq -15$
(D) Neutral	$-15 < \frac{\partial T}{\partial z} \leq -5$
(E) Slightly stable	$-5 < \frac{\partial T}{\partial z} \leq 15$
(F) Moderately stable	$15 < \frac{\partial T}{\partial z} \leq 40$
(G) Extremely stable	$\frac{\partial T}{\partial z} > 40$

Table 26.2 Empirical coefficients given by [8] for estimating horizontal and vertical standard deviations using the empirical laws $\sigma_y = e^{a_y + b_y \ln x + c_y \ln^2 x}$ and $\sigma_z = e^{a_z + b_z \ln x + c_z \ln^2 x}$, respectively, where σ_y and σ_z are in m, x is in km and A-F refer to the Pasquill atmospheric stability classes

Stability	a_y	b_y	c_y	a_z	b_z	c_z
A	5.357	0.8828	-0.0076	6.035	2.1097	0.2770
B	5.058	0.9024	-0.0096	4.694	1.0629	0.0136
C	4.651	0.9181	-0.0076	4.110	0.9201	-0.0020
D	4.230	0.9222	-0.0087	3.414	0.7371	-0.0316
E	3.922	0.9222	-0.0064	3.057	0.6794	-0.0450
F	3.533	0.9181	-0.0070	2.621	0.6564	-0.0540

Table 26.3 Pasquill atmospheric stability classes (see Table 26.1 for definitions of classes A-F) in terms of wind speed, incoming solar radiation and cloudiness (adapted from [9, p. 662]). “Strong” corresponds to a clear summer’s day. “Moderate” corresponds to a summer’s day with broken clouds. “Slight” corresponds to either an overcast summer’s day or anytime during autumn, winter and early spring

Surface wind speed m s^{-1}	Daytime Incoming solar radiation			Night-time Cloudiness	
	Strong	Moderate	Slight	Cloudy ($>4/8$)	Clear ($<3/8$)
<2	A	A-B	B	E	F
2–3	A-B	B	C	E	F
3–5	B	B-C	C	D	E
5–6	C	C-D	D	D	D
>6	C	D	D	D	D

Regulatory Commission (NRC) have recommended instead that stability class be determined from vertical temperature gradient using the criteria given in Table 26.1.

26.4 Effective Stack Height Estimation

The effective stack height, H_e [L], is found from

$$H_e = H_s + H_0 \quad (26.48)$$

where H_s [L] is the actual stack height and H_0 [L] is referred to as the plume rise.

A plume of hot gas exiting a chimney stack will rise due to buoyancy and bend over in the mean wind direction (see Fig. 26.4). Under stable conditions, the buoyancy of the plume is quickly lost. Under neutral or unstable conditions, the plume will rise further but ultimately stop once vertical velocities become comparable to environmental turbulent fluxes. Plume rise, H_0 [L], is an important parameter for stack height design and below we present semi-empirical equations for its estimation along with an associated conceptual model.

26.4.1 Conceptual Model

The conceptual model can be described as follows. Hot gas leaves a chimney stack with a steady vertical velocity, w_0 [LT^{-1}], and steady temperature, T_{p0} [$^\circ\text{C}$]. The temperature of the surrounding air at the same elevation is T_{e0} [$^\circ\text{C}$]. The elevation of the chimney stack exit above the land surface is H_s [L]. The radius of the chimney stack is R_0 [L].

A wind is assumed to blow in the horizontal direction with a constant horizontal velocity, u [LT^{-1}]. The environmental temperature, T_e [$^\circ\text{C}$], is characterised by a

26.4.2 Briggs' Plume Rise Equations

Plume rise is commonly estimated using a set of semi-empirical equations attributed to Briggs [9]. Under neutral or unstable conditions (i.e., $N^2 \leq 0$), the Briggs equation for elevation of a plume centroid above the land surface (see Fig. 26.4), z_p [L], at a given horizontal distance from the source in the principal direction of the wind, x [L], takes the form [9, p. 677]

$$z_p = \frac{1.6F_0^{1/3}x^{2/3}}{u} + H_s, \quad x \leq x_f \quad (26.52)$$

where F_0 [L^4T^{-3}] is known as a buoyancy flux parameter, defined by [3, p. 11]

$$F_0 = \frac{R_0^2 w_0 (T_{p0} - T_{e0})g}{T_{p0}} \quad (26.53)$$

and x_f [L] is a distance at which the maximum plume rise is thought to occur, found from

$$x_f = \begin{cases} 49F_0^{5/8}, & F_0 < 55 \text{ m}^4\text{s}^{-3} \\ 119F_0^{2/5}, & F_0 \geq 55 \text{ m}^4\text{s}^{-3} \end{cases} \quad (26.54)$$

The corresponding plume rise, H_0 , is found from

$$H_0 = \frac{1.6F_0^{1/3}x_f^{2/3}}{u} \quad (26.55)$$

Under stable conditions (i.e., $N^2 > 0$), the Brigg's equation for the plume rise takes the form [9, p. 677]

$$H_0 = \begin{cases} 5F_0^{0.25}(N^2)^{-0.375}, & u < 1.5 \text{ m s}^{-1} \\ 2.6 \left(\frac{F_0}{uN^2} \right)^{1/3}, & u \geq 1.5 \text{ m s}^{-1} \end{cases} \quad (26.56)$$

Equation (26.54) and the case when $u < 1.5 \text{ m s}^{-1}$ in Eq. (26.56) are both empirical equations derived from a combination of measurements from wind tunnels and field observations of atmospheric plume releases from chimney stacks. However, elements of Eqs. (26.52) and (26.56) can be derived from theoretical considerations, as shown below.

26.4.3 Analytical Solution to Provide Theoretical Basis

26.4.3.1 Governing Equations

An analytical solution for the plume rise term, H_0 , can be obtained by solving the following set of steady-state Lagrangian equations for mass conservation, vertical momentum conservation and heat conservation [10]:

$$\frac{\partial M}{\partial s} = 2\pi R \rho_e v_e \quad (26.57)$$

$$\frac{\partial(Mw)}{\partial s} = \pi R^2(\rho_e - \rho_p)g \quad (26.58)$$

$$\frac{\partial(Mh_p)}{\partial s} = 2\pi R\rho_e v_e h_e \quad (26.59)$$

where M [MT^{-1}] is the mass flux of air through the plume, found from

$$M = \pi R^2 v_s \rho_p \quad (26.60)$$

The relevant boundary conditions are [11]:

$$\begin{aligned} R &= 0, & s &= 0 \\ Mw &= 0, & s &= 0 \\ M(h_p - h_e) &= \pi R_0^2 w_0 \rho_{p0}(h_{p0} - h_{e0}), & s &= 0 \end{aligned} \quad (26.61)$$

Challenge 26.10 Use the concepts of specific heat capacity and ideal gas law to write the right-hand-side of Eq. (26.58) in terms of $M(h_p - h_e)$.

The ideal gas law gives that

$$\rho_e T_e = \rho_p T_p \quad (26.62)$$

and the specific heat capacity, c_p [$\text{L}^2\text{T}^{-2}\Theta^{-1}$], can be used to say

$$h = c_p T \quad (26.63)$$

It follows that

$$\begin{aligned} \rho_e - \rho_p &= \rho_p \left(\frac{\rho_e}{\rho_p} - 1 \right) \\ &= \rho_p \left(\frac{T_p}{T_e} - 1 \right) \\ &= \rho_p \left(\frac{h_p}{h_e} - 1 \right) \\ &= \frac{\rho_p}{h_e} (h_p - h_e) \end{aligned} \quad (26.64)$$

Substituting Eqs. (26.60) and (26.64) into Eq. (26.58) leads to

$$\frac{\partial(Mw)}{\partial s} = \frac{gM(h_p - h_e)}{v_s h_e} \quad (26.65)$$

Challenge 26.11 Use Eqs. (26.49), (26.50), (26.57), (26.59), (26.63) and (26.65) to derive an expression for $\frac{\partial}{\partial s}[M(h_p - h_e)]$ in terms of $\frac{h_e N^2 M_w}{v_s g}$.

Note that

$$\frac{\partial}{\partial s}[M(h_p - h_e)] = \frac{\partial}{\partial s}(Mh_p) - h_e \frac{\partial M}{\partial s} - M \frac{\partial h_e}{\partial s} \quad (26.66)$$

Substituting Eq. (26.57) into Eq. (26.59) leads to

$$\frac{\partial}{\partial s}(Mh_p) = h_e \frac{\partial M}{\partial s} \quad (26.67)$$

Substituting Eq. (26.67) into Eq. (26.66) gives us

$$\frac{\partial}{\partial s}[M(h_p - h_e)] = -M \frac{\partial h_e}{\partial s} \quad (26.68)$$

Substituting Eqs. (26.50) and (26.63) into Eq. (26.68) leads to

$$\frac{\partial}{\partial s}[M(h_p - h_e)] = -\frac{Mwh_e}{v_s T_e} \frac{\partial T_e}{\partial z} \quad (26.69)$$

Substituting Eq. (26.49) into Eq. (26.69) gives us

$$\frac{\partial}{\partial s}[M(h_p - h_e)] = -\frac{h_e N^2 M w}{v_s g} \quad (26.70)$$

26.4.3.2 Application of the Boussinesq Approximation

At this stage it is useful to apply the Boussinesq approximation, which involves assuming that density is constant everywhere except where it is present as a difference. From Eqs. (26.62) and (26.63) we have that

$$\frac{\rho_e}{\rho_p} = \frac{T_p}{T_e} = \frac{h_p}{h_e}$$

Invoking the Boussinesq approximation therefore implies that:

$$\rho_e = \rho_p = \rho_{e0} = \rho_{p0}$$

$$T_e = T_p = T_{e0} = T_{p0}$$

$$h_e = h_p = h_{e0} = h_{p0}$$

everywhere except for where we see the difference $h_p - h_e$.

It follows that Eqs. (26.60), (26.57), (26.65) and (26.70) reduce to

$$M = \pi R^2 v_s \rho_{p0} \quad (26.71)$$

$$\frac{\partial M}{\partial s} = 2\pi R \rho_{p0} v_e \quad (26.72)$$

$$\frac{\partial(Mw)}{\partial s} = \frac{gM(h_p - h_e)}{v_s h_{p0}} \quad (26.73)$$

and

$$\frac{\partial}{\partial s}[M(h_p - h_e)] = -\frac{h_{p0} N^2 M w}{v_s g} \quad (26.74)$$

respectively.

26.4.3.3 Solutions for Mw and $M(h_p - h_e)$

Challenge 26.12 Combine Eqs. (26.73) and (26.74) to form a second-order differential equation for Mw , solve for Mw , solve for $M(h_p - h_e)$ and then apply the boundary conditions in Eq. (26.61). Write the final equations in terms of the buoyancy flux parameter, F_0 .

Differentiating both sides of Eq. (26.73) with respect to s and equating the result with Eq. (26.74) leads to

$$\frac{\partial^2(Mw)}{\partial s^2} = -\frac{N^2 Mw}{v_s^2} \quad (26.75)$$

which has the general solution

$$Mw = A_1 \cos\left(\frac{Ns}{v_s}\right) + A_2 \sin\left(\frac{Ns}{v_s}\right) \quad (26.76)$$

where A_1 and A_2 are integration constants.

Noting that $Mw = 0$ at $s = 0$ (recall Eq. (26.61)) it can be understood that $A_1 = 0$ and

$$Mw = A_2 \sin\left(\frac{Ns}{v_s}\right) \quad (26.77)$$

Differentiating Eq. (26.77) with respect to s and equating the result with Eq. (26.73) leads to

$$M(h_p - h_e) = \frac{A_2 h_{p0} N}{g} \cos\left(\frac{Ns}{v_s}\right) \quad (26.78)$$

Noting that $M(h_p - h_e) = \pi R_0^2 w_0 \rho_{p0} (h_{p0} - h_{e0})$ at $s = 0$ (recall Eq. (26.61)) it can be understood that

$$A_2 = \frac{\pi R_0^2 w_0 \rho_{p0} (h_{p0} - h_{e0}) g}{h_{p0} N} \quad (26.79)$$

Substituting Eq. (26.63) into Eq. (26.79) gives us

$$A_2 = \frac{\pi R_0^2 w_0 \rho_{p0} (T_{p0} - T_{e0}) g}{T_{p0} N} \quad (26.80)$$

Substituting Eq. (26.53) into Eq. (26.80) leads to

$$A_2 = \frac{\pi F_0 \rho_{p0}}{N} \quad (26.81)$$

where F_0 [$L^4 T^{-3}$] is the aforementioned buoyancy flux parameter.

Substituting Eq. (26.81) into Eqs. (26.77) and (26.78) gives us

$$Mw = \frac{\pi F_0 \rho_{p0}}{N} \sin\left(\frac{Ns}{v_s}\right) \quad (26.82)$$

and

$$M(h_p - h_e) = \frac{\pi F_0 \rho_{p0} h_{p0}}{g} \cos\left(\frac{Ns}{v_s}\right) \quad (26.83)$$

respectively.

26.4.3.4 Solution for the Plume Rise

Substituting Eqs. (26.51) and (26.71) into the left-hand-side of Eq. (26.72) gives us

$$\frac{\partial M}{\partial s} = \frac{2\alpha M|w|}{Rv_s} \quad (26.84)$$

Substituting Eq. (26.71) into the left-hand-side of Eq. (26.84) gives us

$$\pi v_s \rho_{p0} \frac{\partial R^2}{\partial s} = \frac{2\alpha M|w|}{Rv_s} \quad (26.85)$$

from which it follows that

$$R^2 \frac{\partial R}{\partial s} = \frac{\alpha M|w|}{\pi v_s^2 \rho_{p0}} \quad (26.86)$$

Substituting Eq. (26.82) into Eq. (26.86) gives us

$$R^2 \frac{\partial R}{\partial s} = \frac{\alpha F_0}{v_s^2 N} \left| \sin \left(\frac{Ns}{v_s} \right) \right| \quad (26.87)$$

Interestingly

$$\int_0^x |\sin x| dx = 2 \left\lfloor \frac{x}{\pi} \right\rfloor + 1 - \operatorname{sgn}(\sin x) \cos x$$

where $\lfloor x \rfloor$ represents the integer part of x and $\operatorname{sgn}(x)$ represents the sign of x . Therefore integrating both sides of Eq. (26.87) with respect to s from zero to s (recall from Eq. (26.61) that $R = 0$ at $s = 0$) yields

$$R^3 = \frac{3\alpha F_0}{v_s N^2} \left\{ 2 \left\lfloor \frac{Ns}{\pi v_s} \right\rfloor + 1 - \operatorname{sgn} \left[\sin \left(\frac{Ns}{v_s} \right) \right] \cos \left(\frac{Ns}{v_s} \right) \right\} \quad (26.88)$$

Substituting Eqs. (26.71) and (26.88) into Eq. (26.82) and solving for w leads to

$$w = \frac{\left[\frac{F_0 N}{9\alpha^2 v_s} \right]^{1/3} \sin \left(\frac{Ns}{v_s} \right)}{\left\{ 2 \left\lfloor \frac{Ns}{\pi v_s} \right\rfloor + 1 - \operatorname{sgn} \left[\sin \left(\frac{Ns}{v_s} \right) \right] \cos \left(\frac{Ns}{v_s} \right) \right\}^{2/3}} \quad (26.89)$$

Substituting Eq. (26.89) into Eq. (26.50) gives us

$$\frac{\partial z}{\partial s} = \frac{\left[\frac{F_0 N}{9\alpha^2 v_s^4} \right]^{1/3} \sin \left(\frac{Ns}{v_s} \right)}{\left\{ 2 \left\lfloor \frac{Ns}{\pi v_s} \right\rfloor + 1 - \operatorname{sgn} \left[\sin \left(\frac{Ns}{v_s} \right) \right] \cos \left(\frac{Ns}{v_s} \right) \right\}^{2/3}} \quad (26.90)$$

It can be further stated that

$$\frac{\partial \zeta}{\partial \sigma} = \frac{\left[\frac{\gamma}{9} \right]^{1/3} \sin(\gamma\sigma)}{\left\{ 2 \left\lfloor \frac{\gamma\sigma}{\pi} \right\rfloor + 1 - \operatorname{sgn}[\sin(\gamma\sigma)] \cos(\gamma\sigma) \right\}^{2/3}} \quad (26.91)$$

where

$$\zeta = \frac{z - H_s}{L}, \quad \sigma = \frac{s}{\alpha L}, \quad \gamma^2 = \frac{\alpha^2 N^2 L^2}{v_s^2} \quad (26.92)$$

and $L = F_0 v_s^{-3}$ [L] is a characteristic length.

Equation (26.91) is very difficult to integrate analytically. However, when $N^2 \leq \frac{\pi^2 v^2}{s^2}$ it can be said that $\gamma^2 \sigma^2 \leq \pi^2$. Furthermore, it can be seen that

$$2 \left\lfloor \frac{\gamma \sigma}{\pi} \right\rfloor + 1 - \operatorname{sgn}[\sin(\gamma \sigma)] \cos(\gamma \sigma) = 1 - \cos(\gamma \sigma), \quad \gamma^2 \sigma^2 \leq \pi^2 \quad (26.93)$$

Substituting Eq. (26.93) into Eq. (26.91) leads to

$$\frac{\partial \zeta}{\partial \sigma} = \frac{\left[\frac{\gamma}{9}\right]^{1/3} \sin(\gamma \sigma)}{[1 - \cos(\gamma \sigma)]^{2/3}}, \quad \gamma^2 \sigma^2 \leq \pi^2 \quad (26.94)$$

Making the additional substitution $\xi = \cos(\gamma \sigma)$ then gives us

$$\frac{\partial \zeta}{\partial \xi} = -(9\gamma^2)^{-1/3} (1 - \xi)^{-2/3} \quad (26.95)$$

Integrating both sides of Eq. (26.95) with respect to ξ give us

$$\zeta = \left[\frac{3(1 - \xi)}{\gamma^2} \right]^{1/3} + A_3$$

where A_3 is an another integration constant.

Noting that $\zeta = 0$ at $\sigma = 0$ it follows that $A_3 = 0$. Reversing the ξ substitution then leads to

$$\zeta = \left\{ \frac{3[1 - \cos(\gamma \sigma)]}{\gamma^2} \right\}^{1/3}, \quad \gamma^2 \sigma^2 \leq \pi^2 \quad (26.96)$$

26.4.3.5 Special Cases

For unstable atmospheric conditions, $\gamma^2 < 0$ and γ will be imaginary such that we should consider the fact that

$$\cos(\gamma \sigma) = \cosh(i\gamma \sigma)$$

where i denotes an imaginary number.

For neutral atmospheric conditions, $\gamma^2 = 0$, so we should consider the Maclaurin series $\cos x = 1 - \frac{x^2}{2} + O(x^4)$ and recognise that

$$\lim_{\gamma^2 \rightarrow 0} \left\{ \frac{1}{\gamma^2} [1 - \cos(\gamma \sigma)] \right\} = \frac{\sigma^2}{2}$$

We can then see that [11]

$$\zeta = \begin{cases} \left\{ \frac{3[1 - \cosh(i\gamma \sigma)]}{\gamma^2} \right\}^{1/3}, & \gamma^2 < 0 \\ \left(\frac{3\sigma^2}{2} \right)^{1/3}, & \gamma^2 = 0 \\ \left\{ \frac{3[1 - \cos(\gamma \sigma)]}{\gamma^2} \right\}^{1/3}, & 0 < \gamma^2 \sigma^2 \leq \pi^2 \end{cases} \quad (26.97)$$

Furthermore, it can be shown, by numerical integration of Eq. (26.91) with respect to σ from 0 to ∞ , that [11]

$$\lim_{\gamma^2 \sigma^2 \rightarrow \infty} \zeta = \frac{1.53}{\gamma^{2/3}} \equiv \frac{H_0}{L} \quad (26.98)$$

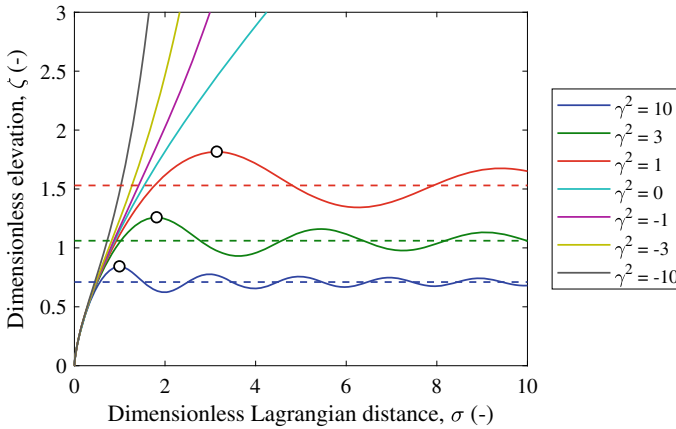


Fig. 26.5 Plots of dimensionless plume rise, ζ , against dimensionless Lagrangian distance, σ , for different dimensionless stability numbers, γ^2 , as indicated by the legend. Results for $\gamma^2\sigma^2 \leq \pi^2$ were obtained using Eq. (26.97). Results for $\gamma^2\sigma^2 > \pi^2$ were obtained by numerically integrating Eq. (26.91). The locations for where $\gamma^2\sigma^2 = \pi^2$ are given by the circular markers. Asymptotic results for $\lim_{\gamma^2\sigma^2 \rightarrow \infty} \zeta$, as given by Eq. (26.98), are shown as an additional set of dashed lines

Plots of ζ against σ for different values of γ^2 are shown in Fig. 26.5. Interestingly, close to the source of the plume, the plume trajectory can be seen to be independent of γ^2 . For stable conditions (i.e., $\gamma^2 > 0$) the plume rises according to a cosine wave up until the maximum value of the cosine wave is reached. The elevation of the plume then behaves like a damped oscillator, eventually settling on the elevation predicted by Eq. (26.98) (as indicated by the dashed lines). For neutral or unstable conditions (i.e., $\gamma^2 \leq 0$), Eq. (26.97) predicts that plumes will continue to rise with distance from source, indefinitely. However, such plumes are perceived to reach a quasi-steady elevation once the vertical velocities within the plume become comparable with those turbulent vertical velocities found naturally present in the surrounding air [12, p. 34].

26.4.3.6 Relating Back to Brigg's Equation

Equation (26.52) can be derived from Eq. (26.97) by setting $s = x$, $v_s = u$, $\alpha = 0.6$ and $N^2 = 0$. An equation very similar to the case in Eq. (26.56), where $u \geq 1.5 \text{ m s}^{-1}$, can be derived from Eq. (26.98) by setting $v_s = u$ and $\alpha = 0.6$.

26.5 Problem Sheet

Problem 26.1 (see Worked Solution 26.1)

(a) A waste gas is discharged from a chimney at a rate of $177 \text{ m}^3 \text{ s}^{-1}$. The NO_2 mass fraction of the waste gas is 713 ppm. The temperature and pressure of the exiting waste gas is 400 K and 100 kPa, respectively. The wind speed is 5 m s^{-1} . The environmental temperature gradient is -10 K km^{-1} . The effective stack height is 100 m.

(i) Determine the emission rate for NO_2 .

(ii) Determine the ground-level mass concentration of NO_2 at 2 km downwind from the stack on the centreline of the plume.

(iii) Repeat part (ii) with the same x and z coordinates but set $y = 100 \text{ m}$.

(b) Write a MATLAB code to calculate concentrations within the plume described in part (a) above.

(i) Construct an $x - z$ contour plot of mass concentration downwind of the stack along the centreline of the plume showing contours from zero to $320 \mu\text{g m}^{-3}$ in increments of $40 \mu\text{g m}^{-3}$.

(ii) Use MATLAB's optimisation tool, `fminsearch`, to determine the location and magnitude of the maximum ground-level concentration.

(iii) Manually change the value of the effective stack height and determine the minimum effective stack height (to the nearest 10 m) required to ensure the maximum ground-level concentration satisfies the annual mean WHO air quality guideline for NO_2 .

(c) Determine the plume rise expected for the scenario described above, assuming the environmental temperature is 280 K.

Problem 26.2 (see Worked Solution 26.2)

Repeat Problem 26.1 but with the environmental temperature gradient set to 10 K km^{-1} .

Problem 26.3 (see Worked Solution 26.3)

Specify the height of chimney required to satisfy the WHO guidelines for both of the scenarios described in Problems 26.1 and 26.2.

26.6 Worked Solutions

Worked Solution 26.1 (see Problem 26.1)

(a) (i) The emission rate can be determined from Eq. (26.2). The density of the gas can be found from Eq. (26.1). Let $p = 10^5$ Pa, $T = 400$ K, $R_u = 8.314$ J mol⁻¹ K⁻¹, $M_d = 28.96$ g mol⁻¹. It follows that $\rho = 870.8$ g m⁻³ or 0.8708 kg m⁻³. Letting $Q = 177$ m³ s⁻¹ and $X_i = 713 \times 10^{-6}$ leads to an emission rate, $M_{i0} = 0.1099$ kg s⁻¹.

(ii) The mass concentration of NO₂ can be determined downwind of the chimney using Eq. (26.36). However, the first step is to determine the standard deviations of the plume. This can be achieved using Table 26.2. Given that the environmental temperature gradient is -10 K km⁻¹, Table 26.1 tells us that the stability class is D. In our case $x = 2$ km. From Table 26.2 we then have that

$$\sigma_y = e^{4.230+0.9222 \ln 2 - 0.0087 \ln^2 2} = 129.7 \text{ m}$$

and

$$\sigma_z = e^{3.414+0.7371 \ln 2 - 0.0316 \ln^2 2} = 49.89 \text{ m}$$

Because we are on the ground, $z = 0$. Because we are on the centreline, $y = 0$. Further letting $M_{i0} = 0.1099$ kg s⁻¹, $H_e = 100$ m and $u = 5$ m s⁻¹, Eq. (26.36) gives that $C = 145.0 \times 10^{-9}$ kg m⁻³, which is 145 µg m⁻³.

(iii) Repeating the exercise but with $y = 100$ m, Eq. (26.36) yields $C = 107.7 \times 10^{-9}$ kg m⁻³, which is 108 µg m⁻³. Note that mass concentrations will always be highest on the centreline at $y = 0$.

(b) (i) The following MATLAB code can be used to develop the contour plot

```
%Specify parameters
Mi0 = 0.1099; %Emission rate (kg/s)
He = 100; %Effective stack height (m)
u=5; %Wind speed (m/s)
dTdz = -10; %Temperature gradient (K/km)
%Specify spatial points to calculate for in m
x = linspace(0, 15000, 101); y = 0;
z = linspace(0, 300, 100)';
%Calculate mass concentration in (kg/m3)
C = DispersionFun(Mi0, He, u, x, y, z, dTdz);
figure(1); clf; %Generate contour plot
contourf(x/1000,z,C*1e9, [0:40:320])
colorbar; caxis([0 320])
ylabel('Elevation above ground surface (m)')
xlabel('Distance from stack (km)')
title('NO_2 concentration (\u00b5gmug m^-^3)')
```

where DispersionFun is a function, given in Listing 26.1, containing the script to calculate the mass concentrations using the standard deviation equations and coefficients due to [8] (given in Table 26.2), the stability class classification due to [7] (given in Table 26.1) along with the analytical solution given in Eq. (26.36). Note the need to multiply by 10^9 to convert kg m^{-3} to $\mu\text{g m}^{-3}$.

Listing 26.1 A MATLAB function to determine pollutant concentrations within a Gaussian plume according to Eq. (26.36), using the standard deviation equations and coefficients due to [8] (given in Table 26.2) along with the stability class classification due to [7] (given in Table 26.1).

```
function [C,Sy,Sz]=DispersionFun(Mi0,He,u,x,y,z,dTdz)
%Coefficients due to McMullen (1975)
abc=[5.357 0.8828 -0.0076 6.035 2.1097 0.2770
5.058 0.9024 -0.0096 4.694 1.0629 0.0136
4.651 0.9181 -0.0076 4.110 0.9201 -0.0020
4.230 0.9222 -0.0087 3.414 0.7371 -0.0316
3.922 0.9222 -0.0064 3.057 0.6794 -0.0450
3.533 0.9181 -0.0070 2.621 0.6564 -0.0540];
%Stability class classification due to NRC (2007)
if dTdz<=-19
n = 1;%Stability Class A
elseif dTdz>-19&dTdz<=-17
n = 2;%Stability Class B
elseif dTdz>-17&dTdz<=-15
n = 3;%Stability Class C
elseif dTdz>-15&dTdz<=-5
n = 4;%Stability Class D
elseif dTdz>-5&dTdz<=15
n = 5;%Stability Class E
elseif dTdz>15&dTdz<=40
n = 6;%Stability Class F
end
xkm=x/1000;%Convert to km
%Calculate standard deviation in x and y
ay=abc(n,1); by=abc(n,2); cy=abc(n,3);
Sy=exp(ay+by*log(xkm)+cy*log(xkm).^2);
az=abc(n,4); bz=abc(n,5); cz=abc(n,6);
Sz=exp(az+bz*log(xkm)+cz*log(xkm).^2);
%Determine concentration within the plume
T1=exp(-y.^2/2./Sy.^2);
T2=exp(-(z-He).^2/2./Sz.^2);
T3=exp(-(z+He).^2/2./Sz.^2);
C=Mi0/2/pi./Sy./Sz/u.*T1.*(T2+T3);
```

The resulting contour plot is shown in Fig. 26.6.

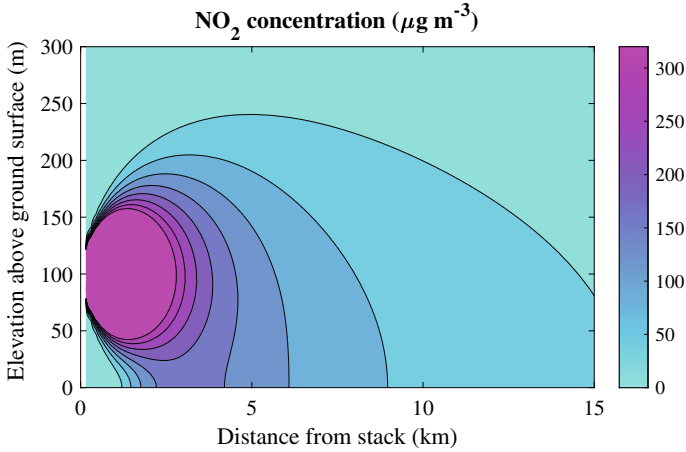


Fig. 26.6 Contour plot of NO_2 concentration within the unstable plume from Problem 26.1b

(ii) The following MATLAB code can be used to find the location and magnitude of the maximum ground-level concentration.

```
%Specify parameters
Mi0 = 0.1099; %Emission rate (kg/s)
He = 100; %Effective stack height (m)
u = 5; %Wind speed (m/s)
dTdz = -10; %Temperature gradient (K/km)
%Determine the location of maximum
%ground concentration, xMAX (m)
xMAXguess = 1000; %Initial estimate of xMAX
FUN = @(x) -DispersionFun(Mi0, He, u, x, 0, 0, dTdz);
xMAX = fminsearch(FUN, xMAXguess);
%Determine the mass concentration at this location
CMAX = DispersionFun(Mi0, He, u, xMAX, 0, 0, dTdz);
```

Note that `fminsearch` is searching for the value of x that gives the smallest value of the negative of the mass concentration returned by `DispersionFun` (see Listing 26.1), which in turn will be the location of the largest value of the mass concentration). `fminsearch` requires an initial value to start its search from. Here we have chosen 1000 m as our starting value but in fact the code is quite robust and not that dependent on this value. We have set y and z to zero in the calling of `DispersionFun` because we want the maximum ground concentration and this will occur somewhere on the centre line. The resulting location of the maximum ground surface concentration is 2960 m downwind of the chimney and its value is $179 \mu\text{g m}^{-3}$.

(iii) The annual mean WHO air quality guideline for NO_2 is $40 \mu\text{g m}^{-3}$ (see Table 24.1). By sequentially increasing the effective stack height by 10 m and rerun-

ning the code, developed for part (ii) above, it is found that a minimum effective stack height of 190 m is required to maintain ground surface concentrations below $40 \mu\text{g m}^{-3}$. This leads to a maximum ground surface concentration of $38.2 \mu\text{g m}^{-3}$, which occurs at a distance of 7830 m downwind of the chimney.

(c) Because the temperature gradient is negative, the plume rise equations for unstable conditions should be used, Eqs. (26.52) and (26.54). The first step is to determine the buoyancy flux parameter, F_0 . Noting that $Q = \pi R_0^2 w_0$ it follows that

$$F_0 = \frac{Q(T_{p0} - T_{e0})g}{\pi T_{p0}}$$

Letting $Q = 177 \text{ m}^3 \text{ s}^{-1}$, $T_{p0} = 400 \text{ K}$, $T_{e0} = 280 \text{ K}$ and $g = 9.81 \text{ m s}^{-2}$ it follows that $F_0 = 165.8 \text{ m}^4 \text{ s}^{-3}$. From Eq. (26.54), it can be determined that the plume centreline will reach its maximum height at $x_f = 919.2 \text{ m}$. The plume rise, H_0 , is found from Eq. (26.55). Noting that $u = 5 \text{ m s}^{-1}$, the plume rise, $H_0 = 166.2 \text{ m}$.

Worked Solution 26.2 (see Problem 26.2)

(a) (i) The emission rate is unchanged by the temperature gradient and remains 0.1099 kg s^{-1} .

(ii) Given that the environmental temperature gradient is 10 K km^{-1} , Table 26.1 tells us that the stability class is E. In our case $x = 2 \text{ km}$. From Table 26.2 we then have that

$$\sigma_y = e^{3.922+0.9222 \ln 2 - 0.0064 \ln^2 2} = 95.41 \text{ m}$$

and

$$\sigma_z = e^{3.057+0.6794 \ln 2 - 0.0450 \ln^2 2} = 33.32 \text{ m}$$

Because we are on the ground, $z = 0$. Because we are on the centreline, $y = 0$. Further letting $M_{i0} = 0.1099 \text{ kg s}^{-1}$, $H_e = 100 \text{ m}$ and $u = 5 \text{ m s}^{-1}$, Eq. (26.36) gives that $C = 24.39 \times 10^{-9} \text{ kg m}^{-3}$, which is $24.4 \mu\text{g m}^{-3}$.

(iii) If we repeat the exercise in (ii) but with $y = 100 \text{ m}$, Eq. (26.36) yields $C = 14.08 \times 10^{-9} \text{ kg m}^{-3}$, which is $14.1 \mu\text{g m}^{-3}$. Note that mass concentrations will always be highest on the centreline at $x = 0$.

(b) (i) By setting the temperature gradient to 10 K km^{-2} in the code developed for Problem 26.1(b) (i), the contour plot shown in Fig. 26.7 is obtained.

(ii) By setting the temperature gradient to 10 K km^{-2} in the code developed for Problem 26.1(b) (ii), it is found that the location of the maximum ground concentration is 5714 m downwind of the chimney and its value is $119.8 \mu\text{g m}^{-3}$. Note that the more stable conditions have led to more lateral dispersion but less vertical dispersion, which in turn leads to lower ground surface concentration. However, this assumes the plume rise is unaffected by stability. In fact, plume rise is much lower in stable conditions, as we will discover shortly.

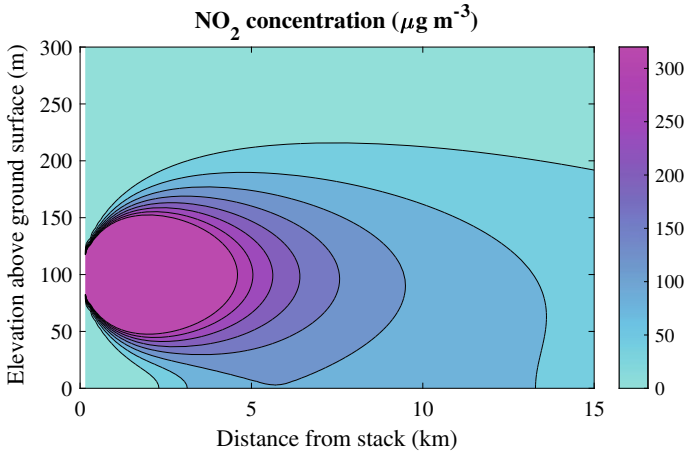


Fig. 26.7 Contour plot of NO_2 concentration within the stable plume from Problem 26.2(b)

(iii) By sequentially increasing the effective stack height by 10 m and rerunning the code developed for part (ii) above it is found that a minimum effective stack height of 150 m is required to maintain ground surface concentrations below $40 \mu\text{g m}^{-3}$. This leads to a maximum ground surface concentration of $38.0 \mu\text{g m}^{-3}$, which occurs at a distance of 12,000 m downwind of the chimney.

(c) Because the temperature gradient is now positive, the plume rise equation for stable conditions should be used, Eq. (26.56). From Worked Solution 26.1c, $F_0 = 165.8 \text{ m}^4 \text{ s}^{-3}$. From Eq. (26.49), $N^2 = \frac{9.81 \times 0.01}{280} = 0.0003504$. Letting $u = 5 \text{ m s}^{-1}$, Eq. (26.56) gives that the plume rise, $H_0 = 118.5 \text{ m}$.

Worked Solution 26.3 (see Problem 26.3)

Based on the scenario described in Problem 26.1, the effective stack height should be 190 m and the plume rise should be 166 m. So the chimney height should be at least 24 m. Based on the scenario described in Problem 26.2, the effective stack height should be 150 m and the plume rise should be 119 m. So the chimney height should be at least 31 m. Therefore, to be safe for both scenarios the chimney height should be at least 31 m.

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Abstract

This chapter introduces key aspects associated with water pollution. Drinking water and wastewater discharge guidelines are compared. A range of relevant pathogenic organisms and toxic substances are discussed. The significance of biochemical oxygen demand (BOD) is explained. The Streeter-Phelps equation, for modelling dissolved oxygen deficit in rivers, is derived using a combination of first-order decay and the two-film model for mass transfer across a liquid gas interface. Empirical equations are provided for estimating oxygen solubility limits and reaeration rate coefficients. Practical applications are presented through a problem sheet with worked solutions.

Notation

A	Cross-sectional area of river channel [L^2].
$B(t)$	Amount of dissolved oxygen that would be consumed after a time-period, t [ML^{-3}].
C	Mass concentration of biodegradable matter [ML^{-3}].
C_D	Downstream mass concentration [ML^{-3}].
C_E	Effluent mass concentration [ML^{-3}].
C_U	Upstream mass concentration [ML^{-3}].
C_0	Initial mass concentration of biodegradable matter [ML^{-3}].
G	Dissolved oxygen deficit [ML^{-3}].
G_0	Initial dissolved oxygen deficit [ML^{-3}].
$G_{\max}$	Maximum dissolved oxygen deficit [ML^{-3}].
H	Mean water depth [L].
k_a	Reaeration rate coefficient [T^{-1}].
k_c	Aerobic consumption rate coefficient [T^{-1}].
L	Ultimate biochemical oxygen demand [ML^{-3}].
L_0	Initial ultimate biochemical oxygen demand [ML^{-3}].

M_{in}	Mass of substance entering a control volume [M].
M_{out}	Mass of substance exiting a control volume [M].
Q_D	Downstream flow rate [L^3T^{-1}].
Q_E	Effluent flow rate [L^3T^{-1}].
Q_U	Upstream flow rate [L^3T^{-1}].
r_a	Reaeration rate [$ML^{-3}T^{-1}$].
r_c	Aerobic consumption rate [$ML^{-3}T^{-1}$].
t	Time [T].
u	Mean velocity of the river flow [LT^{-1}].
U	Dissolved oxygen concentration [ML^{-3}].
U_{min}	Initial dissolved oxygen concentration [ML^{-3}].
U_s	Dissolved oxygen concentration solubility limit [ML^{-3}].
U_0	Initial dissolved oxygen concentration [ML^{-3}].
x	Distance along river [L].
x_{min}	Location of minimum dissolved oxygen concentration [L].
α	Stoichiometric constant [-].
BOD	Biochemical oxygen demand.
BOD ₅	DO consumed after 5 days.
BOD ₂₀	DO consumed after 20 days.
COD	Chemical oxygen demand.
DO	Dissolved oxygen.
SS	Suspended solids.
TDS	Total dissolved solids.
TEP	Trade effluent permit.
THM	Trihalomethane.
WHO	World Health Organisation.

27.1 Introduction

In low income countries, water pollution is the second biggest pollution killer after air pollution (see Table 23.6). Water pollution causes less deaths in high income countries because so much more money is spent on water treatment and wastewater treatment. Water treatment is the treatment of water, to bring it up to a standard, such that it is safe to drink. Wastewater treatment is the treatment of wastewater, to bring it up to a standard, such that it is safe to discharge back to the environment.

In this chapter we explore the principle components of water pollution and some basic modelling techniques to describe pollution transport in rivers. First we look at some key aspects of typical drinking water guidelines. This naturally takes us through a list of relevant microorganisms and substances that lead to water being unsafe to drink. The exercise is then repeated using the EU Urban Wastewater Treatment Directive, which leads to an understanding about what makes wastewater damaging to the environment.

Table 27.1 Comparison of revised drinking water directive (EU) 2020/2184 [1] and WHO guidelines for drinking water quality [2] for selected parameters

Parameter	(EU) 2020/2184	WHO
Coliform bacteria (number/100 ml)	0	Unspecified
Total dissolved solids (mg l^{-1})	1625	Unspecified
Total THM ($\mu\text{g l}^{-1}$)	100	Unspecified
Arsenic ($\mu\text{g l}^{-1}$)	10	10
Benzene ($\mu\text{g l}^{-1}$)	1	10
Boron (mg l^{-1})	1.5	2.4
Mercury ($\mu\text{g l}^{-1}$)	1	6
Nitrate (mg l^{-1})	50	50

It will become apparent that biochemical oxygen demand is a dominant water pollution feature of concern. The final part of this chapter therefore focuses on developing a mathematical model to describe how dissolved oxygen, in river systems, reduces and then recovers, downstream of a pollutant discharger. Some practical applications of these equations are demonstrated through a problem sheet at the end.

27.2 Drinking Water

Drinking water is water deemed suitable for consumption by humans. Drinking water in the UK needs to comply with the Revised Drinking Water Directive (EU) 2020/2184. Table 27.1 shows a selection of parameters specified by both (EU) 2020/2184 [1] and the WHO Drinking Water Guidelines [2]. Each component is discussed below with reference to source, health impact and possible avoidance/treatment methods.

Note that many more parameters are specified by both the EU and the WHO. However, here we focus on representative examples, which are useful for understanding the various water treatment methods discussed later on.

27.2.1 Pathogenic Organisms

The main concern about drinking water are pathogenic organisms (organisms that cause disease). There are a wide range of different water-based pathogenic organisms. Monitoring and detecting all relevant pathogens is not possible. However, because most pathogens originate from faecal matter, an indicator organism can be tested for instead. Analysts normally count coliform bacteria because these are particularly

resistant to disinfection. Drinking Water Directive (EU) 2020/2184, stipulates that there should be zero coliform in any 100 ml sample.

Four relevant categories of organisms include viruses (non-living genetic material), bacteria (single-celled organisms without nuclei), protozoa (larger single-celled organisms with nuclei) and helminths (worm like parasites). Some representative examples of each are discussed below.

Viruses

Outbreaks of many pathogenic viruses have been linked to drinking water supplies including caliciviruses and both hepatitis A and B viruses [2]. Caliciviruses are a major cause of acute viral gastroenteritis with symptoms including nausea, vomiting and abdominal cramps. Hepatitis A and B both cause liver damage. Viruses are excreted in the faeces of infected individuals. Infection can take place by consumption of contaminated drinking water. Unfortunately, viruses tend to be more resistant to disinfection as compared to coliform bacteria. Therefore, avoidance mostly relies on protecting source water from contamination by human wastewater [2].

Bacteria

Relevant bacterial pathogens include *Vibrio*, *Salmonella*, *Escherichia coli* and *Legionella* [2]. *Vibrio* are responsible for cholera infections, which cause watery diarrhoea and dehydration; patients can lose as much as 10–15 litres of liquid per day. *Salmonella* are responsible for typhoid fever. Effects of *Escherichia coli* (*E coli*) include very bloody diarrhoea and meningitis. *Legionella* causes pneumonic illness.

With the exception of *Legionella*, most bacterial pathogens can be avoided through disinfection and checking coliform counts. However, *Legionella* tends to reside within biofilms that develop in warm water distribution systems. Control of *Legionella* in drinking water requires avoiding the temperature range 20–50 °C [2, p. 245].

Protozoa

Protozoa are a particular problem for drinking water because they often produce cysts, oocysts or eggs that are extremely resistant to conventional disinfection processes. One such example includes *Cryptosporidium*, which can cause intense diarrhoea for several weeks. As with many viruses, avoidance mostly relies on protecting source water from contamination by human wastewater [2]. The use of well managed slow sand filtration can help as well [3].

Helminths

One example of a helminth closely associated with drinking water includes *Dracunculus medinensis*, commonly referred to as Guinea worm. This disease has been largely eradicated but 1000s of cases continue to persist in a central belt of counties in sub-Saharan Africa [2, p. 285]. Infection is caused by the accidental consumption of cyclops (small freshwater crustaceans) in drinking water. *Dracunculus medinensis* larvae hatch from cyclops and enter subcutaneous tissues near the intestine of the human host. A female worm can grow up to 700 mm in length. Eventually, the worm

emerges from an ulcer in the lower limb and releases large numbers of larvae when the ulcer is immersed in water. The larvae can move about in the water for up to 3 days during which time they find a new cyclops host.

Main health problems occur when the worm track becomes secondarily infected, which can lead to permanent disability. Guinea worm can be avoided by removing cyclops from drinking water by filtration.

27.2.2 Total Dissolved Solids (TDS)

Water contains dissolved solids and dissolved gases. Groundwater often contains high hydrogen sulphide (H_2S) (which has a rotten egg smell) and carbon dioxide (CO_2) (odourless) concentrations. Water residing in or on the land surface also contains dissolved solids. Total dissolved solids (TDS) can be measured using a conductivity meter. Common cations include aluminium, calcium, sodium, potassium, iron and manganese. Common anions include bicarbonate, chloride, sulphate and nitrate.

Soluble salts of calcium and magnesium form insoluble precipitates with soap, making it difficult to obtain a lather. Hence, TDS associated with calcium and magnesium is referred to as hardness, with measurements reported as equivalent $\text{mg CaCO}_3 \text{ l}^{-1}$. Consumption of soft water (i.e., water with low hardness) is thought to contribute to heart disease. However, there is no hardness guidance within the Drinking Water Directive (EU) 2020/2184.

A comparison of TDS and hardness for different water resources is shown in Table 27.2. Upland water has very low TDS and hardness because that water has spent less time interfacing with rocks and soils on the land surface. Groundwater is high in TDS and hardness because of high levels of contact with water soluble rock minerals. Seawater represents a sink for all terrestrial water and TDS is enriched by evaporation, leading to much higher levels of TDS and hardness.

Limits set on TDS are more to do with taste and excessive scaling in water pipes, heaters and boilers as opposed to health impacts [2]. However, TDS also includes dissolved NaCl , which is generally referred to as salinity. Consumption of water with $>1500 \text{ mg NaCl l}^{-1}$ often leads to vomiting. Furthermore, high salt intake can lead to hypertension. Hence use of saline groundwater or seawater for potable water supply requires desalination.

Table 27.2 Comparison of typical total dissolved solids (TDS) and hardness for different water resources. Data is from [4, p. 6] excluding that for seawater

Source	TDS (mg l^{-1})	Hardness ($\text{mg CaCO}_3 \text{ l}^{-1}$)
Soft upland water	70–150	30–100
Lowland river	200–400	100–250
Groundwater	500	400
Seawater	35,000	6300

27.2.3 Other Toxic Substances

Drinking Water Directive (EU) 2020/2184 also contains safe limits for numerous toxic substance, some of which have been presented in Table 27.1 and include:

Trihalomethanes Chlorine is commonly added to drinking water as a disinfectant. Trihalomethanes (THM) form as a result of chlorination of organic matter. THMs are thought to be carcinogenic and are therefore undesirable in drinking water [2]. THM production can be reduced by removing organic matter prior to disinfection using various combinations of coagulation, flocculation, adsorption, sedimentation and filtration.

Arsenic Elevated arsenic concentrations are often found in groundwater where there are sulphide mineral deposits. Signs of chronic arsenicism include dermal lesions, peripheral neuropathy, skin cancer, bladder and lung cancers and peripheral vascular disease [2]. Arsenic can be removed from water by coagulation and precipitation or adsorption.

Benzene Benzene contamination is mostly derived from hydrocarbon related activities (gasification, oil refinery, fuel storage, etc.). Acute exposure of benzene primarily affects the central nervous system [2]. It is also known to cause cancer in rats. It can be removed from water by adsorption or air-stripping.

Boron Boron compounds are used in the manufacture of glass, soaps, detergents and flame retardants [2]. Consequently, wastewater is often high in boron concentration. High boron concentrations are also found in the sea. High concentrations of boron can lead to leaf damage in plants [5]. This can become a particular problem where drinking water is provided by seawater desalination and wastewater is reused for irrigation. Boron can be removed by ion exchange.

Mercury Mercury is used in the electrolytic production of chlorine, in electrical appliances, dental amalgams and in artisanal gold mining. The toxic effects of inorganic mercury generally manifest themselves in the kidneys [2]. Mercury can be removed through a combination of coagulation, sedimentation, filtration, adsorption and ion exchange.

Nitrate High nitrate concentrations often arise due to exposure of source water to agricultural runoff and/or municipal wastewater effluent. Nitrate in drinking water can lead to methaemoglobinaemia in infants. This is where nitrite reacts with haemoglobin in red blood cells to form methaemoglobin, which binds oxygen tightly and does not release it, thus blocking oxygen transport [2]. There are tentative links with a range of other health conditions as well (see [2, pp. 398–403] for more detail). Nitrates can be removed from water using ion exchange, reverse osmosis, biological denitrification and/or electrodialysis.

Table 27.3 Comparison of a typical municipal wastewater [6, p. 445], limits specified by the EU Urban Wastewater Treatment Directive 91/271/EEC [7] and a typical lake or stream [8, p. 241]

Parameter	Wastewater	91/271/EEC	Lake or stream
BOD ₅ (mg l ⁻¹)	200	25	2–10
COD (mg l ⁻¹)	400–600	125	5–50
SS (mg l ⁻¹)	240	35–60	2–20
Total P (mg l ⁻¹)	10	1–2	Unspecified
Total N (mg l ⁻¹)	35	10–15	<1

27.3 Wastewater

Wastewater, is water produced as a by-product of anthropogenic activity. In the UK, commercial facilities that produce wastewater, containing potentially harmful substances, are required to treat their effluent such that it satisfies the conditions of an Environment Agency regulated trade effluent permit (TEP). Where a TEP is not required (e.g., from homes, shops and offices), wastewater should be collected by sewer systems and transported to wastewater treatment plants. Such water is often referred to as municipal wastewater. Discharges from wastewater treatment plants in the UK need to comply with the Urban Wastewater Treatment Directive 91/271/EEC. Table 27.3 compares parameter values specified in 91/271/EEC with those expected from a typical municipal wastewater and a typical lake or stream.

27.3.1 Dissolved Oxygen (DO)

The main motivation behind the Wastewater Treatment Directive 91/271/EEC is to maintain ambient dissolved oxygen (DO) levels in natural watercourses. High DO levels are required to sustain healthy aqueous ecosystems. Different organisms require varying levels of DO to thrive (see Table 27.4). Low DO levels lead to reduced fish populations, reduced biodiversity and anaerobic environments. Fish are an important food source and also provide a natural pest control function through their feeding on molluscs and insect larvae. Anaerobic environments are undesirable because they lead to the generation of H₂S, which is a harmful gas and smells unpleasant.

27.3.2 Biochemical Oxygen Demand (BOD)

BOD stands for biochemical oxygen demand. BOD₅ represents the quantity of biodegradable matter present in the water in terms of the amount of DO that would be consumed within a 5 day period due to its presence. The standard method for measuring BOD₅ is as follows:

Table 27.4 Examples of different minimum tolerable DO concentrations for different aquatic organisms (Martin Smith, Durham University, 2016, pers. comm.)

Organism	DO (mg l ⁻¹)
Rainbow trout	8.2
Carp	4.2
Larvae of chironomid midges	3.2
Rhabditis (nasty parasitic worm)	3.1
Frogs/toads	1.6
Pike	0.8
Snails and shrimp/krill	0.6
Fiddler crab	0.2
Anaerobic microorganisms	0.0

1. Place a diluted sample of water into a closed vessel.
2. Measure the initial DO concentration of the sample.
3. Leave for five days in darkness at 20 °C.
4. Measure the final DO concentration of the sample.
5. The BOD₅ of the diluted sample is the difference between the two DO measurements.
6. The BOD₅ of the original undiluted sample is obtained by volumetric scaling.

Sometimes people also measure BOD₂₀, which is the same as BOD₅ except that the sample has been incubated for twenty as opposed to five days.

BOD is removed from wastewater using biological treatments that accelerate microbial consumption of biodegradable matter.

27.3.3 Chemical Oxygen Demand (COD)

COD stands for chemical oxygen demand. COD represents the amount of oxygen required to oxidise any organic matter in a water sample using chromic acid, a strong oxidising agent [8].

27.3.4 Suspended Solids (SS)

SS stands for suspended solids. SS represent all undissolved material present in a water. SS in municipal waste are largely made up of organic matter. SS can be indirectly monitored by measuring the turbidity of the water (i.e., how cloudy the water is). Turbidity is caused by the presence of SS and is a measure of the amount of scattering that occurs when light passes through water. Turbidity is measured in

nephelometric turbidity units (NTU). SS is removed from wastewater by screening and clarification.

27.3.5 Total P and N

Phosphorous (P) and nitrogen (N) concentrations are important because these are limiting nutrients required for plant growth. Excessive levels of phosphorous and nitrogen in natural water systems leads to a process known as eutrophication. Excessive nutrient levels lead to excessive algal growth. Algal blooms prevent sunlight reaching other plants and often produce poisonous toxins. Furthermore, the dead plant matter provides additional BOD, which is consumed by benthic organisms, leading to DO depletion and anaerobic environments.

Phosphorus is generally removed from wastewater by chemical precipitation. Nitrogen is removed using a combination of nitrification and denitrification.

27.4 Modelling BOD and DO

In this section we develop some simple mathematical models for simulating BOD and DO transport in rivers. A linear biodegradable matter consumption rate equation is introduced and used to derive an expression relating BOD_5 with ultimate BOD. A mixing equation is derived to determine pollutant concentrations immediately downstream of a pollutant discharger. A two-film model is invoked to describe preparation of river water due to atmospheric interactions. The DO consumption and reaeration models are combined to derive an equation describing how DO reduces and then recovers downstream of a pollutant discharger. Finally some empirical equations are presented for estimating DO solubility limit and reaeration rate coefficient.

27.4.1 BOD Decay

27.4.1.1 Decay of Biodegradable Matter

Consider a sealed and darkened water sample initially containing a mass concentration of biodegradable matter, C_0 [ML^{-3}]. The water sample contains a sufficiently high DO concentration such that, with time, the biodegradable matter is completely consumed by aerobic microorganisms.

Let C [ML^{-3}] be the mass concentration of biodegradable matter at a given time, t [T]. Providing there is sufficient DO, the rate at which aerobic microorganisms consume the biodegradable matter, r_c [$ML^{-3}T^{-1}$], can be described by the following linear equation

$$r_c = k_c C \quad (27.1)$$

where k_c [T^{-1}] is referred to as the aerobic consumption rate coefficient.

Challenge 27.1 Formulate and solve a differential equation describing how the mass concentration of biodegradable matter declines with time.

Given that the water sample is completely sealed, mass conservation dictates that

$$\frac{dC}{dt} = -r_c \quad (27.2)$$

Substituting Eq. (27.1) into Eq. (27.2) leads to

$$\frac{dC}{dt} = -k_c C \quad (27.3)$$

Separating variables and integrating both sides of Eq. (27.3) with respect to t gives us

$$\ln C = -k_c t + A_1 \quad (27.4)$$

where A_1 is an integration constant.

Noting that $C = C_0$ when $t = 0$, it follows that $A_1 = \ln C_0$, which, on substitution into Eq. (27.4), leads to

$$C = C_0 e^{-k_c t} \quad (27.5)$$

27.4.1.2 Decay of DO

Let U [ML^{-3}] be the DO concentration, within the aforementioned water sample, at time t . Suppose that the initial DO concentration is U_0 [ML^{-3}] and that rate of DO consumption is linearly proportional to the rate of biodegradable matter consumption, i.e.,

$$\frac{dU}{dt} = \alpha \frac{dC}{dt} \quad (27.6)$$

where α [-] is a stoichiometric constant.

Challenge 27.2 Use Eqs. (27.5) and (27.6) to derive an equation describing how DO concentration declines with time.

Differentiating Eq. (27.5) with respect to t and substituting the result into Eq. (27.6) leads to

$$\frac{dU}{dt} = -\alpha k_c C_0 e^{-k_c t} \quad (27.7)$$

Integrating both sides of Eq. (27.7) with respect to t give us

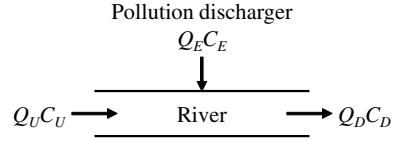
$$U = \alpha C_0 e^{-k_c t} + A_2 \quad (27.8)$$

where A_2 is another integration constant.

Noting that $U = U_0$ when $t = 0$, it follows that $A_2 = U_0 - \alpha C_0$, which, on substitution into Eq. (27.8), leads to

$$U = U_0 - \alpha C_0 (1 - e^{-k_c t}) \quad (27.9)$$

Fig. 27.1 Schematic diagram of a pollution discharger and river system



27.4.1.3 Ultimate BOD

Recall (from Sect. 27.3.2) that a measurement of BOD_5 represents the amount of DO that would be consumed within a 5 day period. Let $B(t)$ [ML^{-3}] be the amount of DO that would be consumed after a time-period, t . It follows from Eq. (27.9) that

$$B(t) \equiv U_0 - U = \alpha C_0 (1 - e^{-k_c t}) \quad (27.10)$$

The ultimate BOD of the sample, L_0 [ML^{-3}], is found from

$$L_0 \equiv \lim_{t \rightarrow \infty} B(t) = \alpha C_0 \quad (27.11)$$

Substituting Eq. (27.11) back into Eq. (27.10) leads to

$$B(t) = L_0 \cdot (1 - e^{-k_c t}) \quad (27.12)$$

which means the ultimate BOD, L_0 , can be determined from a BOD_5 measurement (i.e., $B(t = 5 \text{ days})$) using the expression

$$L_0 = \frac{B(t)}{1 - e^{-k_c t}} \quad (27.13)$$

27.4.2 Mass Balance for a River and Discharger

Consider the situation where a facility is discharging a trade effluent into a nearby river at a volumetric rate of Q_E [$L^3 T^{-1}$] (see Fig. 27.1). The effluent contains a solute at a concentration of C_E [ML^{-3}].

Immediately upstream of the effluent outlet (hereafter referred to as the discharger), the river is flowing at a volumetric rate of Q_U [$L^3 T^{-1}$]. The relevant solute concentration of the river water upstream of the outlet is denoted C_U [ML^{-3}]. Of interest is the resulting solute concentration of the river water immediately downstream of the discharger, C_D [ML^{-3}].

Challenge 27.3 Determine an expression for C_D in terms of C_U , C_E , Q_U and Q_E .

The downstream solute concentration can be determined as follows. Consider an infinitesimal control-volume that encloses the segment of river where the discharger is located. The mass of the solute entering the control volume, M_{in} [M], during an infinitesimal time interval, δt [T], is found from

$$M_{\text{in}} = (Q_U C_U + Q_E C_E) \delta t$$

The mass of the solute exiting the control volume during the same period, M_{out} [M], is found from

$$M_{\text{out}} = Q_D C_D \delta t$$

where Q_D [$\text{L}^3 \text{T}^{-1}$] is the volumetric flow rate immediately downstream of the river.

Assuming steady-state conditions, $M_{\text{in}} = M_{\text{out}}$, such that

$$(Q_U C_U + Q_E C_E) \delta t = Q_D C_D \delta t$$

Furthermore, it can be understood that $Q_D = Q_U + Q_E$ from which it follows that

$$(Q_U C_U + Q_E C_E) \delta t = (Q_U + Q_E) C_D \delta t$$

which can be rearranged to get

$$C_D = \frac{Q_U C_U + Q_E C_E}{Q_U + Q_E} \quad (27.14)$$

27.4.3 DO Consumption in Rivers

Water flows at a steady volumetric flow rate, Q [$\text{L}^3 \text{T}^{-1}$], along a river channel of cross-sectional area, A [L^2]. Let C [ML^{-3}] and U [ML^{-3}] be the mass concentrations of biodegradable matter and DO in the river water, respectively. A polluted effluent discharges into the river such that immediately downstream of the discharger, the mass concentration of biodegradable matter and DO are C_0 [ML^{-3}] and U_0 [ML^{-3}], respectively.

As the polluted water travels away from the discharger, the biodegradable matter decays due to aerobic microbial consumption at a rate, r_c [$\text{ML}^{-3} \text{T}^{-1}$], as defined in Eq. (27.1) (see Fig. 27.2a). DO is simultaneously consumed with the biodegradable matter at a rate, αr_c , where α [-] is the stoichiometric ratio parameter. However, DO is also replenished by gas absorption at the water surface at a rate, r_a [$\text{ML}^{-3} \text{T}^{-1}$], referred to hereafter as the reaeration rate (see Fig. 27.2b).

The reaeration rate is described by the two film model, previously discussed in Sect. 25.4.1 (see Fig. 27.3). The relevant equation takes the form

$$r_a = k_a \cdot (U_s - U) \quad (27.15)$$

where k_a [T^{-1}] is the reaeration rate coefficient and U_s [ML^{-3}] corresponds to the solubility limit of DO.

Considering the two control volume diagrams shown in Fig. 27.4, mass conservation dictates that:

$$QC = Q(C + \delta C) + A \delta x r_c$$

$$QU + A \delta x r_a = Q(U + \delta U) + A \delta x \alpha r_c$$

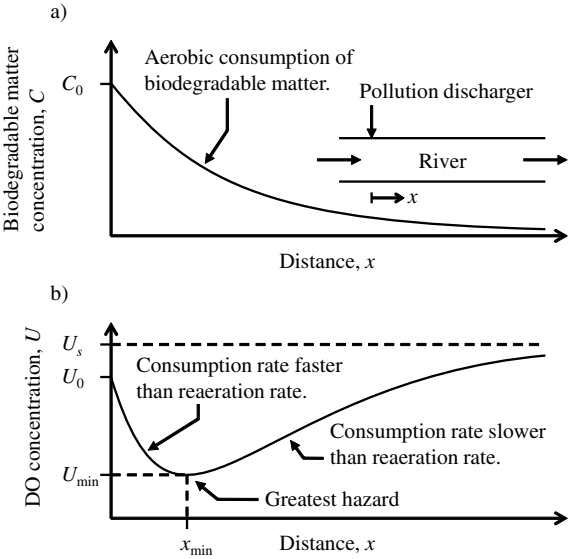


Fig. 27.2 Schematic diagrams showing how biodegradable matter and DO evolve downstream of a pollution discharger

Fig. 27.3 Schematic diagram illustrating how reaeration of rivers can be treated as a two film system

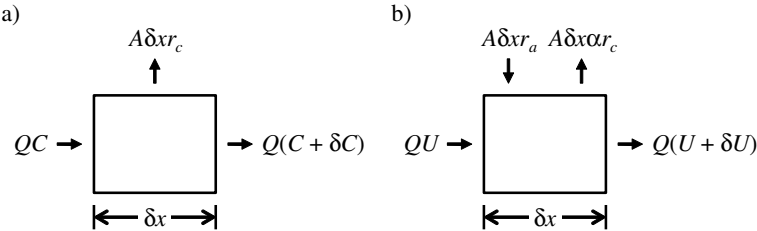
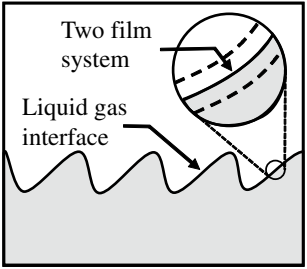


Fig. 27.4 **a** Control volume for the decay of biodegradable matter as it travels down a river. **b** Control volume for the decay and replenishment of DO concentration as it travels down a river

It follows that

$$Q \frac{dC}{dx} = -Ar_c \quad (27.16)$$

$$Q \frac{dU}{dx} = A \cdot (r_a - \alpha r_c) \quad (27.17)$$

The relevant boundary conditions are

$$\begin{aligned} C &= C_0, \quad x = 0 \\ U &= U_0, \quad x = 0 \end{aligned} \quad (27.18)$$

The above set of equations can be solved to derive expressions for the spatial distribution of DO, downstream of the discharger.

27.4.3.1 General Solution

Challenge 27.4 Derive general solutions for C and U .

Substituting Eqs. (27.1) and (27.15) into Eqs. (27.16) and (27.17) leads to

$$Q \frac{dC}{dx} = -Ak_c C \quad (27.19)$$

and

$$Q \frac{dU}{dx} = Ak_a \cdot (U_s - U) - A\alpha k_c C \quad (27.20)$$

respectively.

Equation (27.20) can be rearranged and differentiated to get

$$C = \frac{1}{A\alpha k_c} \left[Ak_a \cdot (U_s - U) - Q \frac{dU}{dx} \right] \quad (27.21)$$

and

$$\frac{dC}{dx} = -\frac{1}{A\alpha k_c} \left[Ak_a \frac{dU}{dx} + Q \frac{d^2 U}{dx^2} \right] \quad (27.22)$$

respectively.

Substituting Eqs. (27.21) and (27.22) into Eq. (27.19) leads to

$$\frac{Q^2}{A^2} \frac{d^2 U}{dx^2} + \frac{Q}{A} (k_a + k_c) \frac{dU}{dx} + k_a k_c \cdot (U - U_s) = 0 \quad (27.23)$$

The general solution of an ordinary differential equation of the form

$$a \frac{d^2 y}{dx^2} + b \frac{dy}{dx} + cy = 0 \quad (27.24)$$

is [9, p. 1093]

$$y(x) = A_3 \exp \left[\left(\frac{-b + \sqrt{b^2 - 4ac}}{2a} \right) x \right] + A_4 \exp \left[\left(\frac{-b - \sqrt{b^2 - 4ac}}{2a} \right) x \right] \quad (27.25)$$

where A_3 and A_4 are unknown constants defined by any associated boundary conditions.

Let us make the substitution, $G = U_s - U$, such that Eq. (27.23) reduces to

$$\frac{Q^2}{A^2} \frac{d^2 G}{dx^2} + \frac{Q}{A} (k_a + k_c) \frac{dG}{dx} + k_a k_c G = 0 \quad (27.26)$$

Comparing Eqs. (27.24) and (27.26) it can be seen that, $a = \frac{Q^2}{A^2}$, $b = \frac{Q}{A} (k_a + k_c)$ and $c = k_a k_c$. The general solution for Eq. (27.24) is therefore

$$G = U_s - U = A_3 \exp \left(-\frac{Ak_c x}{Q} \right) + A_4 \exp \left(-\frac{Ak_a x}{Q} \right) \quad (27.27)$$

Differentiating Eq. (27.27) with respect to x gives us

$$\frac{dU}{dx} = \frac{Ak_c A_3}{Q} \exp \left(-\frac{Ak_c x}{Q} \right) + \frac{Ak_a A_4}{Q} \exp \left(-\frac{Ak_a x}{Q} \right) \quad (27.28)$$

Substituting Eqs. (27.27) and (27.28) into Eq. (27.21) leads to

$$C = \frac{(k_a - k_c) A_3}{\alpha k_c} \exp \left(-\frac{Ak_c x}{Q} \right) \quad (27.29)$$

27.4.3.2 Application of Boundary Conditions

Challenge 27.5 Apply the boundary conditions in Eq. (27.18) to obtain expressions for the two integration constants, A_3 and A_4 .

From Eq. (27.18) we have that $C = C_0$ at $x = 0$. It follows, from Eq. (27.29), that

$$A_3 = \frac{\alpha k_c C_0}{(k_a - k_c)} \quad (27.30)$$

Substituting Eq. (27.30) into Eqs. (27.27) and (27.29) leads to

$$U_s - U = \frac{\alpha k_c C_0}{(k_a - k_c)} \exp \left(-\frac{Ak_c x}{Q} \right) + A_4 \exp \left(-\frac{Ak_a x}{Q} \right) \quad (27.31)$$

and

$$C = C_0 \exp \left(-\frac{Ak_c x}{Q} \right) \quad (27.32)$$

respectively.

Equation (27.18) also gives that $U = U_0$ at $x = 0$. It therefore follows, from Eq. (27.31), that

$$A_4 = U_s - U_0 - \frac{\alpha k_c C_0}{k_a - k_c} \quad (27.33)$$

Substituting Eq. (27.33) into Eq. (27.31) leads to

$$U_s - U = \frac{\alpha k_c C_0}{k_a - k_c} \left(e^{-\frac{Ak_c x}{Q}} - e^{-\frac{Ak_a x}{Q}} \right) + (U_s - U_0) e^{-\frac{Ak_a x}{Q}} \quad (27.34)$$

27.4.3.3 Streeter-Phelps Equation

Often Eqs. (27.32) and (27.34) are written in terms of ultimate BOD, $L = \alpha C$, and DO deficit, $G = U_s - U$, such that:

$$L = L_0 e^{-\frac{Ak_c x}{Q}} \quad (27.35)$$

$$G = \frac{k_c L_0}{k_a - k_c} \left(e^{-\frac{Ak_c x}{Q}} - e^{-\frac{Ak_a x}{Q}} \right) + G_0 e^{-\frac{Ak_a x}{Q}} \quad (27.36)$$

where L_0 [ML^{-3}] and G_0 [ML^{-3}] are the ultimate BOD and DO deficit immediately downstream of the pollution discharger. Equation (27.36) is attributed to [10] and widely referred to as the Streeter-Phelps equation.

27.4.3.4 Minimum DO Concentration

Challenge 27.6 Determine the location of the minimum DO concentration.

Differentiating Eq. (27.36) with respect to x leads to

$$\frac{dG}{dx} = -\frac{Ak_c L_0}{Q \cdot (k_a - k_c)} \left(k_c e^{-\frac{Ak_c x}{Q}} - k_a e^{-\frac{Ak_a x}{Q}} \right) - \frac{Ak_a G_0}{Q} e^{-\frac{Ak_a x}{Q}}$$

The location of the minimum DO concentration, $x_{\min}$, is found by setting $\frac{dG}{dx} = 0$ at $x = x_{\min}$ and solving for $x_{\min}$ yielding

$$x_{\min} = \frac{Q}{A \cdot (k_a - k_c)} \ln \left[\frac{k_a}{k_c} \left(1 - \frac{G_0}{L_0} \left(\frac{k_a - k_c}{k_c} \right) \right) \right] \quad (27.37)$$

A value for the maximum DO deficit, $G_{\max}$, is obtained by setting $x = x_{\min}$ in Eq. (27.36). The associated minimum DO concentration, $U_{\min} = U_s - G_{\max}$.

Table 27.5 Empirical parameters for the DO solubility limit equation, Eq. (27.38) due to [11]

i	a_i
0	-1.393441×10^2
1	1.575701×10^5
2	-6.642308×10^7
3	1.243800×10^{10}
4	-8.621949×10^{11}

Table 27.6 Empirical parameters for determining reaeration rates, k_a , in days^{-1} , using Eq. (27.39), as specified by [12, p. 56]. Mean velocity of river flow, u , is in m s^{-1} . Mean water depth in river channel, H , is in m

Source	a	b	c	Condition
[14]	5.32	0.67	1.85	$H < 0.61$
[15]	3.93	0.5	1.5	$H \geq 0.61$ & $H > 3.45u^{2.5}$
[16]	5.026	0.969	1.673	$H \geq 0.61$ & $H \leq 3.45u^{2.5}$

27.4.3.5 Auxiliary Equations

The solubility limit for dissolved oxygen in freshwater, U_s , can be obtained, in mg l^{-1} , from the following empirical equation due to [11]

$$\ln U_s = \sum_{i=0}^4 \frac{a_i}{T^i} \quad (27.38)$$

where T [°] is temperature in Kelvin and a_i are empirical parameters listed in Table 27.5.

The reaeration rate coefficient, k_a , is often determined from the following empirical equation [12]

$$k_a = \frac{au^b}{H^c} \quad (27.39)$$

where u [LT^{-1}] is the mean velocity of the river flow and H [L] is the mean water depth in the channel.

In the absence of additional information, [12] suggests the use of a method specified by [13] to obtain appropriate values for the empirical parameters a , b and c , which is presented in Table 27.6.

27.5 Problem Sheet

Problem 27.1 (see Worked Solution 27.1)

It is planned to construct a new toasted sandwich maker factory in the nearby industrial estate of Belmont. The planned industrial process involves a trade effluent with elevated mercury concentrations. Following an environmental impact assessment, it was decided that the factory should include a private wastewater treatment plant for trade effluent to be discharged to the River Wear. The anticipated trade effluent discharge rate from the factory is $0.12 \text{ m}^3 \text{ s}^{-1}$. The mean flow rate of the River Wear at Sunderland Bridge is $5.90 \text{ m}^3 \text{ s}^{-1}$. The mercury concentration in the river water immediately upstream of the proposed factory is found to be $0.1 \mu\text{g l}^{-1}$ (this is made up by the way). Determine a suitable limit for mercury concentration in the proposed trade effluent from the factory. Hint: design the system such that the downstream mercury concentration is no more than 50% of the associated drinking water standard limit.

Problem 27.2 (see Worked Solution 27.2)

As part of a routine monitoring exercise, a sample of wastewater was collected from the Durham Colleges Sewage Treatment Works on Hollingside Lane. Technicians placed 10 ml of the sample into a 200-ml BOD bottle. They then filled the bottle (such that there is now 200 ml of liquid) with dilution water (containing zero BOD). The initial DO of the mixture was 8.5 mg l^{-1} . After incubating the mixture at 20°C in the dark for 5 days, the technicians measured the DO to be 6.15 mg l^{-1} . After incubating another identical mixture under the same conditions for 20 days, technicians measured the DO to be 3.77 mg l^{-1} .

- (a) Calculate the BOD_5 of the sample prior to dilution.
- (b) Calculate the BOD_{20} of the sample prior to dilution.
- (c) Determine the ultimate BOD of the sample prior to dilution along with the aerobic consumption rate coefficient for the biodegradable matter in the water.

Problem 27.3 (see Worked Solution 27.3)

Trade effluent from the Bearpark dairy is discharged into the River Browney at a rate of $0.15 \text{ m}^3 \text{ s}^{-1}$. The effluent has a BOD_5 of 90 mg l^{-1} and a DO concentration of 2.3 mg l^{-1} . The river flow immediately upstream of the discharger is $0.9 \text{ m}^3 \text{ s}^{-1}$.

The river water immediately upstream of the discharger has a BOD_5 of 2 mg l^{-1} and a DO concentration of 8 mg l^{-1} . The biodegradable matter aerobic consumption rate coefficient associated with the River Browney is 0.4 day^{-1} . The mean width of the river channel is 10 m. The mean water depth in the river channel is 1 m. The temperature of the river water is 10°C .

- (a) Determine the ultimate BOD and DO concentration of the water immediately downstream of the discharger.
- (b) Determine the DO solubility limit.
- (c) Determine the reaeration rate coefficient.
- (d) Determine the DO levels at 0.5 and 15 km away from the discharger.
- (e) Determine the minimum DO level expected in the river as a consequence of the discharger.

27.6 Worked Solutions

Worked Solution 27.1 (see Problem 27.1)

According to Table 27.1, the (EU) 2020/2184 drinking water limit for mercury is $1 \text{ }\mu\text{g l}^{-1}$. A suitable limit we should apply to the trade effluent can be obtained by determining C_E from Eq. (27.14) where C_D is set to 50% of the drinking water standard (i.e., $0.5 \text{ }\mu\text{g l}^{-1}$). From the information given, $Q_U = 5.90 \text{ m}^3 \text{ s}^{-1}$, $Q_E = 0.12 \text{ m}^3 \text{ s}^{-1}$ and $C_U = 0.1 \text{ }\mu\text{g l}^{-1}$. It follows that

$$C_E = \frac{(Q_U + Q_E)C_D - Q_U C_U}{Q_E} = \frac{(5.90 + 0.12)0.5 - 5.90 \times 0.1}{0.12} = 20.17$$

therefore, Mercury concentrations in the trade effluent should be less than $20.17 \text{ }\mu\text{g l}^{-1}$.

Worked Solution 27.2 (see Problem 27.2)

(a) For the diluted sample $BOD_5 = 8.5 - 6.15 = 2.35 \text{ mg/L}$.
For the undiluted sample $BOD_5 = 2.35 \times 200/10 = 47 \text{ mg/L}$.

(b) For the diluted sample $BOD_{20} = 8.5 - 3.77 = 4.73 \text{ mg/L}$.
For the undiluted sample $BOD_{20} = 4.73 \times 200/10 = 94.6 \text{ mg/L}$.

(c) The ultimate BOD, L_0 , and the aerobic consumption rate coefficient, k_c , can be found using Eq. (27.13). From the BOD₅ measurement, $B(5)$, we can say

$$L_0 = \frac{B(5)}{1 - e^{-5k_c}}$$

From the BOD₂₀ measurement, $B(20)$, we can say

$$L_0 = \frac{B(20)}{1 - e^{-20k_c}}$$

It follows that

$$\frac{B(5)}{B(20)} - \frac{1 - e^{-5k_c}}{1 - e^{-20k_c}} = 0$$

which can be iteratively solved using MATLAB's function, `fzero`.

The following MATLAB code can be used obtain both the aerobic consumption rate coefficient and the ultimate BOD:

```
B5 = 47; %Define BOD5 (mg/l)
B20 = 94.6; %Define BOD20 (mg/l)
kcGUESS = 5; %Guess consumption rate (day-1)
%Now use fzero to obtain actual value of kc
FUN = @(kc) B5/B20 - (1-exp(-5*kc)) / (1-exp(-20*kc));
kc = fzero(FUN, kcGUESS);
%Determine ultimate BOD (mg/l)
L0 = B5 / (1-exp(-5*kc));
```

which gives that $k_c = 0.120 \text{ day}^{-1}$ and $L_0 = 104 \text{ mg l}^{-1}$.

Worked Solution 27.3 (see Problem 27.3)

(a) The first step is to calculate the ultimate BOD of the sample, L_E , and the upstream river water, L_U . From Eq. (27.13)

$$L_E = \frac{90}{1 - \exp(-0.4 \times 5)} = 104.1 \text{ mg l}^{-1}$$

$$L_U = \frac{2}{1 - \exp(-0.4 \times 5)} = 2.313 \text{ mg l}^{-1}$$

and considering Eq. (27.14), the BOD immediately downstream of the discharger is found from

$$L_D = \frac{0.9 \times 2.313 + 0.15 \times 104.1}{0.9 + 0.15} = 16.85 \text{ mg l}^{-1}$$

The DO immediately downstream of the discharger is

$$U_D = \frac{0.9 \times 8 + 0.15 \times 2.3}{0.9 + 0.15} = 7.186 \text{ mg/L}$$

(b) The DO solubility limit, U_s , can be determined using Eq. (27.38) using the following MATLAB code:

```
T = 10 + 273.2; %Define temperature in Kelvin
%Define empirical coefficients
a = [-1.393441e2 1.575701e5 ...
     -6.642308e7 1.243800e10 -8.621949e11];
%Determine the DO solubility limit, Us
Us = exp(sum(a./T.^[0:4]));
```

which gives that $U_s = 11.27 \text{ mg l}^{-1}$.

(c) The reaeration rate coefficient, k_a , can be determined from Eq. (27.39) in conjunction with Table 27.6. The water velocity, $u = \frac{0.15+0.9}{10 \times 1} = 0.105 \text{ m s}^{-1}$ and so $3.45u^{2.5} = 0.0123$. Given that the water depth, $H = 1 \text{ m}$, Eq. (27.39) in conjunction with Table 27.6 lead to the following equation

$$k_a = \frac{3.93u^{0.5}}{H^{1.5}}$$

where k_a is the reaeration rate coefficient in day^{-1} and u is the water velocity in m s^{-1} . Therefore $k_a = 1.274 \text{ day}^{-1}$.

(d) The DO deficit, G , can be determined from Eq. (27.36). Let $k_c = 0.4 \text{ day}^{-1}$, $k_a = 1.274 \text{ day}^{-1}$, $L_0 = 16.85 \text{ mg l}^{-1}$, $G_0 = 11.27 - 7.186 = 4.089 \text{ mg l}^{-1}$, $\frac{Q}{A} = \frac{(0.15+0.9) \times 24 \times 60^2}{10 \times 1 \times 1000} = 9.072 \text{ km day}^{-1}$. It follows that at $x = 0.5 \text{ km}$ and 15 km , $G = 4.167 \text{ mg l}^{-1}$ and 3.541 mg l^{-1} , respectively. It follows that the DO concentration at 0.5 km and 15 km would be 7.108 mg l^{-1} and 7.733 mg l^{-1} , respectively.

(e) From Eq. (27.37), the location of the minimum DO concentration is 4.189 km . From Eq. (27.36), the maximum DO deficit is 4.401 mg l^{-1} . It follows that the minimum DO concentration is 6.874 mg l^{-1} .

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Abstract

This chapter focuses on water treatment technologies. A range of relevant processes are explained including screening, dissolved air floatation, clarification, coagulation, flocculation, filtration, adsorption, disinfection, aeration, desalination, ion exchange and remineralisation. Mathematical models are developed for rapid sand filters concerning head loss estimation, filtration efficiency estimation and the specification of backwash rates for filter cleaning. Mathematical models are developed for reverse osmosis desalination systems concerning concentration polarisation, osmotic pressure calculation and feed rate estimation. Practical applications are presented through a problem sheet with worked solutions.

Notation

A	Cross-sectional area of filter or membrane [L^2].
A_c	Cross-sectional area of channel [L^2].
b	Diffusion film thickness [L].
c_p	Specific heat capacity [$L^2T^{-2}\Theta^{-1}$].
c_0	Laminar flow shape factor [-].
C	Mass concentration [ML^{-3}].
C_f	Feed rate salt concentration [ML^{-3}].
C_p	Permeate rate salt concentration [ML^{-3}].
C_r	Retentate rate salt concentration [ML^{-3}].
C_s	Salt concentration on the feed-side of a membrane [ML^{-3}].
C_0	Boundary mass concentration [ML^{-3}].
D	Diameter of spherical particle [L].
D_0	Molecular diffusion coefficient [L^2T^{-1}].
D_p	Diameter of suspended particles [L].
E	Fraction of SS removed by the granular filter [-].
f	Darcy-Weisbach friction factor [-].

g	Gravitational acceleration [LT^{-2}].
h_L	Hydraulic head loss [L].
H	Channel thickness [L].
k	Mass transfer coefficient [LT^{-1}].
k_f	SS removal rate coefficient [T^{-1}].
L	Length [L].
L_c	Characteristic length [L].
L_E	Expanded length [L].
m	Hydraulic radius of a channel [L].
m_g	Volume to surface area ratio of solid grains [L].
N	Number of moles [-].
Nu	Nusselt number [-].
p	Pressure [$\text{ML}^{-1}\text{T}^{-2}$].
P_c	Wetted perimeter of a channel [L].
Pr	Prandtl number [-].
q	Darcy flux [LT^{-1}].
q_B	Backflow rate [LT^{-1}].
q_c	Convective mass flux [$\text{ML}^{-2}\text{T}^{-1}$].
q_h	Convective heat flux [MT^{-3}].
Q	Flow rate [L^3T^{-1}].
Q_f	Feed rate [L^3T^{-1}].
Q_p	Permeate rate [L^3T^{-1}].
Q_r	Retentate rate [L^3T^{-1}].
r_f	SS removal rate [$\text{ML}^{-3}\text{T}^{-1}$].
R	Universal ideal gas constant [$\text{ML}^2\text{T}^{-2}\Theta^{-1}$].
Re	Reynolds number [-].
s	Distance in the direction of flow [L].
Sh	Sherwood number [-].
T	Temperature [Θ].
T_r	Temperature of surrounding fluid [Θ].
T_s	Temperature of a heat source [Θ].
V_m	Volume of liquid [L^3].
W	Channel width [L].
α	Osmotic pressure coefficient [L^2T^{-2}].
ε	Void ratio [-].
ε_E	Expanded void ratio [-].
κ_h	Thermal conductivity [$\text{MLT}^{-3}\Theta^{-1}$].
κ_I	Head loss coefficient due to inertial forces [-].
κ_s	Solute mass transfer coefficient of a membrane [LT^{-1}].
κ_V	Head loss coefficient due to viscous forces [-].
κ_w	Water permeability coefficient of a membrane [$\text{M}^{-1}\text{L}^2\text{T}$].
μ	Dynamic viscosity of water [$\text{ML}^{-1}\text{T}^{-1}$].
π	Osmotic pressure [$\text{ML}^{-1}\text{T}^{-2}$].
ρ	Fluid density [ML^{-3}].
ρ_p	Mass density of the suspended particles [ML^{-3}].

τ	Tortuosity [-].
ϕ	Porosity [-].
ϕ_E	Expanded porosity [-].
AC	Activated carbon.
BOD	Biochemical Oxygen Demand.
BWRO	Brackish water reverse osmosis.
COD	Chemical oxygen demand.
DO	Dissolved oxygen.
GAC	Granular activated carbon.
MED	Multi effect distillation.
MSF	Multi-stage flash.
PAC	Powdered activated carbon.
RO	Reverse osmosis.
SS	Suspended Solids.
SWRO	Seawater reverse osmosis.
TDS	Total dissolved solids.
THM	Trihalomethane.
VOC	Volatile organic compounds.

28.1 Introduction

The purpose of water treatment is to make water suitable for drinking. A potable water is a water deemed to be safe to drink.

Water treatment should make the water palatable, which means it should be colourless, have low turbidity and be free of unpleasant tastes and odours. But in addition to that, the water should be free of pathogenic organisms and dissolved substances should not be present above concentrations perceived to be toxic to humans. The elimination of pathogenic organisms is commonly achieved by chlorination. Therefore, it is important that the water is free of both suspended and dissolved organic matter so as to avoid generation of THMs. Hence removal of suspended solids and dissolved organic matter represents a significant component of many water treatment works. Salt removal is an additional concern when utilizing seawater.

In this chapter we explore the various processes used to treat river water, groundwater and seawater. We then develop some mathematical equations to design key aspects of a rapid sand filter and a reverse osmosis desalination facility.

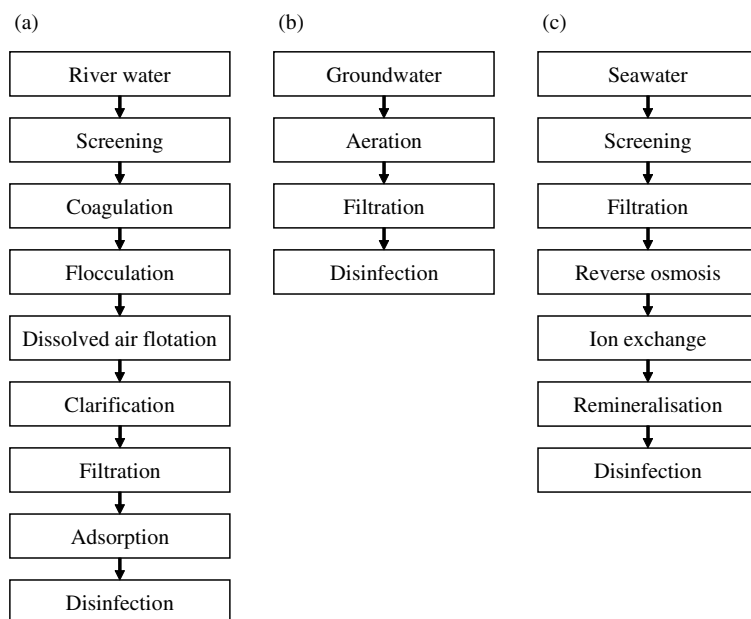


Fig. 28.1 Flow charts for different water treatment systems

28.2 Water Treatment Processes

A comparison of different treatment process required for different water resources is shown in Fig. 28.1. Treatment of river water mostly revolves around removal of suspended solids and dissolved organics (Fig. 28.1a). Less treatment is normally required for groundwater, because it has already been naturally filtered by the aquifer rocks it resides in (Fig. 28.1b). However, aeration is often required to remove unpleasant dissolved gases along with iron (Fe) and manganese (Mn). Seawater can also be used as a potable water resource but requires the special process of desalination (e.g., reverse osmosis), ion exchange (to remove boron) and remineralisation (to increase the pH, alkalinity and hardness) (Fig. 28.1c). Further details about these individual processes are described below.

28.2.1 Screening

The first step often involves screening the water to remove larger objects by passing the water through an array of sub-vertical bars, around 25 mm in diameter and spaced around 100 mm apart [1].

28.2.2 Dissolved Air Floatation

Floatation is used to remove buoyant particles in water such as fats, oils and grease [2]. Dissolved air floatation involves injecting water supersaturated with air at the base of a floatation tank [1]. Bubbles nucleate around solid particles and rise to the surface. The resulting foam at the surface is skimmed and collected.

28.2.3 Clarification

Clarification is used to remove non-buoyant suspended solids (SS) by gravitational settling. A schematic diagram of a circular clarifier is shown Fig. 28.2. The influent is injected into the centre of the tank. Water then overtops a circular decanting trough and flows towards an effluent outlet. The residence time needs to be sufficient such that SS can settle out within the sludge zone. A rotational sludge scraper routinely scrapes out the sludge for removal. Particles with settling velocities greater than the overflow-rate are unable to exit with the effluent. The overflow-rate equals the volume input rate divided by the plan area of clarifier. The larger the particle, the faster the settling rate and the smaller the plan area required.

28.2.4 Coagulation and Flocculation

Colloids are particles ranging between 10 nm and 10 μm (see Table 28.1). Colloids are typically negatively charged and hence repel each other, making them difficult to aggregate. Coagulation and flocculation are two combined processes often used to aggregate colloids to form larger particles, known as flocs, which can be more easily separated out by clarification.

Coagulation involves adding a chemical, known as a coagulant, to encourage colloids to stick together. Typical coagulants include aluminium or ferric salts such as alum ($\text{Al}_2(\text{SO}_4)_3 \cdot 14\text{H}_2\text{O}$), ferric sulfate ($\text{Fe}_2(\text{SO}_4)_3$) and ferric chloride (FeCl_3) [1]. Such materials reduce negative surface charge and hence reduce repulsion between colloids. Coagulants also form precipitates, which trap additional particles.

Flocculation involves gentle mixing of the water to increase the number of contacts between colloids and speed up the formation of flocs. Mixing needs to be gentle because over aggressive mixing leads to floc destruction [1].

28.2.5 Filtration

Additional SS and BOD can be removed by filtration through a packed sand bed. Note that sand particle size ranges between 0.4 and 1.5 mm yet sand filters are expected to remove particles of the order of a few microns. The removal process in a sand filter is therefore more complicated than mere straining [1].

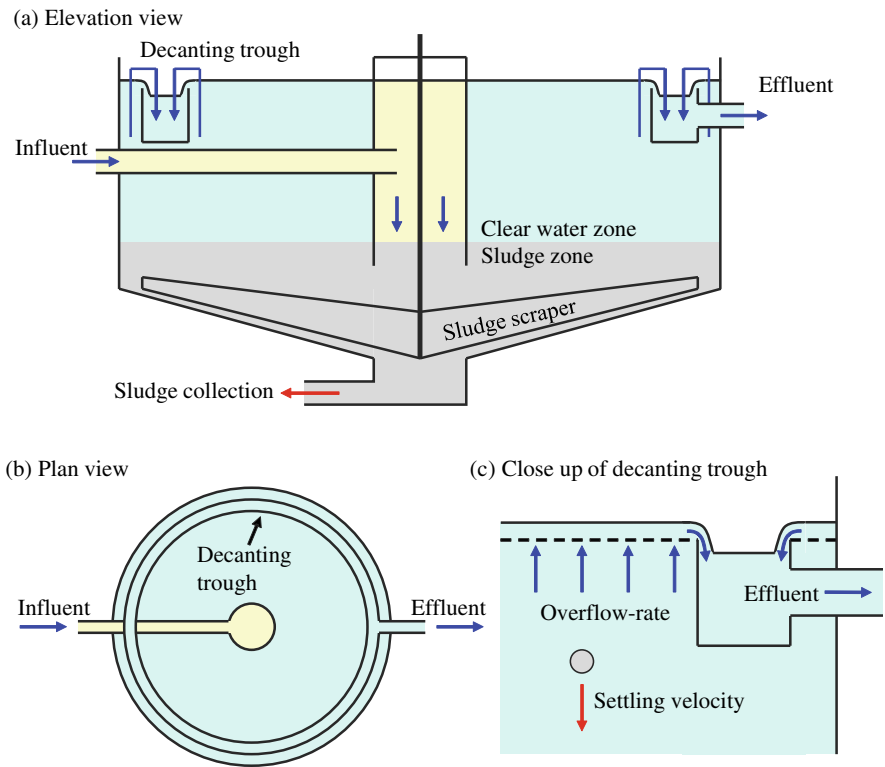


Fig. 28.2 Schematic diagrams describing a circular clarifier

Table 28.1 Size range of particles of concern in water treatment (modified from [1])

Particle type	Size range (m)
Molecules	$10^{-10} - 10^{-8}$
Colloids	$10^{-8} - 10^{-5}$
Suspended particles	$10^{-6} - 10^{-2}$
Viruses	$10^{-8} - 10^{-7}$
Bacteria	$10^{-7} - 10^{-5}$
Pathogenic protozoa	$10^{-6} - 10^{-5}$
Algae	$10^{-6} - 10^{-4}$

Slow sand filters Older sand filters are generally referred to as slow sand filters, due to their relatively slow loading rate. The loading rate, in this context is a term used to describe the volumetric inflow rate per unit cross-sectional area of filter. A typical setup, for a slow sand filter, is shown in Fig. 28.3a. A biofilm, known as the *schmutzedecke* (a German word meaning “layer of dirt”), develops on the surface of the sand within the upper 30 cm of the sand bed. The biofilm consumes both suspended and dissolved BOD as the water slowly moves through the filter.

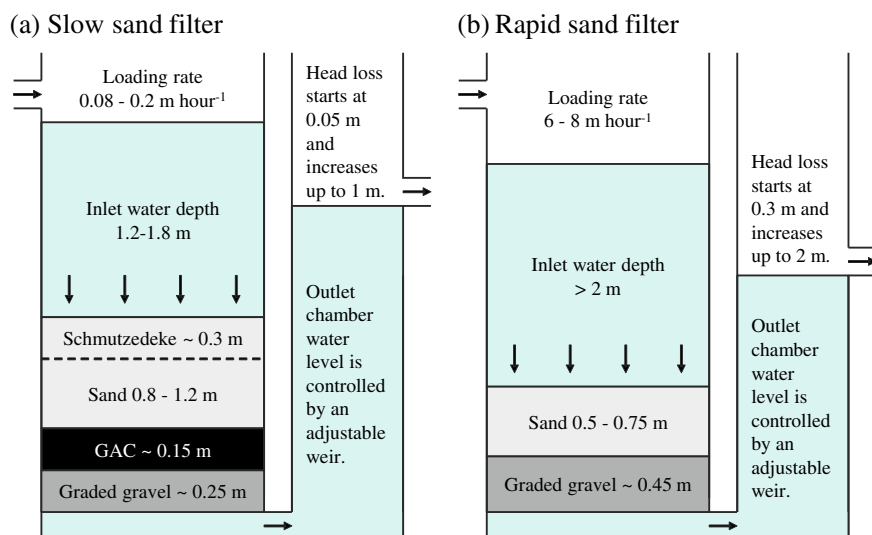


Fig. 28.3 Schematic diagrams for a slow and rapid sand filter based on data provided by [1]

Furthermore, the biofilm reduces the size of the pores within the filter such that smaller particles, including cryptosporidium oocysts, can be removed by straining and adsorption [3].

Eventually the biofilm grows to such an extent that it blocks the pores within the sand such that the head loss across the filter is too great to sustain the design load rate. When this happens, the top 20 mm of sand is scraped off. Once repeated cleaning reduces the sand bed to around 450 mm, the filter is re-sanded and the schmutzedeke has to be carefully re-established [1].

A layer of granular activated carbon (GAC) can also be included to remove organic chemicals such as pesticides [1].

Rapid sand filters A disadvantage of slow sand filters is that they require large plan areas. Rapid sand filters have a similar setup (see Fig. 28.3b) but allow faster loading rates and hence smaller plan areas. However, fast loading rates tend to prohibit the development of a schmutzedeke. Instead, coagulants are added to feed water such that smaller particles are flocculated and strained in between the sand grains. Eventually a mud cake builds up within the pore-space and the head loss becomes prohibitively large. At this point the filter must be cleansed by backwashing with a mixture of water and air, which leads to fluidisation of the bed [1].

Incorporating GAC within a rapid sand filter tends not to be effective due to the relatively short contact times. However the filtrate can be passed through a separate GAC adsorption tower following filtration, if required.

The advantages of slow sand filters as compared to rapid sand filters are that:

1. They do not require coagulants.
2. They do not require backwashing.
3. They provide reliable removal of cryptosporidium oocysts.
4. GAC can be incorporated as an additional layer.

28.2.6 Adsorption

Many dissolved contaminants can be removed by adsorption. Adsorption is a process whereby molecules, atoms or ions, in a gas or liquid, diffuse to the surface of a solid, where they bond with the solid surface or are held by weak intermolecular forces [4]. Organics and metals naturally adsorb to clay minerals in soils and sediments. Organics will also adsorb to other organics [5].

The water industry typically use a product called activated carbon (AC) as an adsorbent. AC can be used to remove toxic organics from both water and air. AC is manufactured by heating carbonaceous materials (e.g., coal, wood or coconut shells). First the heating takes place in the absence of air to drive out mobile volatile substances. It is then heated at high temperatures and reacted with steam, air and CO₂. This removes volatile matter embedded within the pores of the carbon producing a porous structure with a much higher surface area to volume ratio [1].

AC is available as a fine powder (PAC) or in granular form (GAC). PAC can be mixed into water allowing dissolved contaminants to adsorb to the AC particles. The PAC can then be removed by clarification, which leads to the removal of the dissolved contaminants of concern.

GAC requires between 15 and 20 min of contact time to remove pesticides and other organic chemicals [1]. GAC can be packed into the bed of a slow sand filter to provide a layer where adsorption takes place. Alternatively, GAC can be packed into a separate GAC adsorption tower. Once all the adsorption sites have been used up, GAC can be regenerated (or reactivated) by reheating.

28.2.7 Disinfection

Disinfection is the most important water treatment process. Primary disinfection involves inactivating pathogenic organisms present in the water. Secondary disinfection involves maintaining a disinfectant residual in a drinking water distribution system, which provides protection against subsequent pathogenic contamination.

Three commonly applied disinfectants include chlorine, ozone (O₃) and ultraviolet radiation. All three kill viruses and bacteria. Unfortunately oocysts due to protozoa are mostly resistant to these processes and so must be removed by other means (e.g., slow sand filtration). Coliform bacteria are more resistant than most other bacteria hence they are often used as an indicator organism to check that disinfectant has been sufficient to inactivate all pathogenic bacteria in general. However, viruses are

generally more resistant to disinfection than bacteria, so a coliform count of zero per 100 ml may not mean water is free of viral pathogens.

Whilst all three disinfectants can be used for primary disinfection, only chlorine-based disinfectants are persistent and therefore suitable as a secondary disinfectant. However, a problem with chlorine is that it reacts with organic matter to form trihalomethanes (THM), which are thought to be carcinogenic. Consequently, although SS, BOD and COD are not generally covered in drinking water standards, it is important to remove these from water prior to disinfection, so as to avoid chlorine associated THM production.

28.2.8 Aeration

Groundwater often has high concentrations of Fe and Mn, CO_2 and H_2S and low levels of DO [1]. Although Fe, Mn, CO_2 and H_2S are not identified as a health concern in drinking water [6, Table A3.2], they can lead to taste, odour and colour problems. Increasing the DO concentration can also improve the taste of water. Therefore it is desirable to remove Fe, Mn, H_2S , reduce dissolved CO_2 concentrations and increase DO concentrations. This can be achieved by aeration [1].

Aeration oxidises Fe and Mn leading to the formation of precipitates, which can be removed by filtration. Aeration will also increase DO concentrations and reduce concentrations of dissolved CO_2 and H_2S by virtue of Henry's law.

Henry's law states that when a gas and liquid are in equilibrium, the concentration of a given component in a liquid is linearly proportional to its partial pressure in the gas [7, p. 811]. The partial pressures of atmospheric air are relatively low for CO_2 , close to zero for H_2S and relatively high for O_2 . Therefore when a groundwater is brought into equilibrium with the atmosphere, dissolved CO_2 and H_2S concentrations will reduce and DO concentration will increase. The removal of CO_2 and H_2S from water in this way is sometimes referred to as air stripping. Dissolved volatile organic compounds (VOC) can be removed from water by air stripping in the same way.

There are two categories of method used for aeration. One involves injecting air into the water (e.g., using diffusers). The other involves promoting air entrainment by developing a high water-air interface. The latter can be done by spraying the water, cascading the water down a steep slope with obstacles or pouring water over a series of trays [1].

28.2.9 Desalination

The main challenge with seawater concerns desalination. The cost of desalination is strongly linked to the salinity of the original water (see Table 28.2). Potable water provided by seawater desalination can be up to eight times more expensive than that from a freshwater resource [8].

There are two categories of desalination method commonly applied: distillation and reverse osmosis [9]. Distillation involves separating water from salt solution

Table 28.2 Water cost by supply type in the US (after [8]). Prices include all costs to consumers including water treatment and delivery. Note that costs for brackish water and seawater include the additional costs associated with desalination

Supply type	Cost (USD ₂₀₀₇ kgal ⁻¹)
Freshwater (< 1 g l ⁻¹ TDS)	0.90–2.50
Brackish water (1 – 5 g l ⁻¹ TDS)	1.50–3.00
Seawater (30 – 35 g l ⁻¹ TDS)	3.00–8.00

Table 28.3 Energy requirements for different desalination technologies (after [9]). MSF refers to multi-stage flash distillation. MED refers to multi-effect distillation. SWRO refers to reverse osmosis with seawater (30 – 35 g l⁻¹ TDS). BWRO refers to reverse osmosis with brackish water (1 – 5 g l⁻¹ TDS)

Process	Thermal energy (kWh m ⁻³)	Electrical energy (kWh m ⁻³)	Total cost (USD ₂₀₁₃ m ⁻³)
MSF	7.5–12	2.5–4	0.8–1.5
MED	4–7	1.5–2	0.7–1.2
SWRO	–	3–4	0.5–1.2
BWRO	–	0.5–2.5	0.2–0.4

by evaporation and condensation. Two commonly applied distillation methods are multi-stage flash (MSF) distillation and multi effect distillation (MED). Differences between the two methods concern how energy is recovered during the condensation of the distillate [10,11]. Reverse osmosis (RO) involves separating water from salt solution by high pressure displacement across a semi-permeable membrane.

A large part of the cost of desalination is due to energy requirements, with distillation methods requiring considerably more energy than RO (see Table 28.3). However, the bulk of the energy required for distillation plants is thermal energy. Therefore, it is often found that distillation plants are preferred where a ready source of co-generated heat is available (e.g., near a power station). In the absence of a cheap heat source, RO is better value and hence more widely used [8].

28.2.10 Ion Exchange

Some solutes can be removed by ion exchange. The process typically involves passing a solution through a packed bed containing ion exchange resin beads. The most widely used ion exchanger beads are synthetic, organic-polymer resins [4]. The idea is that ions of positive charge (cations) or negative charge (anions) in a liquid solution replace dissimilar and displaceable ions, called counterions, of the same charge contained within a solid ion exchange resin [4]. Once all the exchange sites have been used up the resin can be regenerated by flushing the resin with a regenerant

solution [1]. Ion exchange is often used in the water industry for water softening, nitrate removal [1] and, importantly in the context of seawater reverse osmosis, boron removal [12].

28.2.11 Remineralisation

Water produced by reverse osmosis generally has a very low pH and is highly corrosive. Therefore it is necessary to increase the pH, alkalinity and hardness. This is often achieved by moving the water through a packed bed containing crushed limestone [1].

28.3 Granular Filtration Theory

Here we will develop some simple mathematical models to aid in the design of rapid sand filters. First we will look at the hydraulic head loss across the filter; this is required to determine the energy required to pass water through a filter. We will then develop equations to predict how efficient a filter will be at removing suspended solids. Finally we will derive an equation to determine the backwash rate required to clean a filter.

28.3.1 Hydraulic Head Loss

Hydraulic head loss, h_L [L], (see Sect. 1.3.4) in granular filters is typically modelled using the Ergun equation [13] (see Sect. 12.8.2)

$$h_L = \frac{c_0 \mu \tau^2 L q}{\rho g \phi \varepsilon^2 m_g^2} + \frac{f \tau^3 L q^2}{2 g \phi^2 \varepsilon m_g} \quad (28.1)$$

where L [L] is the length of the granular filter, c_0 [-] is a laminar flow shape factor, μ [$\text{ML}^{-1}\text{T}^{-1}$] is dynamic viscosity, τ [-] is a tortuosity factor, q [LT^{-1}] is the flow per unit area (sometimes referred to as the Darcy flux), ϕ [-] is the porosity, ε [-] is the void ratio, m_g [L] is the volume to surface area ratio of solid grains, ρ [ML^{-3}] is the fluid density, g [LT^{-2}] is gravitational acceleration and f [-] is the Darcy-Weisbach friction factor.

Table 28.4 Recommended empirical parameters for Eq. (28.6) [14]

Medium	κ_V (-)	κ_I (-)	ϕ (-)
Sand	110–115	2.0–2.5	0.40–0.43
Anthracite	210–245	3.5–5.3	0.47–0.52

The porosity represents the volume fraction of the filter media comprised of pore-space, i.e.,

$$\phi = \frac{\text{volume of pore-space in filter media}}{\text{volume of filter media}} \quad (28.2)$$

The void ratio is related to porosity via the relationship (see Sect. 12.3)

$$\varepsilon = \frac{\phi}{1 - \phi} \quad (28.3)$$

For spherical particles of diameter, D [L],

$$m_g = \frac{D}{6} \quad (28.4)$$

In the context of granular filters, the following empirical coefficients are invoked

$$\kappa_V = 36c_0\tau^2 \quad \text{and} \quad \kappa_I = 3f\tau^3 \quad (28.5)$$

where κ_V [-] is referred to as a head loss coefficient due to viscous forces and κ_I [-] is referred to as a head loss coefficient due to inertial forces. Some typical parameters for sand and anthracite are given in Table 28.4. Substituting Eqs. (28.3), (28.4) and (28.5) into Eq. (28.1) gives us [14, p. 745]

$$h_L = \frac{\kappa_V(1 - \phi)^2\mu Lq}{\phi^3 D^2 \rho g} + \frac{\kappa_I(1 - \phi)Lq^2}{\phi^3 Dg}. \quad (28.6)$$

28.3.2 Filtration Efficiency

Filtration efficiency, E [-], commonly represents the fraction of SS removed by a granular filter. Consider water, with a SS concentration, C_0 [ML⁻³], being fed at a constant volumetric flow rate, Q [L³T⁻¹], through a filter bed of cross-sectional area, A [L²], and length, L [L].

Let r_f [ML⁻³T⁻¹] be the rate at which SS is removed from a unit-volume of pore-space. Noting the definition of porosity given in Eq. (28.2), the rate at which SS is removed from a unit-volume of filter media is ϕr_f .

Recall the development of Eq. (27.16) to describe transport and aerobic consumption of biodegradable matter in a river. An analogous equation to describe transport and filtration of SS in a sand filter takes the form

$$Q \frac{dC}{ds} = -A\phi r_f \quad (28.7)$$

where C [ML⁻³] is the SS concentration within the filter bed and s [L] is distance along the flow direction of the filter. The SS removal rate can be written in terms of SS concentration and an SS removal rate coefficient, k_f [T⁻¹], i.e.,

$$r_f = k_f C \quad (28.8)$$

The relevant boundary condition is

$$C(s = 0) = C_0 \quad (28.9)$$

Immediately after backwashing, k_f is quite small. However, k_f increases with increasing filtration time as more SS are retained within the pore-space, leading to a reduction in pore size. Nevertheless, k_f tends to stabilise with time and can be treated as a constant.

Challenge 28.1 Derive an expression for the fraction of SS removed by the granular filter as a whole.

Substituting the Eq.(28.8) into Eq.(28.7), dividing both sides by C , integrating both sides with respect to s and applying the boundary condition, given in Eq. (28.9), leads to (analogous to Eq.27.32)

$$C = C_0 \exp\left(-\frac{A\phi k_f s}{Q}\right) \quad (28.10)$$

The fraction of SS removed by the granular filter, E , is found by setting $s = L$, subtracting C from C_0 , and dividing the result by C_0 to get

$$E \equiv \frac{C_0 - C}{C_0} = 1 - \exp\left(-\frac{A\phi k_f L}{Q}\right). \quad (28.11)$$

28.3.3 Removal Rate Coefficient Correlations

Many semi-empirical expressions have been derived to estimate k_f under different situations [14, p. 759]. Such expressions are often written in terms of dimensionless groups and seek to incorporate multiple trapping processes including interception, sedimentation and diffusion. Many of these expressions take on complicated functional forms, which can make it difficult to understand the important controlling mechanisms. However, by studying these equations and fixing some of the properties as constants it is possible to provide a more simplified function.

If we consider the work of [15] and decide on the temperature being 20°C and the fluid being water it is possible to arrive at

$$k_f = \frac{3.894 \times 10^{-13} q^{0.285}}{\phi \varepsilon^{0.850} D_p^{0.796} D^{1.634}} \quad (28.12)$$

where $q = \frac{Q}{A}$ and D_p [L] is the diameter of the suspended particles and all terms are in SI units.

From Eq.(28.12), it can be understood that removal rate decreases with increasing void ratio, increasing suspended particle size and increasing media particle size. The k_f parameter increases with increasing loading rate but overall, removal decreases with increasing loading rate due to the presence of the loading rate in the denominator of the exponential argument in Eq.(28.11).

That k_f increases with decreasing suspended particle size is testament to the reality that straining is not a significant filtration process in this context. In fact, diffusion is much more important. The smaller a suspended particle, the more likely

it is to diffuse from the main flow pathway, collide with a filter media particle and become immobile.

28.3.4 Backwash Hydraulics

As suspended solids are progressively entrained within a filter, the porosity reduces leading to an increase in hydraulic head loss. Eventually the head loss becomes too high for economic operations and the filter must be cleaned. Cleaning is achieved by forcing water upwards through the filter at a sufficiently high rate to suspend the granular media (a process known as fluidisation). Backwashing typically aims to expand filter bed length by around 37% for sand filters and around 25% for anthracite filters [14, p. 754].

Consider a filter bed with an initial length, L [L], and initial porosity, ϕ . It is often of interest to determine the necessary backwash rate, q_B [LT^{-1}], required to achieve an expanded length, L_E [L], during the fluidisation process (see Fig. 28.4).

Given Eq. (28.6), the hydraulic head loss, h_L [L], for a given backwash rate, q_B [LT^{-1}], can be estimated from [14, p. 752]

$$h_L = \frac{\kappa_V(1 - \phi_E)^2 \mu L_E q_B}{\phi_E^3 D^2 \rho g} + \frac{\kappa_I(1 - \phi_E) L_E q_B^2}{\phi_E^3 D g} \quad (28.13)$$

where ϕ_E [-] is the porosity of the expanded filter bed.

Equation (28.2) gives that the expanded pore-volume = $\phi_E L_E A$ where A [L^2] is the cross-sectional area of the filter bed. It follows that the volume of sand grains contained within the fluidised column = $(1 - \phi_E) L_E A$ and the associated weight of the suspended sand, F_g [MLT^{-2}], is found from

$$F_g = (1 - \phi_E) L_E A \rho_p g \quad (28.14)$$

where ρ_p [ML^{-3}] is the mass density of the suspended particles.

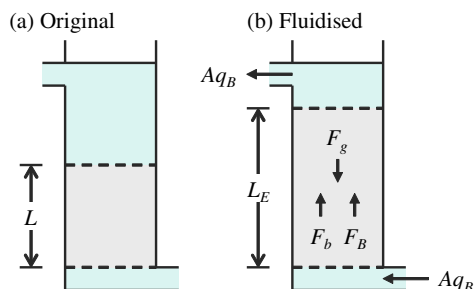
There is a corresponding, upward acting, buoyancy force (see Sect. 1.2.4.1)

$$F_b = (1 - \phi_E) L_E A \rho g \quad (28.15)$$

Backwashing gives rise to an additional upward force

$$F_B = h_L A \rho g \quad (28.16)$$

Fig. 28.4 Schematic diagram illustrating how the length of a filter bed expands from L to L_E during the fluidisation process associated with backwashing



which supports the weight of the suspended sand in the fluidised column.

During backwashing, the fluidised column of sand can be assumed static, which implies that (see Fig. 28.4)

$$F_g = F_b + F_B \quad (28.17)$$

Substituting Eqs. (28.14), (28.15) and (28.16) into Eq. (28.17) and solving for h_L leads to [14, p. 751]

$$h_L = \frac{(\rho_p - \rho)(1 - \phi_E)L_E}{\rho} \quad (28.18)$$

Equating Eqs. (28.13) and (28.18) then gives

$$\frac{(\rho_p - \rho)\phi_E^3}{\rho} = \frac{\kappa_V(1 - \phi_E)\mu q_B}{D^2 \rho g} + \frac{\kappa_I q_B^2}{Dg} \quad (28.19)$$

which can be solved for q_B to obtain the backwash rate required to sustain a fluidised expanded length, L_E .

Interestingly, the expanded length, L_E , is not directly present within Eq. (28.19). However, a relationship between the expanded porosity, ϕ_E , and the expanded length, L_E , can be determined by assuming the volume of sand grains is unchanged by the fluidisation process.

Challenge 28.2 Determine an expression for the expanded porosity, ϕ_E , in terms of the original porosity, ϕ , the expanded length, L_E , and the original length, L , assuming that the volume of sand grains is unchanged by the fluidisation process.

Equation (28.2) gives that the original pore-volume = ϕLA where $A [L^2]$ is the cross-sectional area of the filter bed. It follows that the original volume of sand grains = $(1 - \phi)LA$. In the same way, it can be said that the fluidised pore-volume = $\phi_E L_E A$ and the associated volume of sand grains = $(1 - \phi_E)L_E A$. Given that the volume of sand grains has not actually changed, it follows that $(1 - \phi)LA = (1 - \phi_E)L_E A$ and therefore

$$\phi_E = 1 - (1 - \phi) \frac{L}{L_E} \quad (28.20)$$

Another important constraint is that the backwash rate should be less than the settling velocity (see Sect. 24.7.2) of the granular particles that comprise the filter. If the backwash rate is greater than the settling velocity of the particles, the filter bed will be washed away with the backwash water. Providing the backwash rate is less than the settling velocity, the filter bed should resettle close to its original form once backwashing is complete.

28.4 Reverse Osmosis Theory

Reverse osmosis (RO) for desalination typically takes place using spiral wound membrane elements, packed within a cylindrical pressure cell (see Fig. 28.5). Saline

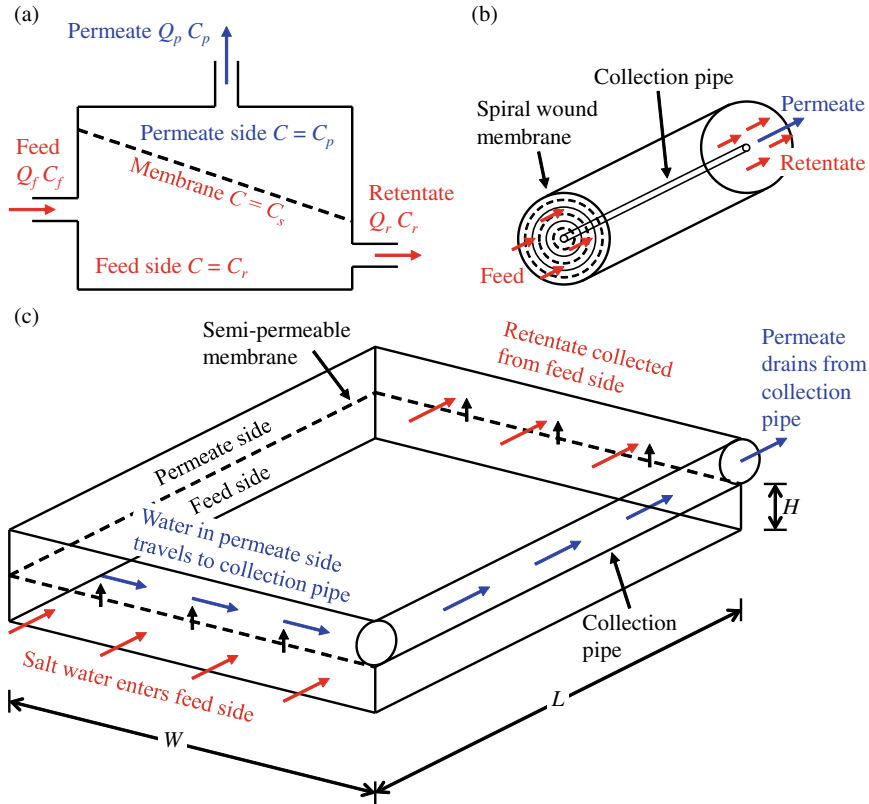


Fig. 28.5 Schematic diagrams of a spiral wound membrane for reverse osmosis. **a** Mass conservation system. **b** Cylindrical pressure cell containing a rolled up membrane with a central collection tube. **c** Unravalled membrane showing how water flows within the system

feed water is injected into the feed side of the membrane at high pressure. The portion of water that is displaced through the membrane is referred to as the permeate. The permeate will have a lower salinity because the membrane excludes salt molecules. The remaining water is referred to as the retentate. This water will have a higher salinity than the feed water because it contains the rejected salt.

Spiral wound membranes consist of a sheet of semi-permeable membrane enclosed within two impermeable sheets. Feed water is fed into the feed side of the membrane. Permeate is collected from the permeate side of the membrane. The sheet is rolled up and packed into a cylindrical pressure cell with a collection pipe at the centre (see Fig. 28.5b).

Consider a diagram of an unrolled membrane sheet (see Fig. 28.5c). Salt water is forced into the feed side of the membrane and travels in a longitudinal direction. Because of the high pressure of the feed water, some of the water is able to transfer

across the semi-permeable membrane to the permeate side of the membrane. This latter water is the permeate.

The permeate travels along the permeate side of the membrane in a spiral direction towards the central collection pipe, from which it is drained and taken away. Some of the feed water does not make it through the membrane and exits the feed side of the membrane at the other end of the cylindrical pressure cell, this is the retentate.

An important design consideration concerns the volume of feed water required to produce a desired volume of permeate. Relevant physical processes include Darcy's law for water movement across the membrane, diffusion for solute movement within the feed water and across the membrane and osmosis, which describes the additional resistance to flow caused by the difference in salinity between the feed-water and the permeate. Below we will derive a simple mathematical model to describe these different processes and design some key aspects of an RO facility.

First we define mass conservation statements for water and salt in an RO pressure cell. We then look at the concept of concentration polarisation, which is needed to determine the salt concentration on the feed side of the membrane. An empirical equation is provided that relates permeate rate to pressure difference and osmotic pressure difference. It is then explained how to determine osmotic pressure from salt concentration. An empirical equation is provided to describe solute transport across the membrane, which enables us to determine the salt concentration on the permeate side of the membrane for a given salt concentration on the feed side of the membrane. Finally a sequence of algebraic manipulations is performed to determine the feed rate required for a given permeate rate.

28.4.1 Reverse Osmosis Explained

Semi-permeable membranes are special porous membranes that are selectively permeable to different substances. Typical membranes used for RO include cellulosic derivatives and polyamide derivatives [14, p. 1350]. Such membranes are permeable to water but impermeable to salt.

To help understand the concept of RO let us consider three different scenarios each involving two aqueous solutions either side of a semi-permeable membrane.

Scenario 1: Both fluids are pure water. One of the fluids is at a higher pressure than the other. Accordingly water will flow through the membrane from the high pressure side to the low pressure side, according to Darcy's law.

Scenario 2: Both fluids are at the same pressure. One of the fluids has a higher salinity than the other. Accordingly water will flow through the membrane from the low salinity side to the high salinity side. This is due to a process known as osmosis, whereby water travels through a semi-permeable membrane from low salt concentration to high salt concentration. The reason this happens is that although the pressures are the same on both sides of the membrane, the chemical potential of water is higher on the low salinity side. Water will move across the membrane from

where it has a high chemical potential to where it has a low chemical potential. Salt does not travel across the membrane because the membrane excludes it.

Scenario 3: One of the fluids has a high salinity and high pressure. The other fluid has a low salinity and low pressure. Providing the pressure of the fluid on the high salinity side is sufficiently high, the net movement of water across the membrane will be from the high salinity side to the low salinity side. The reason this happens is that the rate at which water moves due to the pressure difference is greater than the rate at which water moves in the opposite direction due to the chemical potential difference. Furthermore, because the membrane excludes salt, water that travels across the membrane is stripped of its salinity. This scenario describes the process of reverse osmosis.

28.4.2 Conservation Equations

The mass conservation equation for water within an RO pressure cell takes the form

$$\rho Q_f = \rho Q_r + \rho Q_p \quad (28.21)$$

where Q_f [L^3T^{-1}] is the volumetric feed rate, Q_r [L^3T^{-1}] is the volumetric retentate rate and Q_p [L^3T^{-1}] is the volumetric permeate rate. Note that the fluid density, ρ , is assumed to be unaffected by salt concentration.

The associated mass conservation equation for salt takes the form (see Fig. 28.5a)

$$Q_f C_f = Q_r C_r + Q_p C_p \quad (28.22)$$

where C_f [ML^{-3}], C_r [ML^{-3}] and C_p [ML^{-3}] are the mass concentrations of salt in the feed, retentate and permeate, respectively.

28.4.3 Concentration Polarisation

The exclusion of salt by the membrane leads to a build-up in salt concentration on the feed-side of the membrane (see Fig. 28.6). Consider a control-volume of feed water immediately adjacent to the membrane (see Fig. 28.7). Mass balance dictates that [16, p. 89]

$$Q_p C = Q_p C_p - A D_0 \frac{\partial C}{\partial s} \quad (28.23)$$

where A [L^2] is the area of semi-permeable membrane (for Fig. 28.5c, $A = WL$) and D_0 [L^2T^{-1}] is the molecular diffusion coefficient of the salt in the water.

The relevant boundary conditions are:

$$\begin{aligned} C &= C_s, \quad s = 0 \\ C &= C_r, \quad s = b \end{aligned} \quad (28.24)$$

where C_s [ML^{-3}] is the salt concentration on the feed-side of the membrane and b [L] is the diffusion film thickness, beyond which the concentration is the same as the retentate.

Fig. 28.6 Schematic diagram illustrating concentration polarisation during reverse osmosis

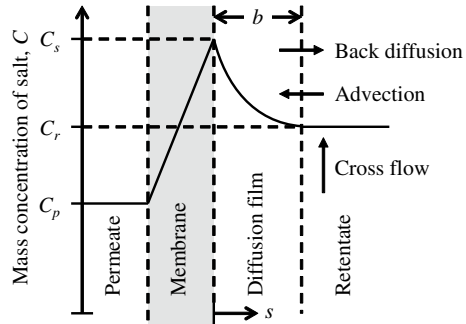
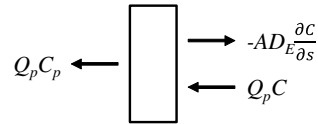


Fig. 28.7 Mass balance for a control-volume of feed water immediately adjacent to the membrane



The idea that salt is advected towards the membrane by the feed water but is diffused in a counter direction, away from the membrane, due to salt buildup at the membrane, is referred to as concentration polarisation.

Challenge 28.3 Use Eq. (28.23) to derive an expression for C_s in terms of C_r , C_p , Q_p , A and k .

Separating variables in Eq. (28.23) and integrating both sides with respect to s leads to the general solution

$$-\frac{Q_p s}{AD_0} = \ln(C - C_p) + A_0 \quad (28.25)$$

where A_0 is an integration constant.

From Eq. (28.24), $C = C_s$ at $s = 0$. Equation (28.25) therefore gives that

$$A_0 = -\ln(C_s - C_p) \quad (28.26)$$

Substituting Eq. (28.26) into Eq. (28.25) leads to

$$-\frac{Q_p s}{AD_0} = \ln\left(\frac{C - C_p}{C_s - C_p}\right) \quad (28.27)$$

From Eq. (28.24), $C = C_r$ at $s = b$. Equation (28.27) therefore gives that

$$-\frac{Q_p b}{AD_0} = \ln\left(\frac{C_r - C_p}{C_s - C_p}\right) \quad (28.28)$$

Solving Eq. (28.28) for C_s leads to [16, p. 90]

$$C_s = (C_r - C_p)e^{\frac{Q_p b}{Ak}} + C_p \quad (28.29)$$

where $k = \frac{D_0}{b}$ [LT^{-1}] is referred to as the concentration polarisation mass-transfer coefficient.

28.4.3.1 Mass Transfer Coefficient Estimation

The concentration polarisation mass transfer coefficient, k [LT^{-1}], can be determined by using existing correlations associated with convective heat transfer.

Consider mass transfer from a mass source dissolving into a surrounding fluid. The convective mass flux from the mass source, q_c [$\text{ML}^{-2}\text{T}^{-1}$], is found from [17, p. 756]

$$q_c = \frac{D_0 \text{Sh}}{L_c} (C_s - C_r)$$

where D_0 [LT^{-2}], is the molecular diffusion coefficient of the solute in the fluid, Sh [-] is the Sherwood number, L_c [L] is a characteristic length, C_s [ML^{-3}] is the mass concentration of the substance on the surface of the mass source and C_r [ML^{-3}] is the mass concentration in the surrounding fluid. The aforementioned mass transfer coefficient, k [LT^{-1}], is found from

$$k = \frac{D_0 \text{Sh}}{L_c} \quad (28.30)$$

Analogous to the above problem, consider heat transfer from a constant temperature heat source into a surrounding moving fluid. The convective heat flux from the source, q_h [MT^{-3}], is found from [17, p. 756]

$$q_h = \frac{\kappa_h \text{Nu}}{L_c} (T_s - T_r)$$

where κ_h [$\text{MLT}^{-3}\Theta^{-1}$], is the thermal conductivity of the fluid, Nu [-] is the Nusselt number and L_c [L] is a characteristic length, T_s [Θ] is the temperature of the heat source and T_r [Θ] is the temperature of the surrounding fluid.

Many empirical correlations exist for predicting the Nusselt number under different convection scenarios. The transport problem associated with spiral bound membranes is analogous to laminar flow across a flat plate of fixed temperature where [17, p. 761]

$$\text{Nu} = 0.664 \text{Re}^{1/2} \text{Pr}^{1/3}$$

where Re [-] is the Reynolds number and Pr [-] is the Prandtl number, further defined by

$$\text{Re} = \frac{\rho v L_c}{\mu} \quad (28.31)$$

and

$$\text{Pr} = \frac{c_p \mu}{\kappa_h} \quad (28.32)$$

respectively, with ρ [ML^{-3}] being the fluid density, v [LT^{-1}] being the fluid velocity, μ [$\text{ML}^{-1}\text{T}^{-1}$] being the dynamic viscosity of the fluid and c_p [$\text{L}^2\text{T}^{-2}\Theta^{-1}$] being the specific heat capacity of the fluid.

The Sherwood number is the mass transfer analogue to the Nusselt number [17, p. 756]. An associated expression for laminar flow across a flat plate takes the form [17, p. 761]

$$\text{Sh} = 0.664 \text{Re}^{1/2} \text{Sc}^{1/3} \quad (28.33)$$

where Sc [-] is the Schmidt number found from

$$Sc = \frac{\mu}{\rho D_0} \quad (28.34)$$

For fluid flow between two parallel plates, $L_c = 4m$ where $m = \frac{A_c}{P_c}$ [L] is the hydraulic radius (see Sect. 2.4.1) of the flowing channel, A_c [L²] is the cross-sectional area of the channel and P_c [L] is the wetted perimeter of the channel. For a rectangular channel of width, W [L], and thickness, H [L] (consider again Fig. 28.5c):

$$A_c = WH, \quad P_c = 2W + 2H, \quad m = \frac{WH}{2W + 2H}, \quad L_c = \frac{2WH}{W + H}$$

For the case where $H \ll W$, it can be further stated that $L_c = 2H$ [14, p. 1371].

28.4.4 Osmotic Pressure

Water travels through the membrane due to reverse osmosis and the rate is controlled by the following Darcy-law-like equation [16, p.255]

$$Q_p = A\kappa_w \cdot (\Delta p - \Delta\pi) \quad (28.35)$$

where A [L²] is the area of the membrane, Δp [ML⁻¹T⁻²] and $\Delta\pi$ [ML⁻¹T⁻²] are the pressure difference and osmotic pressure difference across the membrane, respectively, and κ_w [M⁻¹L²T] is the water permeability coefficient of the membrane.

The osmotic pressure is found using the van't Hoff equation [14, p. 1354]

$$\pi = \frac{NRT}{V_m} \quad (28.36)$$

where N [-] is the number of moles associated with a given salt dissolved in a volume of liquid, V_m [L³], R [ML²T⁻²Θ⁻¹] (= 8.314 J mol⁻¹ K⁻¹) is the universal ideal gas constant and T [Θ] is temperature. Equation (28.36) is analogous to the equation used to describe partial pressures for ideal gas mixtures (see Sect. 18.3.2).

Challenge 28.4 Derive an expression relating osmotic pressure to mass concentration of NaCl at 20°C.

The molecular mass of NaCl is 58.44 g mol⁻¹. When dissolved in water



so every one mole of solid NaCl produces two moles in solution. It follows that mass concentration of salt, C , in mg l⁻¹, is related to $\frac{N}{V_m}$ via the relationship

$$\frac{N}{V_m} = \frac{2C}{58.44} \quad (28.37)$$

Substituting Eq. (28.37) into Eq. (28.36) and setting $T = 293.15$ K (i.e., 20° C) leads to

$$\pi = \frac{2C \times 8.314 \times 293.15}{58.44} = \alpha C \quad (28.38)$$

where $\alpha = 83.41$ Pa m³ g⁻¹. (Note that the salinity of seawater is 35,000 mg l⁻¹, so the corresponding osmotic pressure would be 2.92 MPa.)

It follows that for the system described in Fig. 28.6, $\Delta\pi = \alpha \cdot (C_s - C_p)$, which on substitution into Eq. (28.35) leads to

$$Q_p = A\kappa_w \cdot [\Delta p - \alpha \cdot (C_s - C_p)]. \quad (28.39)$$

28.4.5 Solute Diffusion Through the Membrane

Solute travels through the membrane due to diffusion, with the rate being controlled by the following mass transfer equation [16, p. 255]

$$Q_p C_p = A\kappa_s \cdot (C_s - C_p) \quad (28.40)$$

where κ_s [LT⁻¹] is the solute mass transfer coefficient of the membrane.

Challenge 28.5 Use Eqs. (28.21), (28.22), (28.29) and (28.40) to derive an expression for C_p in terms of Q_f , A , κ_s , C_f , Q_p , and k .

Substituting Eq. (28.29) into Eq. (28.40) leads to

$$Q_p C_p = A\kappa_s \cdot (C_r - C_p) e^{\frac{Q_p}{Ak}} \quad (28.41)$$

From Eqs. (28.21) and (28.22) we have that

$$C_r = \frac{Q_f C_f - Q_p C_p}{Q_f - Q_p} \quad (28.42)$$

Substituting Eq. (28.42) into Eq. (28.41) give us

$$Q_p C_p = \frac{Q_f A\kappa_s \cdot (C_f - C_p) e^{\frac{Q_p}{Ak}}}{Q_f - Q_p} \quad (28.43)$$

Solving Eq. (28.43) for C_p leads to

$$C_p = \frac{Q_f A\kappa_s C_f}{(Q_f - Q_p) Q_p e^{-\frac{Q_p}{Ak}} + Q_f A\kappa_s} \quad (28.44)$$

Challenge 28.6 Use Eq. (28.29) to derive an expression for C_s in terms of Q_f , Q_p , A , κ_s , C_f and k .

Substituting Eq. (28.42) into Eq. (28.29) leads to

$$C_s = \frac{Q_f C_f e^{\frac{Q_p}{Ak}} + [Q_f(1 - e^{\frac{Q_p}{Ak}}) - Q_p]C_p}{Q_f - Q_p} \quad (28.45)$$

Substituting Eq. (28.44) into Eq. (28.45) gives us

$$C_s = \frac{Q_f(Q_p + A\kappa_s)C_f}{(Q_f - Q_p)Q_p e^{-\frac{Q_p}{Ak}} + Q_f A\kappa_s}. \quad (28.46)$$

28.4.6 Feed Rate Estimation

Challenge 28.7 Use Eqs. (28.39), (28.44) and (28.46) to derive an expression for Q_f in terms of Q_p , A , κ_w , α , C_f , Δp , κ_s and k .

Substituting Eqs. (28.44) and (28.46) into Eq. (28.39) leads to

$$Q_p = A\kappa_w \cdot \left[\Delta p - \frac{\alpha Q_f Q_p C_f}{(Q_f - Q_p)Q_p e^{-\frac{Q_p}{Ak}} + Q_f A\kappa_s} \right] \quad (28.47)$$

Solving Eq. (28.47) for Q_f gives us

$$Q_f = \frac{Q_p}{1 - \left(\frac{A\kappa_w \alpha C_f}{A\kappa_w \Delta p - Q_p} - \frac{A\kappa_s}{Q_p} \right) e^{\frac{Q_p}{Ak}}} \quad (28.48)$$

from which it can be seen that, for a given permeate rate, Q_p , the required feed rate, Q_f , increases with increasing feed salinity, C_f , whereas it decreases with increasing κ_s and/or k .

The required feed rate increases with increasing salinity because this leads to the osmotic pressure difference becoming harder to overcome. The required feed rate decreases with increasing κ_s because this parameter describes how easily salt is transmitted through the membrane, which will reduce the osmotic pressure difference across the membrane. The required feed rate decreases with increasing k because this parameter describes how efficiently the cross flow of feed water over the membrane reduces the effect of concentration polarisation.

28.5 Problem Sheet

Problem 28.1 (see Worked Solution 28.1)

(a) Determine the maximum overflow rate (in m day^{-1}) for a circular clarifier designed to remove all particles of size $> 20 \mu\text{m}$ in diameter. Assume the density and viscosity of water to be 1000 kg m^{-3} and 10^{-3} Pa s , respectively, and the density of the suspended particles to be 2650 kg m^{-3} .

(b) Given the overflow rate determined in part (a), calculate the diameter of clarifier required to treat $2000 \text{ MI year}^{-1}$.

Problem 28.2 (see Worked Solution 28.2)

A rapid sand filter contains a 0.6 m thick sand bed. The loading rate of the filter is 7 m hour^{-1} . The median diameter of the sand grains is 0.5 mm . The head-loss parameters of the sand are $\kappa_V = 112$ and $\kappa_I = 2.2$. The density and viscosity of the influent are 1000 kg m^{-3} and 10^{-3} Pa s , respectively. The initial porosity of the sand is 0.4 .

(a) Determine the initial head loss across the filter.

(b) As time passes, suspended solids are entrained within the filter leading to a reduction in porosity and a corresponding increase in head loss. Determine the porosity of the sand when the head loss has reached 2 m .

(c) Calculate the percentage of suspended solids removed from the influent (i) at the beginning of the filtration cycle and (ii) at the end of the filtration cycle. Assume the particles being removed have a diameter of $0.1 \mu\text{m}$.

(d) Calculate the backwash rate required to expand the filter bed by an additional 37% and verify that sand grains greater than 0.2 mm will not be washed away during the backwash process. Assume the density of the sand is 2650 kg m^{-3} .

(e) Determine the plan area of sand filter required to produce $2000 \text{ MI year}^{-1}$ of potable water.

Problem 28.3 (see Worked Solution 28.3)

A spiral wound membrane contains a sheet of membrane of 32.5 m width and 1 m length. The feed channel thickness, $H = 0.125 \text{ mm}$. The water mass transfer

coefficient, $\kappa_w = 7.97 \times 10^{-12} \text{ m s}^{-1} \text{ Pa}^{-1}$. The solute mass transfer coefficient, $\kappa_s = 1.71 \times 10^{-7} \text{ m s}^{-1}$. The desired permeate rate is $26.8 \text{ m}^3 \text{ day}^{-1}$. The concentration polarisation mass transfer coefficient, $k = 3.93 \times 10^{-4} \text{ m s}^{-1}$.

(a) Determine the required feed rate and the resulting permeate concentration when:

(i) The feed water has a NaCl concentration of 2000 mg l^{-1} and the applied pressure difference is 1.39 MPa .

(ii) The feed water has a NaCl concentration of 2000 mg l^{-1} and the applied pressure difference is 4.5 MPa .

(iii) The feed water has a NaCl concentration of $35,000 \text{ mg l}^{-1}$ and the applied pressure difference is 4.5 MPa .

(b) Use the heat convection analogy to estimate the concentration polarisation mass transfer coefficient for part (a) (i). Assume the density and dynamic viscosity of water are 1000 kg m^{-3} and 10^{-3} Pa s , respectively, and that the molecular diffusion coefficient of NaCl in water is $1.35 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$.

(c) Determine the number of spiral wound membrane cells required to produce $2000 \text{ Ml year}^{-1}$ of potable water.

28.6 Worked Solutions

Worked Solution 28.1 (see Problem 28.1)

(a) The maximum overflow rate will be equal to the settling velocity of the smallest particle to be removed, $v \text{ [LT}^{-1}\text{]}$, which can be determined from (Eq. 24.9)

$$v^2 = \frac{4D(\rho_p - \rho)g}{3\rho C_d}$$

where $D \text{ [L]}$ is the particle diameter, $\rho_p \text{ [ML}^{-3}\text{]}$ is the density of the particle, $\rho \text{ [ML}^{-3}\text{]}$ is the density of the fluid the particle is settling in, $g \text{ [LT}^{-2}\text{]}$ is gravitational acceleration and $C_d \text{ [-]}$ is the drag coefficient, found from (Eq. 24.20)

$$C_d = \begin{cases} \frac{432}{K^3}, & K < 3.302 \\ \frac{55.46}{K^{1.282}}, & 3.302 < K < 43.53 \\ 0.44, & 43.53 < K < 2363 \end{cases}$$

where $K \text{ [-]}$ represents a dimensionless settling regime number found from (Eq. (24.17))

$$K = \left[\frac{D^3 \rho (\rho_p - \rho) g}{\mu^2} \right]^{1/3}$$

From the information given: $D = 20 \text{ }\mu\text{m}$, $\rho = 1000 \text{ kg m}^{-3}$, $\mu = 10^{-3} \text{ Pa s}$ and $\rho_p = 2650 \text{ kg m}^{-3}$. It follows that $K = 0.5059$, $C_d = 3336$ and $v = 3.597 \times 10^{-4}$

m s^{-1} which is equal to 31.08 m day^{-1} . So the maximum overflow rate should be 31.1 m day^{-1} .

(b) The clarifier is required to treat $2000 \text{ Ml year}^{-1}$, which corresponds to $5479 \text{ m}^3 \text{ day}^{-1}$. Given that the maximum overflow rate is 31.08 m day^{-1} , the required area of the clarifier is $5479 \div 31.08 = 176.3 \text{ m}^2$. So the diameter of the clarifier needs to be greater than 15.0 m .

Worked Solution 28.2 (see Problem 28.2)

(a) The initial head loss can be determined using the Ergun equation. Let $L = 0.6 \text{ m}$, $q = 0.001944 \text{ m s}^{-1}$, $D = 0.0005 \text{ m}$, $\kappa_V = 112$, $\kappa_I = 2.2$, $\rho = 1000 \text{ kg m}^{-3}$, $\mu = 10^{-3} \text{ Pa s}$ and $\phi = 0.4$. It follows from Eq. (28.6) that the initial hydraulic head loss, $h_L = 0.309 \text{ m}$.

(b) Equation (28.6) can be rearranged to get

$$h_L \phi^3 - a \phi^2 + (2a + b)\phi - a - b = 0$$

where

$$a = \frac{\kappa_V \mu L q}{D^2 \rho g} \quad \text{and} \quad b = \frac{\kappa_I L q^2}{D g}$$

The above equation can be solved using the MATLAB function, `roots`, as follows:

```
phi=roots([hL -a 2*a+b -a-b]);
```

Using the parameter values provided in part (a) along with $h_L = 2 \text{ m}$ leads to our cubic equation having just one real root, which is 0.2489 . So the final porosity is 0.249 .

(c) The fraction of suspended solids removed by the filter, E , is found from Eq. (28.11). From the information given in Problem 26.2a, $L = 0.6 \text{ m}$, $\frac{Q}{A} = 0.001944 \text{ m s}^{-1}$, $D = 0.0005 \text{ m}$. The removal rate coefficient, k_f , can be found from Eq. (28.12). From the information given in Problem 28.2c, $D_p = 10^{-7} \text{ m}$.

(i) At the beginning of the filtration cycle, $\phi = 0.4$, $\varepsilon = 0.6667$ (from Eq. 28.3), $k_f = 0.02144 \text{ s}^{-1}$ and $E = 0.9291$. So the percentage removal of suspended solids is 92.9% .

(ii) At the end of the filtration cycle, $\phi = 0.2489$, $\varepsilon = 0.3313$, $k_f = 0.06244 \text{ s}^{-1}$ and $E = 0.9917$. So the percentage removal of suspended solids is 99.2% .

(d) If the filter bed is to be expanded by 37% , the expanded length, $L_E = 1.37 \times 0.6 = 0.8220 \text{ m}$. Assuming the porosity and length are initially 0.4 and 0.6 m , respectively,

Eq. (28.20) gives that the expanded porosity, $\phi_E = 0.5620$. The backwash rate can be found from Eq. (28.19). The only positive root of Eq. (28.19) is

$$q_B = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$$

where

$$a = \frac{\kappa_I}{Dg}, \quad b = \frac{\kappa_V(1-\phi_E)\mu}{D^2\rho g} \quad \text{and} \quad c = -\frac{(\rho_p - \rho)\phi_E^3}{\rho}$$

with $D = 0.0005$ m, $\kappa_V = 112$, $\kappa_I = 2.2$, $\rho = 1000$ kg m⁻³, $\mu = 10^{-3}$ Pa s and $\rho_p = 2650$ kg m⁻³. It follows that $q_B = 0.01162$ m s⁻¹. So the backwash rate should be 41.8 m hour⁻¹.

To verify that sand grains greater than 0.2 mm will not be washed away we need to determine the settling velocity of a 0.2 mm diameter grain. Following the steps used to solve Problem 28.1a, the settling velocity is determined as 0.0249 m s⁻¹, which is greater than the backwash rate. So it is confirmed that sand grains greater than 0.2 mm diameter will be retained.

(e) Given that the loading rate of the sand filter is 7 m hour⁻¹, the plan area of filter required to produce 2000 Ml year⁻¹ would be $2 \times 10^6 \div (365 \times 24 \times 7) = 32.62$ m². Rounding up to 3 significant figures then gives us 32.7 m².

Worked Solution 28.3 (see Problem 28.3)

(a) The feed rate, Q_f , can be determined from Eq. (28.48). The permeate concentration, C_p , can be determined from Eq. (28.44). Let $A = 32.5$ m², $\kappa_w = 7.97 \times 10^{-12}$ m s⁻¹ Pa⁻¹, $\kappa_s = 1.71 \times 10^{-7}$ m s⁻¹, $Q_p = 3.102 \times 10^{-4}$ m³ s⁻¹, $k = 3.93 \times 10^{-4}$ m s⁻¹. For NaCl, $\alpha = 83.41$ Pa m³ g⁻¹. It follows that

	Δp (MPa)	C_f (mg l ⁻¹),	Q_f (m ³ day ⁻¹)	C_p (mg l ⁻¹)
(i)	1.39	2000	205.5	41.35
(ii)	4.5	2000	27.73	709.4
(iii)	4.5	35,000	237.9	709.4

As the pressure difference is increased less feed water is required to generate the same quantity of permeate but the consequence is that the permeate salinity is increased. As the feed water salinity is increased, much more feed water is required to achieve the same rate of permeate production because the osmotic pressure difference has been increased.

(b) The mass transfer coefficient, k , can be calculated from Eq. (28.30) and the Sherwood number, Sh , can be calculated from Eq. (28.33). Let $L_c = 2H = 2.5 \times 10^{-4}$ m, $\rho = 1000$ kg m⁻³, $\mu = 10^{-3}$ Pa s and $D_0 = 1.35 \times 10^{-9}$ m² s⁻¹. The velocity, $v = \frac{Q_f}{WH} = \frac{205.5}{24 \times 60^2 \times 32.5 \times 1.25 \times 10^{-4}} = 0.5855$ m s⁻¹. It follows that the Reynolds

number, $Re = 146.4$ and the Schmidt number, $Sc = 740.7$. So the Sherwood number, $Sh = 72.69$ and $k = 3.93 \times 10^{-4} \text{ m s}^{-1}$.

(c) Given that each spiral wound membrane cell produces $26.8 \text{ m}^3 \text{ day}^{-1}$, the number of cells required to produce $2000 \text{ Ml year}^{-1}$ would be $2 \times 10^6 \div (365 \times 26.8) = 204.5$. Rounding up to a whole number of cells then gives us 205.

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Abstract

This chapter focuses on wastewater treatment technologies. The difference between preliminary, primary, secondary and tertiary treatment are discussed. A range of different biological treatment methods are explained, including trickling filters, rotating biological contactors, activated sludge reactors and waste stabilization ponds. Mathematical models are developed for describing basic activated sludge processes. A completely mixed model is derived using Monod equations. An incompletely mixed model is derived using the advection dispersion equation combined with a linear reaction term and Danckwerts' boundary conditions. The efficiency of plug flow conditions and completely mixed flow conditions are compared. Practical applications are presented through a problem sheet with worked solutions.

Notation

a	Dimensionless group [-].
A	Flowing cross-sectional area of a aeration tank [L^2].
C	Dissolved BOD concentration [ML^{-3}].
C_0	Dissolved BOD concentration of a primary clarifier effluent [ML^{-3}].
C_e	Dissolved BOD concentration of an aeration tank effluent [ML^{-3}].
C_i	BOD concentration of incoming fluid for an aeration tank [ML^{-3}].
k_c	BOD consumption rate coefficient [T^{-1}].
k_{c0}	Zeroth order BOD consumption rate coefficient [T^{-1}].
k_d	Microbial death rate coefficient [T^{-1}].
k_g	Microbial growth rate coefficient [T^{-1}].
$k_{g,max}$	Maximum possible microbial growth rate coefficient [T^{-1}].
H	Water depth [L].
K	Dispersion tensor [L^2T^{-1}].
J_x	Mass flux of BOD in the x direction [$ML^{-2}T^{-1}$].

K_c	Half-velocity constant for BOD [ML^{-3}].
K_{xx}	Dispersion coefficient in x direction [L^2T^{-1}].
L	Length of reactor or channel [L].
Pe	Peclet number [-].
Q_0	Inflow rate from a primary clarifier [L^3T^{-1}].
Q_G	Air injection rate [L^3T^{-1}].
Q_r	Recycle flow rate of sludge from a secondary clarifier [L^3T^{-1}].
r_c	Microbial consumption rate of BOD [$\text{ML}^{-3}\text{T}^{-1}$].
r_d	Microbial death rate [$\text{ML}^{-3}\text{T}^{-1}$].
r_g	Microbial growth rate [$\text{ML}^{-3}\text{T}^{-1}$].
t	Time [T].
u	Velocity in x direction [LT^{-1}].
$\mathbf{u}$	Velocity vector [LT^{-1}].
V	Volume of an aeration tank [L^3].
W	Width of channel [L].
W_d	Width of the air diffuser [L].
x	Distance along a reactor [L].
X	Active microbial mass concentration [ML^{-3}].
X_e	Active microbial mass concentration of an aeration tank effluent [ML^{-3}].
X_r	Active microbial mass concentration of a recycled sludge [ML^{-3}].
β	Mass of BOD consumed per unit mass of microorganisms [-].
γ	Dimensionless BOD consumption rate [-].
γ_i	Another dimensionless BOD consumption rate [-].
ε	Dimensionless small parameter [-].
BOD	Biochemical oxygen demand.
COD	Chemical oxygen demand.
DO	Dissolved oxygen.
SS	Suspended solids.

29.1 Introduction

Wastewater, is water produced as a by-product of an anthropogenic activity. In this chapter, we focus on the treatment of municipal wastewater. First we look at the various processes generally applied. Then we develop some mathematical theory to design key features of an activated sludge system.

29.2 Wastewater Treatment Processes

The objective of wastewater treatment is to reduce BOD, COD, SS, total P and total N (recall Table 27.3). A typical set of processes to achieve these objectives are shown in Fig. 29.1.

Within a typical wastewater treatment plant it is common to distinguish between preliminary, primary, secondary and tertiary treatment [1, p. 313]. Preliminary treatment includes screening, grit removal and dissolved air flotation (DAF) so as to remove coarse SS, fats, oils and grease. Screening and DAF are as described in Chap. 28, concerning water treatment. Grit removal is normally achieved using a clarifier with a relatively short residence time (so as to only retain the larger particles).

Primary treatment concerns removing the remainder of the SS using a (primary) clarifier. Sometimes this can be combined with coagulation and flocculation, as described in Chap. 28. Following primary treatment, the wastewater will have low turbidity and appear to be very clean. However, the water will remain high in BOD and nutrients due to high dissolved concentrations of organic matter, ammonium and often nitrates and phosphates.

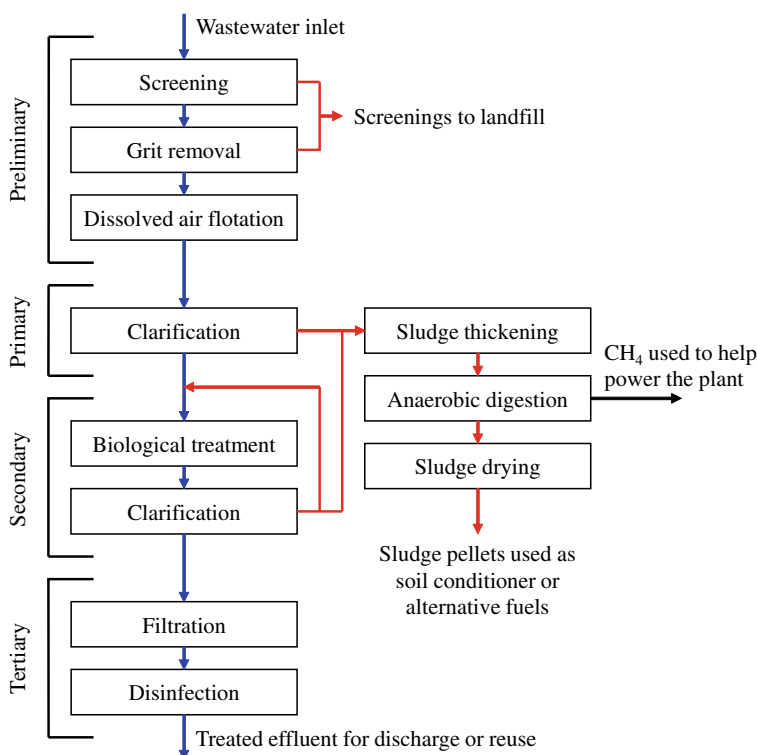


Fig. 29.1 Flow chart for a typical wastewater treatment plant

Secondary treatment involves removal of biodegradable organic matter and nutrients using various biological methods, which convert dissolved constituents into solid biomass referred to as sludge. A coagulant is then added to precipitate any remaining phosphorus. Sludge and precipitate are then removed using an additional clarifier, referred to as a secondary clarifier.

Tertiary treatment is not always available but can include filtration, disinfection and/or an additional nitrogen removal step.

Biological treatment involves promoting the growth of microorganisms to consume organic matter, nitrify ammonium (NH_4^+) and denitrify nitrate (NO_3^-). The most efficient methods for consuming biodegradable matter involve promoting aerobic microbial systems. This is because aerobic organisms generally grow much faster than anaerobic organisms. Consequently shorter residence times and hence smaller land areas are required. However, denitrification requires anaerobic conditions and so anaerobic environments must also be provided. Two important categories of biological reactors include attached growth reactors and suspended growth reactors.

29.2.1 Attached Growth Reactors

Attached growth reactors involve providing a surface for microorganisms to grow. Two examples commonly applied in the UK include trickling filters and rotating biological contactors.

29.2.1.1 Trickling Filters

Trickling filters have provided biological treatment at municipal wastewater treatment plants for over 100 years [1, p. 890]. They generally comprise a cylindrical casing of between 10 and 20 m in diameter and 2–3 m deep, which is filled with crushed rock or plastic filter media (see Fig. 29.2).

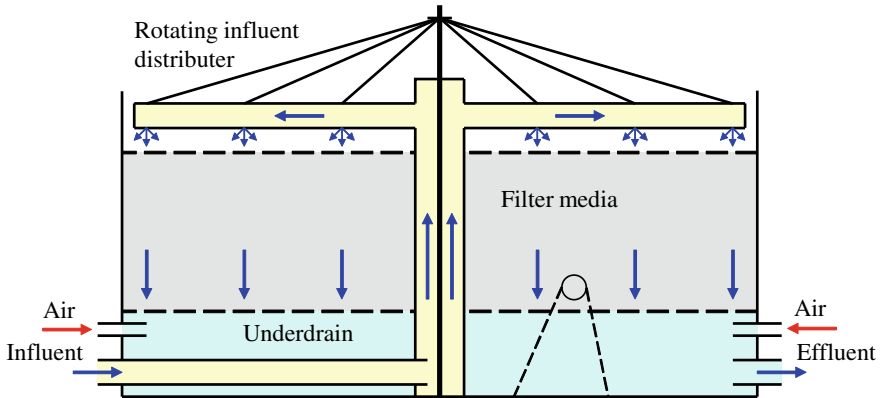
Primary treated effluent (i.e., wastewater after primary clarification) is trickled over the filter media via a set of rotating distributor arms. The water then seeps through the media and is collected from a drain at the base. Air is fed into the base of the filter media to maintain unsaturated conditions.

The filter media provides a surface for biofilm to grow. The biofilm comprises microorganisms that consume the biodegradable matter in the water as it trickles through the filter. The unsaturated conditions provides a high interfacial area between wastewater and air such that aerobic conditions are maintained throughout.

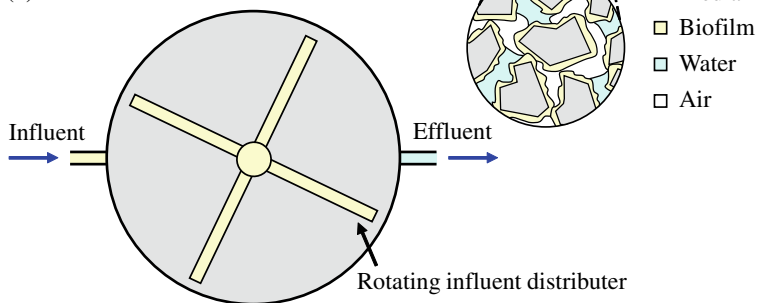
29.2.1.2 Rotating Biological Contactors (RBC)

Rotating biological contactors (RBC) comprise a series of plastic circular media disks that rotate on a horizontal shaft (Fig. 29.3). As the disks rotate, portions of the media are periodically submerged within a primary treated effluent. A biofilm grows on the surface of the disk, fuelled by the BOD in the wastewater. The rotation of

(a) Elevation view



(b) Plan view

**Fig. 29.2** Schematic diagrams describing a trickling filter

the disks enables the biofilm to be periodically exposed to the air such that aerobic conditions can be continuously maintained.

The surface of the disks are carefully designed to maximise the area available for biofilm growth. A 7.5 m length stack of disks of 3.5 m diameter can be expected to have a surface area of around 9300 m² [1, p. 931]. A higher level of treatment (for the same plan area) is expected from RBC as compared to trickling filters due to a longer contact time (8–10 times greater) [2]. Consequently RBC systems are often attractive for dense urban environments.

29.2.1.3 Secondary Clarification

Primary treated effluent is low in SS but high in dissolved BOD. The resulting effluent from a trickling filter or an RBC is low in dissolved BOD but high in SS. The SS comes about due to biofilm sloughing from the media as biofilm grows excessively thick. The sloughed biofilm should subsequently be removed using an additional clarifier referred to as a secondary clarifier.

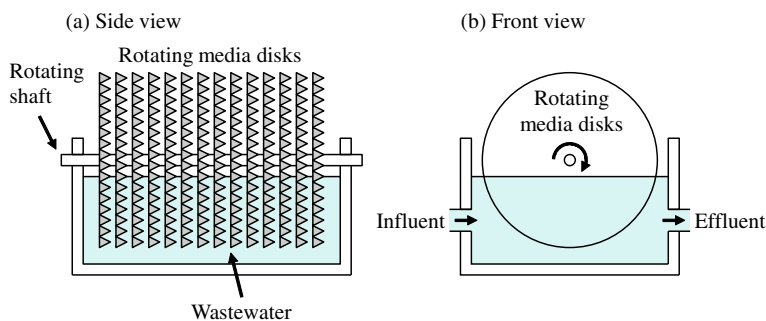


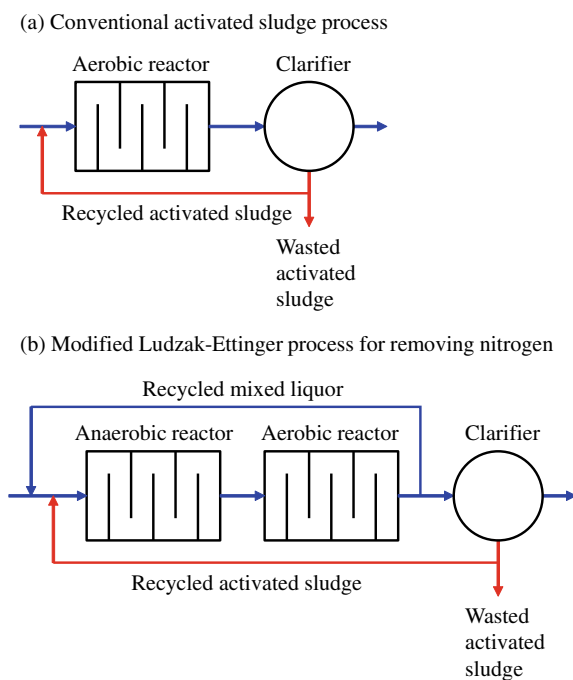
Fig. 29.3 Schematic diagram of a rotating contactor

29.2.2 Suspended Growth Reactors

There are a number of different suspended growth reactor types, but here we will focus on the activated sludge method, whereby an activated mass of microorganisms is developed and maintained to consume biodegradable matter.

A typical scheme is illustrated in Fig. 29.4a. Primary treated wastewater is mixed with recycled activated sludge from a secondary clarifier and then pushed through an aerobic reactor [1, p. 661].

Fig. 29.4 Schematic diagrams describing two typical activated sludge process configurations



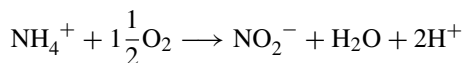
An aerobic reactor typically comprises an open vessel with baffles and air diffusers at the base. The air diffusers maintain aerobic conditions. The baffles maintain “plug flow” conditions such that wastewater is unable to shortcut the system. Microorganisms within the activated sludge grow and reproduce as they consume the BOD. The length of the reactor passage needs to be designed such that sufficient residence time is provided to allow the BOD to reduce to an acceptable level.

The reactor effluent is discharged to a secondary clarifier where the activated sludge is removed. Some of the sludge is sent off for thickening but a portion of the sludge is recycled and sent back to the aerobic reactor inlet, to maintain the microbial population within the reactor.

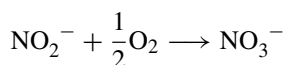
29.2.3 Nitrogen Removal

Nitrogen is present within wastewater as ammonium (NH_4^+), nitrite (NO_2^-) and nitrate (NO_3^-). As mentioned earlier in Chap. 27, nitrate pollution is a problem in natural water systems because it can cause algal blooms and eutrophication. Ammonium is also a problem because it is toxic to fish and can nitrify to form nitrite.

Ammonium is transformed to nitrate alongside aerobic degradation of organic matter in aerobic reactors due to a two stage nitrification process [3, p. 337]. First *Nitrosomonas* bacteria convert ammonium to nitrite

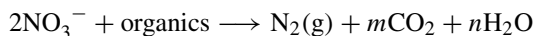


Then *Nitrobacter* bacteria convert nitrite to nitrate



It can therefore be appreciated that effluents from trickling filters, RBC and conventional activated sludge reactors will remain high in NO_3^- .

An anaerobic reactor can be used to convert nitrate to gaseous molecular nitrogen. In the absence of oxygen, denitrifying bacteria use the nitrate as an oxidising agent to consume organic matter [3, p. 338]



Any aerobic reactor facility can be made anaerobic by removing the air supply. In the past, nitrate was often removed by passing the effluent from an aerobic reactor into an anaerobic reactor. However, a problem arises due to there being insufficient organic matter to maintain the denitrifying bacteria.

Another idea is to pass the primary effluent through an anaerobic reactor before using an aerobic reactor. The problem here is that the denitrifying bacteria are not exposed to NO_3^- formed as a result of nitrification in the aerobic reactor.

The so-called modified Ludzak-Ettinger process [1, p. 791] seeks to overcome this latter problem by mixing a portion of the aerobic reactor effluent with the primary treated influent (Fig. 29.4b). See Tchobanoglous et al [1, p. 749] for details about additional methods for removing nitrogen in this way.

29.2.4 Waste Stabilization Ponds

Many secondary and tertiary treatment objectives can be achieved in simple waste stabilization ponds (WSP). Shallow ponds naturally aerate and the UV from the sun can act as a natural disinfectant. Deep ponds will quickly develop anaerobic conditions such that denitrification will occur and nitrates are removed. WSP retention times to meet some WHO standards are provided in Table 29.1.

WSP are considerably cheaper to construct and operate as compared to conventional wastewater treatment methods (see Table 29.2). However, WSP require considerably more land area to be effective. WSPs become a preferable option when land prices are below 15–20 USD₂₀₁₀ m⁻² [4].

29.2.5 Sludge Disposal and Reuse

Solid material from screening and grit removal is normally sent to landfill. However, the sludge removed from both the primary and secondary clarifiers is very high in organic content and can therefore be exploited as both an energy resource and/or a soil conditioner.

The first stage is to thicken the sludge, normally by centrifugal dewatering [1, p. 1559]. The sludge is then sent to a sealed vessel where it is kept warm under anaerobic conditions for anaerobic digestion [1, p. 1505]. Anaerobic microorganisms digest the organic matter by methanogenesis, which results in the production of methane (CH₄) and CO₂. The CH₄ is normally passed onto an on-site generator where heat and power are co-generated for use around the wastewater treatment plant.

The remaining sludge is further dewatered, sometimes in greenhouses [1, p. 1576], and the final product can be reused as an alternative fuel or as a soil conditioner.

Table 29.1 Required WSP retention times for different parameters regarding WHO standards [4]

Parameter	Residence time (days)
BOD	5
Coliform bacteria	16
Nematode eggs	18

Table 29.2 Capital (capex) and annual operation and maintenance (opex) costs of various wastewater treatment processes for a population of 1000 in France in 1997 [5]

Treatment process	Capex (€ ₁₉₉₇ capita ⁻¹)	Annual opex (€ ₁₉₉₇ capita ⁻¹)
Trickling filter	180	7.00
Rotating biological contactor	220	7.00
Activated sludge	230	11.50
Waste stabilization ponds	120	4.50

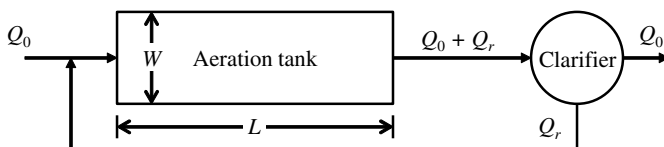
Sludge products often contain high levels of pathogenic organisms. Therefore, rules about how such products can be used for agriculture are very strict so as to avoid the transferring of pathogens back into the food chain (e.g., [6]).

29.3 Activated Sludge Theory

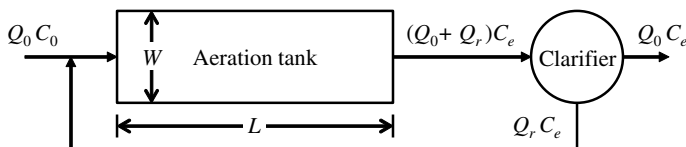
Consider the simplified activated sludge system illustrated in Fig. 29.5. Effluent from a primary clarifier is discharged at a constant rate of Q_0 [L^3T^{-1}] with a dissolved BOD concentration of C_0 [ML^{-3}]. The water is mixed with sludge from a secondary clarifier, which is provided at a constant rate of Q_r [L^3T^{-1}] with a dissolved BOD concentration of C_e [ML^{-3}] and an active microbial mass concentration of X_r [ML^{-3}]. Water exits the aeration tank at a constant rate of $Q_0 + Q_r$ [L^3T^{-1}] with a dissolved BOD concentration of C_e [ML^{-3}] and an active microbial mass concentration of X_e [ML^{-3}].

In what follows we will develop the necessary equations to design various aspects of the above system according to various engineering criteria of interest. The first step is to form conservation equations for BOD and microbial mass. These equations are coupled using a Monod growth rate equation and solved assuming completely mixed conditions. A linearisation is then introduced to allow incomplete mixing conditions

(a) Mass conservation for water



(b) Mass conservation for BOD



(c) Mass conservation for microorganisms

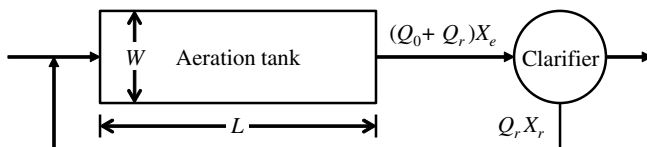


Fig. 29.5 Mass conservation diagrams for an activated sludge system

to be considered using the advection dispersion equation. Boundary conditions are defined and an analytical solution is derived. It is then shown how to obtain the two extreme cases of plug flow conditions and completely mixed conditions. Plug flow conditions is shown to be a more favourable situation. Finally an empirical equation is provided to estimate dispersion coefficients in aeration tanks, which can be used to assess the extent to which plug flow conditions are reached.

29.3.1 Mass Conservation Statements

Under steady-state conditions, mass conservation for BOD within the aeration tank dictates that

$$Q_0 C_0 + Q_r C_e - (Q_0 + Q_r) C_e - A \int_0^L r_c dx = 0 \quad (29.1)$$

where A [L^2] and L [L] are the flowing cross-sectional area and length of the aeration tank, respectively, x [L] is distance along the aeration tank and r_c [$ML^{-3}T^{-1}$] is the microbial consumption rate of BOD within the aeration tank.

Mass conservation for active microorganisms within the aeration tank dictates that

$$Q_r X_r - (Q_0 + Q_r) X_e + A \int_0^L (r_g - r_d) dx = 0 \quad (29.2)$$

where r_g [$ML^{-3}T^{-1}$] and r_d [$ML^{-3}T^{-1}$] are the growth and death rates of microorganisms within the aeration tank, respectively.

The consumption, growth and death rates are all assumed to be first-order kinetic processes. It follows that

$$r_c = k_c C \quad (29.3)$$

$$r_g = k_g X \quad (29.4)$$

and

$$r_d = k_d X \quad (29.5)$$

where k_c [T^{-1}], k_g [T^{-1}] and k_d [T^{-1}] are the BOD consumption rate coefficient, microbial growth rate coefficient and microbial death rate coefficient, respectively, C [ML^{-3}] is the dissolved BOD concentration in the aeration tank and X [ML^{-3}] is the active microbial mass concentration in the aeration tank.

29.3.2 Monod Equation

The growth rate of microorganisms is dependent on many different properties including BOD, DO, temperature and pH. Biodegradable matter associated with BOD is required to provide food for the microbes to consume. DO is required to enable the microbes to perform aerobic respiration. For aerobic reactors, DO is maintained at

high levels throughout by using mechanical aerators. The objective is to provide an optimal environment such that BOD is the only significant limiting factor for growth. The limiting nature of BOD can be incorporated mathematically using an empirical Monod equation, attributed to the French 20th century biochemist, Jacques Monod.

An appropriate Monod equation takes the form [7, p. 194]

$$k_g = \frac{k_{g,\max} C}{K_c + C} \quad (29.6)$$

where $k_{g,\max}$ [T^{-1}] represents the maximum possible microbial growth rate coefficient and K_c [ML^{-3}] is the half-velocity constant for BOD.

The assumption here is that microbial growth is only limited by availability of biodegradable matter associated with BOD. If an infinite supply of biodegradable matter is available then $k_g = k_{g,\max}$, hence $k_{g,\max}$ is referred to as the maximum possible growth rate coefficient. If $C = K_c$ then $k_g = k_{g,\max}/2$, hence K_c is referred to as a half-velocity constant for BOD. If $C = 0$ then $k_g = 0$ because there is no biodegradable matter available for the microorganisms to feed on.

The Monod equation, Eq. (29.6), leads to a coupling of the mass conservation statement for microorganisms, Eq. (29.2), with the mass conservation statement for BOD, Eq. (29.1). The latter is coupled to the microorganisms conservation statement by virtue of the yield coefficient, β [-], which represents the mass of BOD consumed per unit mass of microorganisms formed. In this way, it can be said that

$$r_c = \beta r_g. \quad (29.7)$$

29.3.3 Completely Mixed Conditions

When modelling chemical transport in reactor vessels it is common to differentiate between plug flow and completely mixed conditions. Under plug flow conditions, fluid particles in reactor vessels travel along parallel and identical pathways such that each particle spends the same amount of time in the reactor vessel. This leads to the mass concentration of reactive chemicals gradually varying (due to reaction processes) with distance along a reactor vessel, from the influent concentration, C_i , to the effluent concentration, C_e (see the “Plug flow” line in Fig. 29.6).

The effect of mixing within a reactor causes pathways to become chaotic with some particles experiencing much shorter residence times than others. A consequence of this mixing is that mass concentrations immediately drop below the influent concentration on entry within the reactor (see the “non-Plug flow” lines in Fig. 29.6).

The extent of mixing is often expressed through the Peclet number, Pe [-], which represents the ratio of fluid velocity to chemical dispersion (see Sect. 6.6.3). Plug flow conditions occur when $Pe \rightarrow \infty$. As the Pe number becomes progressively smaller, the system can be considered to be more vigorously mixed. Completely mixed conditions occur when $Pe \rightarrow 0$ and represents a scenario where mixing is sufficiently vigorous such that mass concentration, throughout a reactor vessel, is equal to the mass concentration of the reactor effluent (see the “Completely mixed” line in Fig. 29.6).

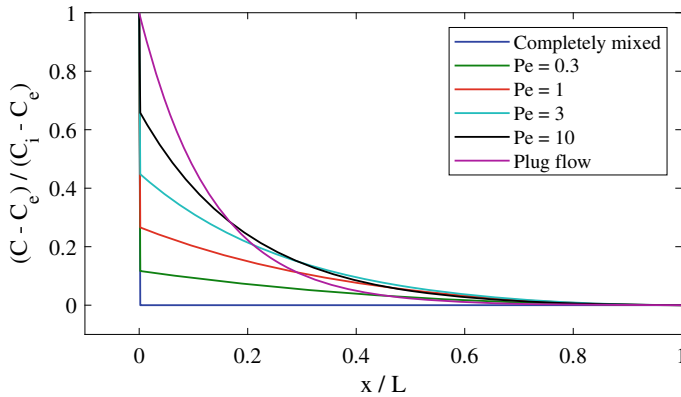


Fig. 29.6 Plot of normalised mass concentration, C , against distance, x , along a reactor vessel of length, L , for different Peclet numbers, Pe . Note that C_i and C_e represent the influent and effluent concentrations, respectively

Combining the conservation equations in Sect. 29.3.1 with the Monod equation in Sect. 29.3.2 leads to a non-linear set of equations, which are very difficult to solve analytically. However, if we assume completely mixed conditions, mass concentrations within the reactor will be constant with distance and equal to the corresponding mass concentrations in the reactor effluent, leading to a significantly simplified mathematical problem.

29.3.3.1 Consumption Rate Coefficient

Challenge 29.1 Assume completely mixed conditions and use the set of equations, given in Sects. 29.3.1 and 29.3.2, to determine a useful expression for the consumption rate coefficient, k_c , that is free of X_e terms.

For a completely mixed reactor, $C = C_e$ and $X = X_e$ for $x \in (0, L]$ such that Eqs. (29.3)–(29.6) reduce to:

$$r_c = k_c C_e \quad (29.8)$$

$$r_g = k_g X_e \quad (29.9)$$

$$r_d = k_d X_e \quad (29.10)$$

$$k_g = \frac{k_{g,\max} C_e}{K_c + C_e} \quad (29.11)$$

Substituting Eq. (29.11) into Eq. (29.9) leads to

$$r_g = \frac{k_{g,\max} C_e X_e}{K_c + C_e} \quad (29.12)$$

Substituting Eq. (29.12) into Eq. (29.7) gives us

$$r_c = \frac{\beta k_{g,\max} C_e X_e}{K_c + C_e} \quad (29.13)$$

The X_e terms can be eliminated by considering Eq. (29.2). Substituting Eqs. (29.7) and (29.10) into Eq. (29.2) leads to

$$Q_r X_r - (Q_0 + Q_r) X_e + A \int_0^L \left(\frac{r_c}{\beta} - k_d X_e \right) dx = 0 \quad (29.14)$$

The completely mixed conditions implies that everything within the integral term of Eq. (29.14) is constant and therefore

$$Q_r X_r - (Q_0 + Q_r) X_e + AL \cdot \left(\frac{r_c}{\beta} - k_d X_e \right) = 0 \quad (29.15)$$

Solving Eq. (29.15) for X_e gives us

$$X_e = \frac{Q_r X_r + \frac{V r_c}{\beta}}{Q_0 + Q_r + V k_d} \quad (29.16)$$

where $V = AL [L^3]$ is the volume of the aeration tank.

Substituting Eq. (29.16) into Eq. (29.13) gives us

$$r_c = \frac{k_{g,\max} C_e \cdot (\beta Q_r X_r + V r_c)}{(K_c + C_e)(Q_0 + Q_r + V k_d)} \quad (29.17)$$

Solving Eq. (29.17) for r_c leads to

$$r_c = \frac{k_{g,\max} C_e \beta Q_r X_r}{(Q_0 + Q_r + V k_d) K_c + (Q_0 + Q_r + V \cdot (k_d - k_{g,\max})) C_e} \quad (29.18)$$

Equating Eqs. (29.8) with (29.18) gives us

$$k_c = \frac{k_{g,\max} \beta Q_r X_r}{(Q_0 + Q_r + V k_d) K_c + (Q_0 + Q_r + V \cdot (k_d - k_{g,\max})) C_e} \quad (29.19)$$

Further insight can be gained by making the substitutions

$$k_{c0} = \frac{k_{g,\max} \beta Q_r X_r}{(Q_0 + Q_r + V k_d) K_c} \quad (29.20)$$

and

$$\varepsilon = \left(1 - \frac{V k_{g,\max}}{Q_0 + Q_r + V k_d} \right) \frac{C_0}{K_c} \quad (29.21)$$

such that Eq. (29.19) reduces to

$$k_c = \frac{k_{c0}}{1 + \varepsilon \frac{C_e}{C_0}} \quad (29.22)$$

Noting that $\frac{1}{1+x} = 1 - x + x^2 + O(x^3)$, it can be further stated that

$$k_c = k_{c0} + O(\varepsilon) \quad (29.23)$$

29.3.3.2 Solving for Effluent Concentration

Challenge 29.2 Derive an analytical solution for the effluent BOD concentration.

Substituting Eq. (29.22) into Eq. (29.8) and then substituting the result into Eq. (29.1) leads to

$$Q_0(C_0 - C_e) - \frac{Vk_{c0}C_e}{1 + \varepsilon \frac{C_e}{C_0}} = 0 \quad (29.24)$$

Equation (29.24) can be rearranged into the following quadratic equation

$$\varepsilon \left(\frac{C_e}{C_0} \right)^2 + (1 + \gamma - \varepsilon) \frac{C_e}{C_0} - 1 = 0 \quad (29.25)$$

where

$$\gamma = \frac{Vk_{c0}}{Q_0} \quad (29.26)$$

The positive root of Eq. (29.25) is found from

$$\frac{C_e}{C_0} = \frac{-(1 + \gamma - \varepsilon) + \sqrt{(1 + \gamma - \varepsilon)^2 + 4\varepsilon}}{2\varepsilon} \quad (29.27)$$

which can be expanded for small ε to get

$$\frac{C_e}{C_0} = \frac{1}{1 + \gamma} + O(\varepsilon) \quad (29.28)$$

29.3.4 Incompletely Mixed Conditions

Under incompletely mixed conditions, transport of BOD can be described using an advection dispersion equation (similar to Eq. 26.13) with a reaction term due to microbial consumption as follows

$$\frac{\partial C}{\partial t} = -\nabla \cdot (\mathbf{u}C - \mathbf{K}\nabla C) - r_c \quad (29.29)$$

where t [T] is time, $\mathbf{u}$ [LT^{-1}] is the fluid velocity vector and $\mathbf{K}$ [L^2T^{-1}] is the dispersion tensor.

For simplicity, we will assume that $\varepsilon \ll 1$ such that

$$r_c = k_{c0}C \quad (29.30)$$

where k_{c0} is the zeroth-order consumption rate coefficient defined by Eq. (29.20).

Substituting Eq. (29.30) into Eq. (29.29) gives us

$$\frac{\partial C}{\partial t} = -\nabla \cdot (\mathbf{u}C - \mathbf{K}\nabla C) - k_{c0}C \quad (29.31)$$

29.3.4.1 Danckwerts' Boundary Conditions

If we assume steady-state conditions and that the reactor is completely mixed in the y and z directions but incompletely mixed in the x direction, Eq. (29.31) reduces to

$$K_{xx} \frac{d^2 C}{dx^2} - u \frac{dC}{dx} - k_{c0} C = 0 \quad (29.32)$$

where K_{xx} [$L^2 T^{-1}$] is the dispersion coefficient in the x direction and u [LT^{-1}] is the velocity in the x direction, found from

$$u = \frac{Q_0 + Q_r}{A} \quad (29.33)$$

Writing Eq. (29.32) in a mass conservative form gives us

$$0 = \frac{dJ_x}{dx} + k_{c0} C \quad (29.34)$$

where J_x [$ML^{-2}T^{-1}$] is the mass flux of BOD, found from

$$J_x = uC - K_{xx} \frac{dC}{dx} \quad (29.35)$$

The dispersion is caused by turbulent mixing. However, at the inlet and outlet of the reactor, all the flow paths are brought together through a narrow pipe, which significantly reduces the effect of dispersion (see Fig. 29.7). It is therefore common to assume that dispersion is negligible at the boundaries. Consequently, at the reactor inlet (i.e., $x = 0$) it can be stated that $J_x = uC_i$, where C_i [ML^{-3}] is the BOD of the incoming fluid. At the reactor outlet (i.e., $x = L$) it can be simply stated that $J_x = uC$. The resulting set of boundary conditions are

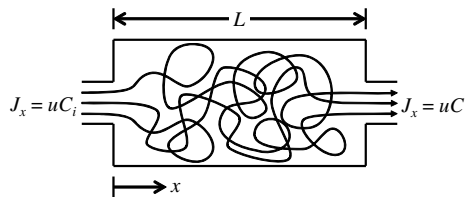
$$\begin{aligned} uC - K_{xx} \frac{dC}{dx} &= uC_i, & x = 0 \\ \frac{dC}{dx} &= 0, & x = L \end{aligned} \quad (29.36)$$

The BOD of the incoming fluid is found from

$$C_i = \frac{Q_0 C_0 + Q_r C_e}{Q_0 + Q_r} \quad (29.37)$$

The boundary conditions asserted in Eq. (29.36) are often referred to as Danckwerts' boundary conditions and attributed to Danckwerts [8].

Fig. 29.7 Schematic diagram illustrating Danckwerts' idea that flow pathways are brought together at the inlet and outlet of a reactor



29.3.4.2 General Solution

Challenge 29.3 Derive a general solution for Eq. (29.32).

The general solution of an ordinary differential equation of the form

$$a \frac{d^2 y}{dx^2} + b \frac{dy}{dx} + cy = 0 \quad (29.38)$$

is [9, p. 1093]

$$y(x) = A_1 \exp \left[\left(\frac{-b + \sqrt{b^2 - 4ac}}{2a} \right) x \right] + A_2 \exp \left[\left(\frac{-b - \sqrt{b^2 - 4ac}}{2a} \right) x \right] \quad (29.39)$$

where A_1 and A_2 are unknown constants defined by any associated boundary conditions.

By comparing Eqs. (29.32) and (29.38) it can be understood that $a = K_{xx}$, $b = -u$ and $c = -k_{c0}$. The general solution for Eq. (29.32) is therefore

$$C = A_1 e^{m_1 x} + A_2 e^{m_2 x} \quad (29.40)$$

where

$$m_1 = \frac{u + \sqrt{u^2 + 4K_{xx}k_{c0}}}{2K_{xx}} \quad \text{and} \quad m_2 = \frac{u - \sqrt{u^2 + 4K_{xx}k_{c0}}}{2K_{xx}} \quad (29.41)$$

29.3.4.3 Application of Boundary Conditions

Challenge 29.4 Apply the boundary conditions in Eq. (29.36) to find expressions for the two integration constants in Eq. (29.40).

Differentiating both sides of Eq. (29.40) yields

$$\frac{dC}{dx} = A_1 m_1 e^{m_1 x} + A_2 m_2 e^{m_2 x} \quad (29.42)$$

Substituting Eq. (29.42) into the $x = L$ boundary condition, given in Eq. (29.36), and solving for A_2 leads to

$$A_2 = -\frac{m_1}{m_2} e^{(m_1 - m_2)L} A_1 \quad (29.43)$$

Substituting Eq. (29.43) into Eqs. (29.40) and (29.42) gives us

$$C = A_1 \left[e^{m_1 x} - \frac{m_1}{m_2} e^{(m_1 - m_2)L} e^{m_2 x} \right] \quad (29.44)$$

and

$$\frac{dC}{dx} = A_1 m_1 \left[e^{m_1 x} - e^{(m_1 - m_2)L} e^{m_2 x} \right] \quad (29.45)$$

respectively.

Substituting Eqs. (29.44) and (29.45) into the $x = 0$ boundary condition, given in Eq. (29.36), leads to

$$uA_1 \left[1 - \frac{m_1}{m_2} e^{(m_1-m_2)L} \right] - K_{xx}A_1m_1 \left[1 - e^{(m_1-m_2)L} \right] = uC_i \quad (29.46)$$

Solving Eq. (29.46) for A_1 gives us

$$A_1 = \frac{C_i}{1 - \frac{K_{xx}m_1}{u} - \left(\frac{m_1}{m_2} - \frac{K_{xx}m_1}{u} \right) e^{(m_1-m_2)L}} \quad (29.47)$$

29.3.4.4 Definition of Peclet Number

Now consider the substitutions

$$a = \sqrt{1 + \frac{4\gamma_i}{\text{Pe}}}, \quad \gamma_i = \frac{Lk_{c0}}{u} \quad \text{and} \quad \text{Pe} = \frac{uL}{K_{xx}} \quad (29.48)$$

From Eq. (29.41) it can be said that

$$\frac{K_{xx}m_1}{u} = \frac{1+a}{2}, \quad \frac{m_1}{m_2} = \frac{1+a}{1-a}, \quad (m_1 - m_2)L = a\text{Pe}$$

Substituting the above expressions into Eqs. (29.43) and (29.47) leads to

$$A_2 = - \left(\frac{1+a}{1-a} \right) e^{a\text{Pe}} A_1 \quad (29.49)$$

and

$$A_1 = \frac{C_i}{\left[\frac{1+a}{2} - \left(\frac{1+a}{1-a} \right) \right] e^{a\text{Pe}} + \frac{1-a}{2}} \quad (29.50)$$

respectively.

The dimensionless Pe term is referred to as the Peclet number. It represents the ratio of advection to dispersion. A small Peclet number means that the system is dominated by dispersion. A large Peclet number means that the system is dominated by advection. The limiting case when $\text{Pe} \rightarrow \infty$ represents plug flow conditions. The limiting case when $\text{Pe} \rightarrow 0$ represents completely mixed conditions.

29.3.4.5 Analytical Solution for the Effluent BOD

Challenge 29.5 Derive a simplified equation for the effluent concentration of an incompletely mixed reactor.

An analytical solution for the effluent BOD is obtained by setting $x = L$. Substituting Eqs. (29.50) and (29.49) into Eq. (29.40) and setting $x = L$ leads to

$$\frac{C_e}{C_i} = \frac{1}{\left[\frac{1+a}{2} - \left(\frac{1+a}{1-a} \right) \right] e^{a\text{Pe}} + \frac{1-a}{2}} \left[e^{\frac{(1+a)\text{Pe}}{2}} - \left(\frac{1+a}{1-a} \right) e^{a\text{Pe}} e^{\frac{(1-a)\text{Pe}}{2}} \right] \quad (29.51)$$

After some further rearrangement it can be shown that [8]

$$\frac{C_e}{C_i} = \frac{4a}{(1+a)^2 e^{-\frac{(1-a)\text{Pe}}{2}} - (1-a)^2 e^{-\frac{(1+a)\text{Pe}}{2}}} \quad (29.52)$$

29.3.5 Limiting Cases

29.3.5.1 Plug Flow Conditions

Challenge 29.6 Use the expansion, $\sqrt{1+x} = 1 + \frac{x}{2} + O(x^2)$, to determine the limit of Eq. (29.52) for plug flow conditions.

Under plug flow conditions, $Pe \rightarrow \infty$. Given that $\sqrt{1+x} = 1 + \frac{x}{2} + O(x^2)$, the a term in Eq. (29.48) can be expanded to get

$$a = 1 + \frac{2\gamma_i}{Pe} + O\left(\frac{1}{Pe^2}\right) \quad (29.53)$$

Substituting Eq. (29.53) into Eq. (29.52) gives us

$$\frac{C_e}{C_i} = \frac{4\left[1 + \frac{2\gamma_i}{Pe} + O\left(\frac{1}{Pe^2}\right)\right]}{\left[2 + \frac{2\gamma_i}{Pe} + O\left(\frac{1}{Pe^2}\right)\right]^2 e^{\gamma_i + O\left(\frac{1}{Pe}\right)} - \left[\frac{2\gamma_i}{Pe} + O\left(\frac{1}{Pe^2}\right)\right]^2 e^{-Pe - \gamma_i + O\left(\frac{1}{Pe}\right)}}$$

from which it follows that

$$\lim_{Pe \rightarrow \infty} \left\{ \frac{C_e}{C_i} \right\} = e^{-\gamma_i} \quad (29.54)$$

29.3.5.2 Completely Mixed Conditions

Challenge 29.7 Use the expansion, $\sqrt{1+x} = \sqrt{x} + O\left(\frac{1}{\sqrt{x}}\right)$, to determine the limit of Eq. (29.52) for completely mixed conditions.

Under completely mixed conditions, $Pe \rightarrow 0$. Given that $\sqrt{1+x} = \sqrt{x} + O\left(\frac{1}{\sqrt{x}}\right)$, the a term in Eq. (29.48) can be expanded to get

$$a = \sqrt{\frac{4\gamma_i}{Pe}} + O\left(\sqrt{Pe}\right) \quad (29.55)$$

Substituting Eq. (29.55) into Eq. (29.52) gives us

$$\begin{aligned} \frac{C_e}{C_i} &= \frac{4\left[\sqrt{\frac{4\gamma_i}{Pe}} + O\left(\sqrt{Pe}\right)\right]}{\left[1 + \sqrt{\frac{4\gamma_i}{Pe}} + O\left(\sqrt{Pe}\right)\right]^2 e^{\sqrt{\gamma_i Pe} + O(Pe)} - \left[1 - \sqrt{\frac{4\gamma_i}{Pe}} + O\left(\sqrt{Pe}\right)\right]^2 e^{-\sqrt{\gamma_i Pe} + O(Pe)}} \\ &= \frac{4\left[\sqrt{\frac{4\gamma_i}{Pe}} + O\left(\sqrt{Pe}\right)\right]}{\left[1 + \sqrt{\frac{4\gamma_i}{Pe}} + O\left(\sqrt{Pe}\right)\right]^2 \left[1 + \sqrt{\gamma_i Pe} + O(Pe)\right] - \left[1 - \sqrt{\frac{4\gamma_i}{Pe}} + O\left(\sqrt{Pe}\right)\right]^2 \left[1 - \sqrt{\gamma_i Pe} + O(Pe)\right]} \end{aligned}$$

$$\begin{aligned}
&= \frac{8\sqrt{\frac{\gamma_i}{\text{Pe}}} + O(\sqrt{\text{Pe}})}{\left[1 + 4\sqrt{\frac{\gamma_i}{\text{Pe}}} + \frac{4\gamma_i}{\text{Pe}}\right] \left[1 + \sqrt{\gamma_i \text{Pe}}\right] - \left[1 - 4\sqrt{\frac{\gamma_i}{\text{Pe}}} + \frac{4\gamma_i}{\text{Pe}}\right] \left[1 - \sqrt{\gamma_i \text{Pe}}\right] + O(\text{Pe})} \\
&= \frac{8\sqrt{\frac{\gamma_i}{\text{Pe}}} + O(\sqrt{\text{Pe}})}{8(1 + \gamma_i)\sqrt{\frac{\gamma_i}{\text{Pe}}} + O(\sqrt{\text{Pe}})}
\end{aligned}$$

from which it follows that

$$\lim_{\text{Pe} \rightarrow 0} \left\{ \frac{C_e}{C_i} \right\} = \frac{1}{1 + \gamma_i} \quad (29.56)$$

Also note that if we substitute Eqs. (29.26) and (29.33) into the expression for γ_i in Eq. (29.48) we get

$$\gamma_i = \frac{Q_0 \gamma}{Q_0 + Q_r} \quad (29.57)$$

Substituting both Eqs. (29.37) and (29.57) into Eq. (29.56) then leads to Eq. (29.28).

29.3.5.3 Comparison of Limits

It is interesting to compare the plug flow and completely mixed models to see which is more efficient for BOD removal. Noting that

$$e^{-\gamma_i} = \frac{1}{e^{\gamma_i}} = \frac{1}{1 + \gamma_i + \frac{\gamma_i^2}{2} + O(\gamma_i^3)}$$

it can be understood that the plug flow mode provides more efficient removal for the same γ_i value.

Plug flow conditions are often encouraged within activated sludge reactors so as to promote more efficient treatment. The reason that completely mixed conditions are less beneficial in this respect is that the mixing leads to fluid particles short-cutting across the reactor, reducing the time they spend experiencing treatment.

Plug flow conditions can be encouraged by providing baffles within the reactor (as illustrated in Fig. 29.4) such that fluid has to “snake” through the reactor and has less opportunity to mix. Perfect plug flow conditions are impossible to obtain. However, Eq. (29.52) can be used to estimate how close a system is to plug flow conditions for a given Peclet number. Below, we will look at a simple empirical model that can be used to estimate the Peclet number for a given rectangular open channel reactor.

29.3.6 Dispersion Coefficient Estimation

The longitudinal dispersion coefficient, K_{xx} , for an aeration tank can be estimated, in m^2s^{-1} , using the following empirical correlation due to [10]

$$K_{xx} = \frac{2}{3} \left(\frac{H}{H + W} \right) \sqrt{\frac{Q_G W_d (L + W)}{2L}} \quad (29.58)$$

where H (m) is the water depth in the aeration tank, W (m) is the width of the channel, L (m) is the length of the channel, W_d (m) is the width of the air diffuser and Q_G ($\text{m}^3 \text{s}^{-1}$) is the air injection rate. In many cases it can be assumed that $W_d = W$.

The required air injection rate is a function of the rate at which BOD is to be removed within the aeration tank. [11, p. 596] suggests that around 46.1 m^3 of air is required for every kg of BOD_5 to be removed. [11] also recommend using an additional safety factor of 2. Therefore, a conservative air injection rate should typically provide 92.2 m^3 of air for every kg of BOD_5 to be removed.

29.4 Problem Sheet

Problem 29.1 (see Worked Solution 29.1)

A primary clarifier produces a clear effluent at a rate of 18.9 Ml day^{-1} with a BOD_5 of 250 mg l^{-1} . An activated sludge aeration tank is required to reduce the BOD_5 to 7.4 mg l^{-1} . The effluent from the primary clarifier is to be mixed with recycled sludge collected from a subsequent secondary clarifier, which is supplied at rate of 14.3 Ml day^{-1} .

The recycled sludge contains 8000 mg of microorganisms per litre. Microbial growth within the aeration tank is described by the Monod equation given in Eq. (29.6). The maximum growth rate coefficient is 2 day^{-1} . The death rate coefficient is 0.06 day^{-1} . The half-velocity constant for BOD_5 is 84.6 mg l^{-1} . The yield coefficient is 1.54 mg BOD_5 per mg of microorganisms. No baffles are to be provided within the tank such that completely mixed conditions are assumed to apply.

- (a) Determine the minimum volume of aeration tank required.
- (b) Determine the concentration of microorganisms that would be expected within such an aeration tank.
- (c) Determine the BOD_5 of the same aeration tank effluent if the rate at which recycled sludge is supplied is reduced to 2 Ml day^{-1} .

Problem 29.2 (see Worked Solution 29.2)

Repeat the analysis in Problem 29.1 but assuming $\varepsilon = 0$.

Problem 29.3 (see Worked Solution 29.3)

Consider again the scenario described by Problem 29.2 (c). It turns out that the reactor channel water depth is 4 m and the air injection takes place at a constant rate of 400 Ml day^{-1} through an evenly spaced array of diffusers.

(a) Write a MATLAB programme to calculate the expected effluent BOD_5 assuming incomplete mixing with the following reactor channel widths: 80 m, 40 m, 20 m, 10 m, 5 m, 2 m and 1 m. You can assume that $r_c = k_{c0}C$ where k_{c0} is defined by Eq. (29.20).

(b) Compare your results with those that you would expect assuming plug flow conditions.

Problem 29.4 (see Worked Solution 29.4)

Estimate the size of waste stabilisation pond required to produce a similar level of treatment as provided by the activated sludge facility described in Problem 29.1.

29.5 Worked Solutions**Worked Solution 29.1** (see Problem 29.1)

(a) Substituting Eq. (29.18) into Eq. (29.1) leads to

$$Q_0(C_0 - C_e) - \frac{V k_{g,\max} C_e \beta Q_r X_r}{(Q_0 + Q_r + V k_d) K_c + (Q_0 + Q_r + V \cdot (k_d - k_{g,\max})) C_e} = 0$$

Solving for V then yields

$$V = \frac{Q_0(C_0 - C_e)(K_c + C_e)(Q_0 + Q_r)}{k_{g,\max} C_e \beta Q_r X_r - Q_0(C_0 - C_e)[(K_c + C_e)k_d - k_{g,\max} C_e]}$$

Let $Q_0 = 18,900 \text{ m}^3 \text{ day}^{-1}$, $C_0 = 250 \text{ mg l}^{-1}$, $C_e = 7.4 \text{ mg l}^{-1}$, $Q_r = 14,300 \text{ m}^3 \text{ day}^{-1}$, $X_r = 8000 \text{ mg l}^{-1}$, $k_{g,\max} = 2 \text{ day}^{-1}$, $k_d = 0.06 \text{ day}^{-1}$, $K_c = 84.6 \text{ mg l}^{-1}$ and $\beta = 1.54$. It follows that $V = 5285 \text{ m}^3$ or 5.29 Ml .

(b) Substituting Eq. (29.18) into (29.16) leads to

$$X_e = \frac{(K_c + C_e) Q_r X_r}{(Q_0 + Q_r + V k_d)(K_c + C_e) - V k_{g,\max} C_e}$$

Using the values from part (a) above it is then found that $X_e = 3502 \text{ mg l}^{-1}$. So the concentration of microorganisms in the aeration tank is 3500 mg l^{-1} .

(c) Now the volume of the aeration tank is determined, we can use Eq. (29.27) to calculate the effluent BOD₅ that would be expected if Q_r is reduced to 2 Ml day^{-1} .

Substituting Eq. (29.20) into Eq. (29.26) leads to

$$\gamma = \frac{V k_{g,\max} \beta Q_r X_r}{Q_0(Q_0 + Q_r + V k_d) K_c} = 7.677$$

and from Eq. (29.21)

$$\varepsilon = \left(1 - \frac{V k_{g,\max}}{Q_0 + Q_r + V k_d} \right) \frac{C_0}{K_c} = 1.483$$

such that Eq. (29.27) yields

$$C_e = C_0 \left[\frac{-(1 + \gamma - \varepsilon) + \sqrt{(1 + \gamma - \varepsilon)^2 + 4\varepsilon}}{2\varepsilon} \right] = 33.81$$

So the effluent BOD₅ would be raised to 33.8 mg l^{-1} .

Worked Solution 29.2 (see Problem 29.2)

(a) If we assume that $\varepsilon = 0$ then the volume of the tank required can be determined from Eq. (29.28). Substituting Eq. (29.20) into Eq. (29.26) and then substituting the result into Eq. (29.28) leads to

$$C_e = \frac{C_0}{1 + \frac{V k_{g,\max} \beta Q_r X_r}{Q_0(Q_0 + Q_r + V k_d) K_c}} \quad (29.59)$$

Solving for V then leads to

$$V = \frac{Q_0(Q_0 + Q_r) K_c (C_0 - C_e)}{k_{g,\max} \beta Q_r X_r C_e - Q_0 k_d K_c (C_0 - C_e)}$$

Let $Q_0 = 18,900 \text{ m}^3 \text{ day}^{-1}$, $C_0 = 250 \text{ mg l}^{-1}$, $C_e = 7.4 \text{ mg l}^{-1}$, $Q_r = 14,300 \text{ m}^3 \text{ day}^{-1}$, $X_r = 8000 \text{ mg l}^{-1}$, $k_{g,\max} = 2 \text{ day}^{-1}$, $k_d = 0.06 \text{ day}^{-1}$, $K_c = 84.6 \text{ mg l}^{-1}$ and $\beta = 1.54$. It follows that $V = 4984 \text{ m}^3$ or 4.98 Ml .

(b) The concentration of microorganisms in the reactor is found from Eq. (29.16) where $r_c = k_c C_e$. But recall from Eq. (29.22), if $\varepsilon = 0$, $k_c = k_{c0}$, which is found from Eq. (29.20). Substituting Eq. (29.20) into $r_c = k_{c0} C_e$ and then substituting the result into Eq. (29.16) leads to

$$X_e = \frac{[(Q_0 + Q_r + V k_d) K_c + V k_{g,\max} C_e] Q_r X_r}{(Q_0 + Q_r + V k_d)^2 K_c}$$

Using the values from part (a) above it is then found that $X_e = 3504 \text{ mg l}^{-1}$. So the concentration of microorganisms in the aeration tank is 3500 mg l^{-1} .

(c) Now the volume of the aeration tank is determined, we can use Eq. (29.59) to calculate the effluent BOD₅ that would be expected if Q_r is reduced to 2 Ml day^{-1} . It is found that, using all the values previously specified in part (a) above, whilst also setting $V = 4894 \text{ m}^3$ and $Q_r = 2000 \text{ m}^3 \text{ day}^{-1}$, the effluent BOD₅ is 30.3 mg l^{-1} .

Comparing the results between Problems 29.1 and 29.2 above demonstrates that assuming $\varepsilon = 0$ leads to an underestimate in the volume of aeration tank required. However, it can be seen that the general behaviour of the full model (i.e., with $\varepsilon > 0$) is broadly captured by the zero- ε model. Hence the zero- ε approximation is reasonable for comparing the performance of completely mixed reactors with incompletely mixed reactors and plug flow reactors.

Worked Solution 29.3 (see Problem 29.3)

(a) For incomplete mixing, the effluent concentration can be determined from Eq. (29.52). Noting that the expression for C_i in Eq. (29.37) it follows that

$$C_e = \frac{Q_0 C_0 F}{Q_0 + Q_r \cdot (1 - F)}$$

where

$$F = \frac{4a}{(1+a)^2 e^{-\frac{(1-a)Pe}{2}} - (1-a)^2 e^{-\frac{(1+a)Pe}{2}}}$$

The velocity can be calculated from Eq. (29.33). The dispersion coefficient can be calculated from Eq. (29.58). Given the absence of information concerning the width of the air diffusers we will assume $W_d = W$. The following MATLAB programme can be used:

```
%Define model parameters
Q0=18.9e3; %influent rate (m3/d)
C0=250; %influent BOD5 (mg/L)
Qr=2e3; %recycled sudge rate (m3/d)
Xr=8000; %recycled mircoorganisms (mg/L)
kgMAX=2; %maximum growth rate (day-1)
kd=0.06; %death rate (day-1)
Kc=84.6; %half-velocity constant (mg/l)
B=1.54; %yield coefficient (-)
V=4984; %aerator reactor volume (m3)
Qg=400e3; %air injection rate (m3/d)
H=4; %water depth (m)
W=[80 40 20 10 5 2 1]; %channel width (m)
%Determine rate coefficient
kc0=kgMAX*B*Qr*Xr/(Q0+Qr+V*kd)/Kc;
```

```

L=V./W/H; %Determine reactor length
Qg=Qg/24/60^2; %Convert from m3/day to m3/s
%Determine dispersion coefficient
Kxx=2/3*H./(H+W).*sqrt(Qg*W.*(L+W)/2./L);
Kxx=Kxx*24*60^2; %Convert from m2/s to m2/day
u=(Q0+Qr)/H./W; %Determine fluid velocity
Pe=u.*L./Kxx; %Determine Peclet number
%Determine F=Ce/Ci
Gi=L*kc0./u;
a=sqrt(1+4*Gi./Pe);
T1=(1+a).^2.*exp(-(1-a).*Pe/2);
T2=(1-a).^2.*exp(-(1+a).*Pe/2);
F=4*a./(T1-T2);
%Determine the effluent concentration (mg/l)
Ce=Q0*C0*F./(Q0+Qr*(1-F));

```

The following results are obtained:

W (m)	L (m)	Pe (-)	C_e (mg l ⁻¹)
80	15.57	0.01100	30.00
40	31.15	0.05343	28.83
20	62.30	0.2168	25.03
10	124.6	0.7911	16.82
5	249.2	2.961	7.007
2	623.00	19.67	1.211
1	1246	92.82	0.4826

As the length of channel increases, a progressively higher treatment level is achieved. Another way of thinking about this is that as we increase the aspect ratio of the channel we can achieve the same level of treatment with a smaller reactor volume.

(b) Under plug flow conditions, Eq.(29.54) can be used such that $F = \exp(-\gamma_i)$. The associated effluent concentration is found by appending the following code to the programme listed above.

```

%Under plug flow conditions
F=exp(-Gi(1));
Ce=Q0*C0*F./(Q0+Qr*(1-F));

```

In this case, C_e is found to be 0.3225 mg l⁻¹. Comparing this result to those found in part (a) it can be understood that the channel of our reactor would need to be greater than 1.2 km in length to achieve close to plug flow conditions. In practice there is a financial trade-off between length of channel and volume of reactor.

Worked Solution 29.4 (see Problem 29.4)

The 5.29 MI activated sludge facility, described in Problem 29.1, is designed to treat 18.9 MI day^{-1} . According to Table 29.1, waste stabilization ponds (WSP) require a residence time of around 5 days to provide an acceptable level of BOD reduction. The volume of WSP required to treat the same amount of wastewater is therefore expected to be around $18.9 \times 5 = 94.5 \text{ MI}$.

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Abstract

This chapter looks at the topics of environmental impact assessment (EIA) and handling uncertainty. Key aspects of an EIA are explained including project screening, scoping analysis, impact significance assessment and risk ranking. Sources of model structure uncertainty and parameter uncertainty are discussed. It is shown how to use Monte Carlo simulation to propagate parameter uncertainty through to model outputs. Parameter sensitivity is explored using tornado plots of rank correlation. Practical applications are presented through worked examples and a problem sheet with worked solutions.

Notation

a	Lower bound estimate of a parameter.
b	Upper bound estimate of a parameter.
c	Maximum likelihood estimate of a parameter.
E	Dimensionless efficiency factor [-].
$f(x)$	Probability density function.
$f_{\max}$	Maximum probability density.
$F(x)$	Cumulative distribution function [-].
i	Rank number [-].
j	Sample number [-].
M_{CO_2}	CO ₂ storage capacity [M].
M	Number of parameters [-].
N	Number of samples [-].
P	Probability [-].
R	Correlation coefficient [-].
V	Volume of brine aquifer or volume of absorption tower [L ³].
x	Some specified value.
x_i	Ranked parameter value.

x_j	Un-ranked parameter value.
y_i	Ranked model outputs.
y_i	Un-ranked model outputs.
X	A random variable.
ρ_{CO_2}	Mass density of CO_2 [ML^{-3}].
ϕ	Porosity [-].
CapEx	Capital expenditure.
CDF	Cumulative distribution function.
COD	Chemical oxygen demand.
DO	Dissolved oxygen.
EIA	Environmental impact assessment.
ES	Environmental statement.
IRR	Internal rate of return.
OpEx	Operational expenses.
PDF	Probability density function.
PNE	Probability of non-exceedance.
P10	Value with a 10% PNE.
P50	Value with a 50% PNE.
P90	Value with a 90% PNE.

30.1 Environmental Impact Assessment

Environmental impact assessment (EIA) is “a procedure which serves to provide information to local authority planners, other regulators and authorising bodies, other interested parties and the general public about certain proposed developments and their likely effects on the environment” [1]. The aim of EIA is to protect the environment by ensuring that a local planning authority grants planning permission for projects “in the full knowledge of the likely significant effects, and takes this into account in the decision making process” [2].

30.1.1 Outline of the EIA Process

An EIA process typically includes the following activities [1,2]:

- Screening: Determining whether a project requires an EIA.
- Scoping: Identifying the various issues that should be covered.
- Baseline studies: Characterising relevant aspects of the environment prior to the new project taking place. This might involve just a desk study but it could also include new water quality surveys or ecological surveys.
- Impact significance assessment: Determining the nature and significance of different environmental impacts of a project. An example of an impact might be the doubling of a chemical concentration in a factory effluent. An example of its

significance might be that it exceeds a water quality standard leading to potential harm to an ecosystem.

- **Mitigation:** Incorporating measures into a design to avoid, reduce, remedy or compensate for adverse environmental impacts. For example, this could include establishing a private wastewater treatment plant.
- **Submission of environmental statement:** The findings of the EIA are written up within an environmental statement (ES), which includes an important non-technical summary. The ES is published and stakeholders are invited to provide their comments.
- **Decision making:** The ES, together with comments made on it, are taken into account by the local planning authority and/or the Secretary of State in deciding whether or not to grant consent for the development.

It is important to recognise that an EIA should be considered an iterative process that continually involves public participation. The purpose of an EIA should be to discover new knowledge about how a project will likely affect the environment and to improve the design in light of this knowledge. Continuous public participation is important to ensure public acceptance and to benefit from a wider sphere of knowledge.

30.1.2 Project Screening

Screening is a procedure used to determine whether a project requires an EIA. The “Town and Country Planning (Environmental Impact Assessment) Regulations 2017” differentiates between Schedule 1 and Schedule 2 projects [2]. Schedule 1 projects always require an EIA. Schedule 2 projects require EIA if they exceed certain thresholds and/or are situated in a “sensitive” area.

Schedule 1 projects include (although some of these become Schedule 2 if they are below a certain threshold) [3]:

- Crude oil refineries;
- Power stations;
- Iron, steel and other metal works;
- Railways, airports, motorways, new roads, waterways and ports;
- Wastewater treatment plants;
- Intensive pig and poultry rearing;
- Carbon capture and storage facilities.

Schedule 2 projects along with their thresholds include [4]:

- Fish farming (> 10 tonnes of fish per year);
- Food industry (> 1000 m²);
- Shopping centres (> 1 hectare);
- Marinas (> 1000 m²);

- Motorway service areas (>0.5 hectare);
- Theme parks (>0.5 hectare);
- Camp sites (>1 hectare).

Sensitive areas include [2]:

- Sites of Special Scientific Interest;
- National Parks, the Broads and Areas of Outstanding Natural Beauty;
- World Heritage Sites and scheduled monuments.

Note that the above list of project types and sensitive areas only represents a small and indicative selection from the complete list of Schedule 1 and Schedule 2 project types and sensitive areas specified in the “Town and Country Planning (Environmental Impact Assessment) Regulations 2017”.

30.1.3 Scoping

Scoping is a process that involves identifying all possible issues of relevance to the EIA. Often a scoping matrix is used to help think through the various aspects of a project (e.g. Table 30.1). A more extensive list of possible impacts to consider for a wide range of different projects are presented in [5].

30.1.3.1 Scoping Analysis Example

The idea of a large paper factory being constructed on the outskirts of Langley Park is considered. Following a structured brainstorming session using the scoping matrix

Table 30.1 Example of a scoping matrix modified from [1, p. 19]

Environmental topic	Construction	Operation	Decommissioning
Population			
Transport			
Noise and vibration			
Biodiversity			
Soils, geology & agriculture			
Water			
Air, climate & odour			
Cultural heritage/material assets			
Landscape			

shown in Table 30.1, a group of students identified the following list of possible impacts (in practice the list would be much more extensive).

1. Construction phase:

- (a) Population: Local residents may stray into the site and hurt themselves on equipment.
- (b) Transport: Lorries delivering construction material will lead to congestion on local roads.
- (c) Noise and vibration: Drilling equipment will lead to significant noise.
- (d) Biodiversity: Birds and insects existing on the site will find the construction environment less hospitable.
- (e) Soils, geology and agriculture: Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.
- (f) Water: Inadequate drainage on the site may lead to localised flooding problems.
- (g) Air, climate and odour: Dust from the site may cause local air quality problems.
- (h) Cultural heritage: N/A
- (i) Landscape: Cranes and other equipment may look unsightly.

2. Operation phase:

- (a) Population: Local residents should benefit from new jobs in the area.
- (b) Transport: Lorries delivering construction material will lead to congestion on local roads.
- (c) Noise and vibration: Factory equipment is likely to cause noise and vibrations.
- (d) Biodiversity: Effects associated with noise and water contamination may lead to reduction of habitat quality for local ecologies.
- (e) Soils, geology and agriculture: Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.
- (f) Water: Effluent from plant may be inadequately treated and have high levels of BOD and suspended solids.
- (g) Air, climate and odour: Pulp generation may lead to odour problems.
- (h) Cultural heritage: N/A.
- (i) Landscape: The architecture of the plant may not fit well with the surrounding landscape.

3. Decommissioning phase:

- (a) Population: Site may be insecure and a hazard to future residents.
- (b) Transport: Lorries removing equipment may lead to increased traffic.
- (c) Noise and vibration: Demolition of works may lead to excessive noise and vibrations.

- (d) Biodiversity: Bats may have taken residence in the roof of the works. Demolition may lead to loss of habitat.
- (e) Soils, geology and agriculture: Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.
- (f) Water: Inadequate drainage on the site may lead to localised flooding problems.
- (g) Air, climate and odour: Dust from the site may cause local air quality problems.
- (h) Cultural heritage: The paper factory may have become an important part of the local society. Aspects may need to be preserved for heritage purposes.
- (i) Landscape: The decommissioned site may not fit in well with the aesthetics of the local environments.

30.1.4 Impact Significance Assessment

Regulations typically require a description of the likely significant environmental impacts of the proposed project resulting from [1]:

- The existence of the project,
- The use of natural resources,
- The emission of pollutants,
- The creation of nuisances,
- The elimination of wastes.

SNH [5] propose the following scale to describe the significance of impacts:

- Substantial magnitude: Significant changes, over a significant area, to key characteristics or features or to the landscape's character or distinctiveness for more than 2 years.
- Moderate magnitude: Noticeable but not significant changes for more than 2 years or significant changes for more than 6 months but less than 2 years, over a significant area, to key characteristics or features or to the landscape's character or distinctiveness.
- Slight magnitude: Noticeable changes for less than 2 years, significant changes for less than 6 months, or barely discernible changes for any length of time.
- Negligible or no change: Any change would be negligible, unnoticeable or there are no predicted changes.

30.1.5 Risk Ranking

The scoping approach in EIA aims to provide broad coverage of topics so that as many potential impacts, associated with a project, are incorporated as possible. However,

eventually it is useful to determine the relative importance of the various impacts. Risk ranking provides a methodology for doing this. A general approach to risk ranking is as follows:

- Identify hazards (through scoping);
- Assign hazards a level of consequence;
- Assign hazards a level of likelihood;
- Risk = likelihood × consequence;
- Rank hazards in terms of risk value.

Burgman [6] defines risk as “the chance, within a time frame, of an adverse event with specific consequences”. They define hazard as “a situation that in particular circumstances could lead to harm”. Note that negative impacts identified during EIA are forms of hazards.

Once a list of hazards are identified, experts can assign a consequence score along with an associated likelihood score using subjective belief, “the degree to which a proposition is judged to be true” [6]. Likelihoods and consequences are often classified subjectively using tables similar to Tables 30.2 and 30.3.

30.1.5.1 Risk Ranking Example

Table 30.4 shows results from three assessors risk ranking the impacts identified in the scoping analysis example, previously presented in Sect. 30.1.3.1, using the risk ranking guidelines provided in Tables 30.2 and 30.3. The rank numbers denote the rank of each impact in terms of its risk with rank 1 representing the highest risk impact. It can be seen that each assessor has ranked the impacts differently, as is the nature of this subjective process.

Assessor 1 identified the following highest ranking risks:

Table 30.2 Attempt to quantify likelihood from subjective belief [6, p. 150]

Score	Description	Scenario/details	Probability
16	Highly likely	Expected to occur in most circumstances	Over 85%
12	Likely	Will probably occur in most circumstances	50–85%
8	Fairly likely	Might occur at some time, quite often	21–49%
4	Unlikely	Could occur at some time	1–20%
2	Very unlikely	Not expected to happen	<1%
1	Extremely unlikely	Just possible but very surprising	<0.01%

Table 30.3 Attempt to quantify consequence [6, p. 150]

Score	Description	Scenario/details
1000	Disastrous/catastrophic	Deaths, toxic release off-site with substantial detrimental environmental effects, bankruptcy
100	Sever/major	Extensive injuries, release off-site with detrimental effects, serious threat to business
20	Substantial/moderate	Medical treatment required, toxic release on-site contained with outside assistance, or off-site release with no detrimental effects, significant reduction in profit
3	Marginal/minor	First-aid treatment, on-site release immediately contained, small effect on profit
1	Negligible/insignificant	No injuries, no important environmental effect trivial effect on profit

1. (1d) Biodiversity (Construction phase): Birds and insects existing on the site will find the construction environment less hospitable.
2. (1g) Air, climate and odour (Construction phase): Dust from the site may cause local air quality problems.
3. (3g) Air, climate and odour (Decommissioning phase): Dust from the site may cause local air quality problems.
4. (2d) Biodiversity (Operation phase): Effects associated with noise and water contamination may lead to reduction of habitat quality for local ecologies.
5. (1a) Population (Construction phase): Local residents may stray into the site and hurt themselves on equipment.

Assessor 2 identified the following highest ranking risks:

1. (1e) Soils, geology and agriculture (Construction phase): Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.
2. (1a) Population (Construction phase): Local residents may stray into the site and hurt themselves on equipment.
3. (3e) Soils, geology and agriculture (Decommissioning phase): Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.
4. (2e) Soils, geology and agriculture (Operation phase): Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.
5. (2f) Water (Operation phase): Effluent from plant may be inadequately treated and have high levels of BOD and suspended solids.

Assessor 3 identified the following highest ranking risks:

1. (3e) Soils, geology and agriculture (Decommissioning phase): Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.

Table 30.4 Risk ranking by three experts of the impacts identified in the scoping analysis example (Sect. 30.1.3.1). Note that like. and cons. are abbreviations for likelihood and consequence, respectively

Impact	Assessor 1				Assessor 2				Assessor 3				Sum of ranks
	Like.	Cons.	Risk	Rank	Like.	Cons.	Risk	Rank	Like.	Cons.	Risk	Rank	
1a	12	20	240	5	100	12	1200	2	12	100	1200	2	9
1b	12	3	36	16	1	16	16	15	16	3	48	12	43
1c	16	3	48	12	1	8	8	18	16	1	16	20	50
1d	16	100	1600	1	20	16	320	9	8	3	24	15	25
1e	8	20	160	11	1000	8	8000	1	4	100	400	5	17
1f	8	3	24	20	100	4	400	7	8	20	160	9	36
1g	8	100	800	2	20	8	160	11	8	3	24	15	28
1h	0	0	0	25	0	0	0	26	0	0	0	26	77
1i	8	3	24	20	1	16	16	15	16	1	16	20	55
2a	12	0	0	25	1	8	8	18	12	1	12	23	66
2b	12	3	36	16	3	8	24	13	16	3	48	12	41
2c	16	3	48	12	1	4	4	24	8	3	24	15	51
2d	4	100	400	4	20	8	160	11	8	20	160	9	24
2e	2	100	200	7	100	8	800	4	1	1000	1000	3	14
2f	2	100	200	7	100	8	800	4	2	100	200	8	19
2g	8	3	24	20	1	8	8	18	8	3	24	15	53
2h	0	0	0	25	0	0	0	26	0	0	0	26	77
2i	12	3	36	16	1	8	8	18	12	1	12	23	57
3a	12	20	240	5	100	4	400	7	12	20	240	6	18
3b	12	3	36	16	1	8	8	18	16	3	48	12	46
3c	16	3	48	12	1	8	8	18	12	20	240	6	36
3d	2	100	200	7	3	8	24	13	8	3	24	15	35
3e	2	100	200	7	100	12	1200	2	8	1000	8000	1	10
3f	2	20	40	15	100	8	800	4	8	100	800	4	23
3g	8	100	800	2	20	12	240	10	4	20	80	11	23
3h	2	3	6	24	1	2	2	25	2	3	6	25	74
3i	8	3	24	20	1	12	12	17	16	1	16	20	57

2. (1a) Population (Construction phase): Local residents may stray into the site and hurt themselves on equipment.
3. (2e) Soils, geology and agriculture (Operation phase): Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.
4. (3f) Water (Decommissioning phase): Inadequate drainage on the site may lead to localised flooding problems.
5. (1e) Soils, geology and agriculture (Construction phase): Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.

In many cases it is necessary to aggregate the views of different assessors to derive an overall opinion that is somehow consistent with the individual opinions.

One option would be to rank the impacts on the basis of the sum of the risk scores from each of the assessors. The problem here is that this will bias the results to the opinions of the most risk averse assessors. Interestingly the mean risk score identified in Table 30.4 by Assessors 1, 2 and 3 are 203, 542 and 475, respectively. This would mean that the opinions of Assessors 2 and 3 would be over represented.

A better option is to rank the impacts on the basis of the sum of the ranks from each of the assessors. Obviously the mean rank scores identified in Table 30.4 by Assessors 1, 2 and 3 are identical. The final column in Table 30.4 shows the sum of the ranks for each impact. This would suggest that the group, as a whole, have identified the following highest ranking risks:

1. (1a) Population (Construction phase): Local residents may stray into the site and hurt themselves on equipment.
2. (3e) Soils, geology and agriculture (Decommissioning phase): Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.
3. (2e) Soils, geology and agriculture (Operation phase): Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.
4. (1e) Soils, geology and agriculture (Construction phase): Storm drainage from the site may contain toxic chemicals, which may contaminate local soils.
5. (3a) Population (Decommissioning phase): Site may be insecure and a hazard to future residents.

30.2 Handling Uncertainty

30.2.1 Uncertainty in Model Predictions

Environmental engineering frequently involves applications of complicated mathematical models. Engineers often distinguish between deterministic and stochastic models. Deterministic models do not account for random processes and provide single, supposedly exact, answers. Stochastic models account for random processes and provide results in the form of probability distributions.

Most of the analysis undertaken in previous chapters has involved the use of deterministic models. However, these models are undermined by both model structure uncertainty and parameter uncertainty.

30.2.1.1 Model Structure Uncertainty

Development of mathematical models typically involves at least three processes:

1. The conceptual model: This is where we describe the physical process we are trying to represent.
2. Governing equations: At this stage we tend to make limiting assumptions so that we can describe our conceptual model in terms of mathematical equations, initial conditions and boundary conditions.
3. Analytical or numerical solutions: Our governing equations frequently take the form of partial differential equations describing combinations of mass and energy conservation. These need to be solved to obtain answers. Solution typically involves making additional assumptions and/or applying approximate solution techniques to make the problem tractable.

At each stage we incur a deviation from the process we are trying to represent. Uncertainty about the acceptability of this deviation is what is commonly referred to as model structure uncertainty.

30.2.1.2 Parameter Uncertainty

At the same time, it is necessary to specify the value of the various parameters embedded within the resulting set of equations. For the most part, these parameters are obtained using a process known as model calibration. Model calibration involves finding a set of parameter values such that a given mathematical model simulates a set of previously observed measurements to its best ability.

Unfortunately, there are multiple sources of error embedded within these pre-specified parameters including:

- Measurement error: There will be error in the measurements used to inform the parameter calibration.
- Model structure error: Parameter values based on previous experience often compensate for model structure errors incurred due to model structure uncertainty.
- Equifinality: Often it is not possible to constrain all of the unknown parameters using a given set of measurements. This gives rise to equifinality, whereby multiple combinations of parameter values yield identical model responses within a restricted window of behaviour [7].
- Extrapolation error: The scenario of interest often represents an extrapolation from a previous domain of experience.

Collectively, these errors lead to parameter uncertainty.

30.2.1.3 Uncertainty Propagation

If we account for the randomness associated with model structure and parameter uncertainty within our deterministic model predictions, we end up with a probability distribution of model results and our deterministic models become stochastic.

Uncertainty propagation is the process of propagating knowledge about model structure uncertainty and parameter uncertainty through to model outputs such that model results are stochastic and specified as probability distributions. This is more useful than simple deterministic results because it informs engineers about the range of possibilities they should design for in order to achieve a positive outcome.

30.2.2 Cumulative Distribution Functions

Cumulative distribution functions (CDF) provide a convenient means of describing the uncertainty of input model parameter values and model output results.

Let X be a random variable (cost rate, NO_2 concentration, temperature etc.). The term, $P(X > x)$, denotes the probability that X will be greater than a specified value, x , referred to as the probability of exceedance.

The term $P(X \leq x)$ denotes the probability that X will not be greater than a specified value, x , referred to as the probability of non-exceedance. Probability of exceedance is related to probability of non-exceedance by

$$P(X > x) = 1 - P(X \leq x) \quad (30.1)$$

The CDF, $F(x)$, relates directly to the probability of non-exceedance (PNE), i.e., $F(x) \equiv P(X \leq x)$.

30.2.2.1 Continuous CDF

A continuous CDF can be found from

$$F(x) = \int_{-\infty}^x f(x)dx \quad (30.2)$$

where $f(x)$ is the underlying probability density function (PDF).

A PDF can be thought of as a continuous form of a histogram. However, an important property of the PDF is that

$$\int_{-\infty}^{\infty} f(x)dx = 1 \quad (30.3)$$

30.2.2.2 Empirical CDF

It is possible to construct an empirical CDF from a discrete set of measurements. Consider N number of measurements, x_j ($j = 1, 2, \dots, N$). Let x_i ($i = 1, 2, \dots, N$) be the same set of measurements but ranked from largest to smallest; i is referred to as the rank number. The probability of exceedance for x_i can be found from empirical functions of i and N , referred to as plotting positions.

Table 30.5 Example showing an application of the Gringorten and Weibull plotting positions

Measurements		Ranked data		Gringorten	Weibull
j	x_j	i	x_i	$P(X > x_i)$	$P(X > x_i)$
1	35	1	35	0.11	0.17
2	27	2	30	0.30	0.33
3	30	3	27	0.50	0.50
4	10	4	25	0.70	0.67
5	25	5	10	0.89	0.83

Two popular heuristic plotting positions are the Gringorten formula [8, p. 314]

$$P(X > x_i) = \frac{i - 0.44}{N + 0.12} \quad (30.4)$$

and the Weibull formula [8, p. 316]

$$P(X > x_i) = \frac{i}{N + 1} \quad (30.5)$$

The empirical CDF can be obtained from

$$F(x_i) = 1 - P(X > x_i) \quad (30.6)$$

A simple example is presented in Table 30.5 where probability estimates from the Gringorten and Weibull plotting positions are compared. Of note is that the Gringorten plotting position provides extreme probabilities closer to zero and one. Both plotting positions will provide identical results as the number of measurements approaches infinity.

30.2.3 Parameter Distributions

We often have an idea about upper and lower bound values for parameters and sometimes we might be willing to specify a “most likely” value.

30.2.3.1 Uniform Distribution

In the event that we are only able to specify upper and lower bound values, it is common to assume there is an equal likelihood that the “most appropriate” value for that parameter is any value within the specified range. In this case we should assume that the parameter is described by a uniform PDF.

Consider a uniform PDF of the form

$$f(x) = \begin{cases} f_{\max}, & x \in [a, b] \\ 0, & x \notin [a, b] \end{cases} \quad (30.7)$$

where a and b are the lower and upper bounds, respectively, of a parameter of concern, x , and $f_{\max}$ is the maximum probability density.

Challenge 30.1 Determine an expression for the CDF.

Substituting Eq. (30.7) into (30.2) for $x \in [a, b]$ leads to

$$F(x) = \int_a^x f_{\max} dx = f_{\max} \cdot (x - a)$$

It follows that

$$F(x) = \begin{cases} 0, & x < a \\ f_{\max} \cdot (x - a), & x \in [a, b] \\ f_{\max} \cdot (b - a), & x > b \end{cases} \quad (30.8)$$

Challenge 30.2 Define $f_{\max}$ such that $F(\infty) = 1$.

If we force $F(\infty) = 1$, Eq. (30.8) suggests that

$$f_{\max} = \frac{1}{b - a} \quad (30.9)$$

Substituting Eq. (30.9) into Eqs. (30.7) and (30.8) gives us

$$f(x) = \begin{cases} \frac{1}{b-a}, & x \in [a, b] \\ 0, & x \notin [a, b] \end{cases} \quad (30.10)$$

and

$$F(x) = \begin{cases} 0, & x < a \\ \frac{x-a}{b-a}, & x \in [a, b] \\ 1, & x > b \end{cases} \quad (30.11)$$

respectively.

Challenge 30.3 Rearrange Eq. (30.11) to make x the subject of the formula.

Solving Eq. (30.11) for x leads to

$$x = (b - a)F(x) + a \quad (30.12)$$

Challenge 30.4 Write a MATLAB script to plot the histogram and empirical CDF for 500 random temperature values sampled from a uniform PDF ranging from 4 to 8 °C.

The following MATLAB code generates a histogram and a plot of the CDF for 500 random temperature values sampled from a uniform PDF ranging from 4 to 8 °C:

```

N=500; %Number of samples
a=4; %Minimum temperature (deg C)
b=8; %Maximum temperature (deg C)
F=rand(N,1); %Uniform random values
xj=(b-a)*F+a; %Random samples
xi=sort(xj, 'descend'); %Ranked samples
%Probability of exceedance (fraction)
P=( [1:N] '-0.44)/(N+0.12);
%Probability of non-exceedance (%)
PNE=(1-P)*100;
figure(1); clf
subplot(1,2,1)
histogram(xj, 'FaceColor', [0.9 0.9 0.9])
xlabel('Temperature (^oC)')
ylabel('Frequency')
title('a) Histogram')
subplot(1,2,2)
plot(xi, PNE, 'k-')
xlabel('Temperature (^oC)')
ylabel('Probability of non-exceedance (%)')
title('b) CDF')

```

The resulting plots are shown in Fig. 30.1.

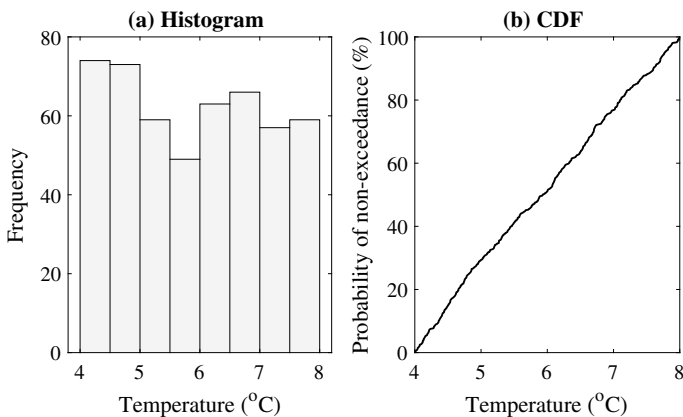


Fig. 30.1 Random sampling from a uniform distribution

30.2.3.2 Triangular Distribution

In the event that we are able to specify upper and lower bound values along with an intermediate value, which is believed to be the most likely value, it is more appropriate to adopt a triangular PDF.

Consider a triangular PDF of the form

$$f(x) = \begin{cases} f_{\max} \cdot \left(\frac{x-a}{c-a} \right), & x \in [a, c) \\ f_{\max} \cdot \left(\frac{b-x}{b-c} \right), & x \in [c, b] \\ 0, & x \notin [a, b] \end{cases} \quad (30.13)$$

where a and b are the lower and upper bounds, respectively, of a parameter of concern, x , and c is the most likely value.

Challenge 30.5 Determine an expression for the CDF.

Substituting Eq. (30.13) into Eq. (30.2) for when $x \in [a, c)$ gives us

$$\begin{aligned} F(x) &= \int_a^x f_{\max} \cdot \left(\frac{x-a}{c-a} \right) dx \\ &= \left[f_{\max} \cdot \left(\frac{x^2 - 2ax}{2(c-a)} \right) \right]_a^x \\ &= f_{\max} \cdot \left(\frac{x^2 - 2ax - a^2 + 2a^2}{2(c-a)} \right) \\ &= \frac{f_{\max}}{2} \frac{(x-a)^2}{(c-a)} \end{aligned}$$

Substituting Eq. (30.13) into Eq. (30.2) for when $x \in [c, b]$ gives us

$$\begin{aligned} F(x) &= \frac{f_{\max}}{2}(c-a) + \int_c^x f_{\max} \cdot \left(\frac{b-x}{b-c} \right) dx \\ &= \frac{f_{\max}}{2}(c-a) + \left[f_{\max} \cdot \left(\frac{2bx - x^2}{2(b-c)} \right) \right]_c^x \\ &= \frac{f_{\max}}{2}(c-a) + f_{\max} \cdot \left(\frac{2bx - x^2 - 2bc + c^2}{2(b-c)} \right) \\ &= \frac{f_{\max}}{2}(c-a) + f_{\max} \cdot \left(\frac{-b^2 + 2bx - x^2 + b^2 - 2bc + c^2}{2(b-c)} \right) \\ &= \frac{f_{\max}}{2}(c-a) + \frac{f_{\max}}{2}(b-c) - \frac{f_{\max}}{2} \frac{(b-x)^2}{(b-c)} \\ &= \frac{f_{\max}}{2}(b-a) - \frac{f_{\max}}{2} \frac{(b-x)^2}{(b-c)} \end{aligned}$$

It follows that

$$F(x) = \begin{cases} 0, & x < a \\ \frac{f_{\max}}{2} \frac{(x-a)^2}{(c-a)}, & x \in [a, c) \\ \frac{f_{\max}}{2} (b-a) - \frac{f_{\max}}{2} \frac{(b-x)^2}{(b-c)}, & x \in [c, b] \\ \frac{f_{\max}}{2} (b-a), & x > b \end{cases} \quad (30.14)$$

Challenge 30.6 Define $f_{\max}$ such that $F(\infty) = 1$.

If we force $F(\infty) = 1$, Eq. (30.14) suggests that

$$f_{\max} = \frac{2}{b-a} \quad (30.15)$$

Substituting Eq. (30.15) into Eqs. (30.13) and (30.14) gives us

$$f(x) = \begin{cases} \frac{2(x-a)}{(b-a)(c-a)}, & x \in [a, c) \\ \frac{2(b-x)}{(b-a)(b-c)}, & x \in [c, b] \\ 0, & x \notin [a, b] \end{cases} \quad (30.16)$$

and

$$F(x) = \begin{cases} 0, & x < a \\ \frac{(x-a)^2}{(b-a)(c-a)}, & x \in [a, c) \\ 1 - \frac{(b-x)^2}{(b-a)(b-c)}, & x \in [c, b] \\ 1, & x > b \end{cases} \quad (30.17)$$

respectively.

Challenge 30.7 Rearrange Eq. (30.17) to make x the subject of the formula.

Solving Eq. (30.17) for x leads to

$$x = \begin{cases} a + \sqrt{(b-a)(b-c)F(x)}, & F(x) \in \left[0, \frac{c-a}{b-a}\right] \\ b - \sqrt{(b-a)(b-c)[1-F(x)]}, & F(x) \in \left[\frac{c-a}{b-a}, 1\right] \end{cases} \quad (30.18)$$

Challenge 30.8 Write a MATLAB script to plot the CDF and histogram for 500 random temperature values sampled from a triangular PDF ranging from 4 to 8 °C with a maximum likelihood value of 7 °C.

The following MATLAB code generates a histogram and a plot of the CDF for 100 random temperature values sampled from a triangular PDF ranging from 4–8 °C with a maximum likelihood value of 7 °C:

```

N=500; %Number of samples
a=4; %Minimum temperature (deg C)
b=8; %Maximum temperature (deg C)
c=7; %Most likely temperature (deg C)
F=rand(N,1); %Uniform random values
%Sample from triangular distribution
xj=a+sqrt((b-a).*(c-a).*F);
xj1=b-sqrt((b-a).*(b-c).*(1-F));
Fc= repmat((c-a)./(b-a),N,1);
xj(F>Fc)=xj1(F>Fc); %Random samples
xi=sort(xj, 'descend'); %Ranked samples
%Probability of exceedance (fraction)
P=( [1:N] '-0.44)/(N+0.12);
%Probability of non-exceedance (%)
PNE=(1-P)*100;
figure(1); clf
subplot(1,2,1)
histogram(xj, 'FaceColor',[0.9 0.9 0.9])
xlabel('Temperature (^oC)')
ylabel('Frequency')
title('a) Histogram')
subplot(1,2,2)
plot(xi,PNE, 'k-')
xlabel('Temperature (^oC)')
ylabel('Probability of non-exceedance (%)')
title('b) CDF')

```

The resulting plots are shown in Fig.30.2.

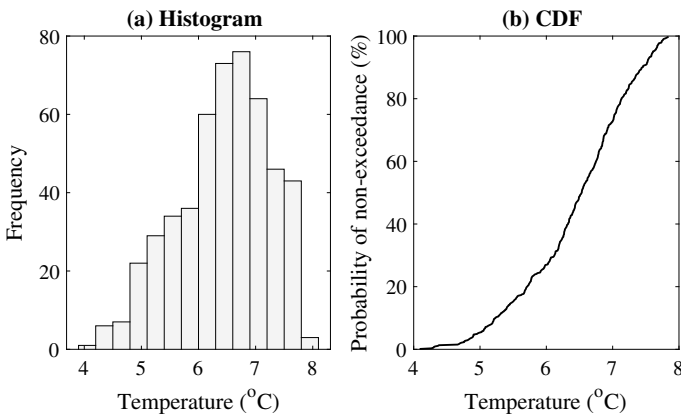


Fig. 30.2 Random sampling from a triangular distribution

30.2.4 Monte Carlo Simulation

Monte Carlo simulation can be used to propagate parameter uncertainty through to model outputs as follows:

1. Specify parameter distributions.
2. Sample a specified number of different parameter sets.
3. Run deterministic model for each parameter set.
4. Collect all the model results to form a cumulative distribution function.

A MATLAB function for performing such a task is provided in Listing 30.1.

Listing 30.1 A MATLAB function for propagating parameter uncertainty to model outputs using Monte Carlo simulation.

```
function [PNE,yi,xj,yj]=MonteCarlo(FUN,abc,N)
%PNE - Probability of non-exceedance (%)
%yi - Ranked model output values
%xj - Unranked random parameter sets
%yj - Unranked model output values
%FUN - Name of function containing model
%abc - Parameter distribution characteristics
%N - Required number of realisations
F=rand(N,size(abc,2)); %Uniform random values
if size(abc,1)==2
%Apply uniform distribution
a=abc(1,:);b=abc(2,:);
xj=(b-a).*F+a;
elseif size(abc,1)==3
%Apply triangular distribution
a=abc(1,:);b=abc(2,:);c=abc(3,:);
xj=a+sqrt((b-a).*(c-a).*F);
xj1=b-sqrt((b-a).*(b-c).*(1-F));
Fc=repmat((c-a)./(b-a),N,1);
xj(F>Fc)=xj1(F>Fc);
end
%Run model for each parameter set
for j=1:N
yj(j,1)=FUN(xj(j,:));
end
yi=sort(yj,'descend'); %Rank outputs
%Probability of exceedance (fraction)
P=( [1:N]' -0.44)/(N+0.12);
%Probability of non-exceedance (%)
PNE=(1-P)*100;
```

30.2.5 Tornado Plots

Parameter sensitivity is often explored using tornado plots, which show bar charts of rank correlation for each parameter with the highest correlating parameters displayed first. Such a plot can be generated using the MATLAB function provided in Listing 30.2.

Listing 30.2 A MATLAB function for generating a tornado plot to explore parameter sensitivity, associated with a Monte Carlo simulation, using rank correlation.

```
function TornadoPlot(xj,yj,Xnames)
%xj - Unranked random paramater sets
%yj - Unranked model output values
%Xnames - Cell array of parameter names
M=size(xj,2); %Number of parameters
%Get rank number for yj values
[~,~,iY]=unique(yj);
for k=1:M
%Get rank number for xj values
[~,~,iX]=unique(xj(:,k));
%Determine rank correlation
%and significant test values
[R,P]=corrcoef(iX,iY);
R(P>0.05)=0; %Reject failed values
Rx(k,1)=R(2,1); %Store rank correlation
end
%Get indices to sort in terms of abs(Rx)
[~,iRx]=sort(abs(Rx));
Rx=Rx(iRx); %Sort rank correlations
Xnames=Xnames(iRx); %Sort parameter name labels
%Plot horizontal bar chart
barh(Rx,'facecolor',[0.9 0.9 0.9])
xlabel('Rank correlation (-)')
xlim([-1 1])
%Label with different parameter names
set(gca,'ytick',1:M)
set(gca,'yticklabel',Xnames)
```

The first step involves determining the rank number of the model outputs and each parameter. The next step is to determine the rank correlation between parameter ranks and output ranks for each parameter. At the same time it is important to determine the P value from a significant test. If $P > 0.05$ a correlation is considered to be not significant, so we set those correlation coefficients to zero. Finally we rank all the rank correlations and order the model parameters accordingly in a bar chart.

Rank correlation is used as opposed to conventional correlation because correlation only picks up linear relationships between two parameters whereas rank correlation will pick up any relationship. The higher the rank correlation the more

Table 30.6 Lower bound, a , upper bound, b , and maximum likelihood, c , parameters for a brine aquifer for which the CO₂ storage capacity is to be determined using Eq. (30.19)

Parameter	a	b	c
ρ_{CO_2} (kg m ⁻³)	600	700	650
V (km ³)	30	80	56
ϕ [-]	0.15	0.3	0.25
E [-]	0.005	0.025	0.02

sensitive the model output is to that parameter. The main purpose of a tornado plot is to inform the user about which parameters should be focused on first where resources are available to acquire additional information.

30.2.6 Simple Example

As a simple example, we will revisit Problem 25.1 (a) where the CO₂ storage capacity of a brine aquifer, M_{CO_2} [M], is to be determined from (recall Eq. 25.4)

$$M_{\text{CO}_2} = \rho_{\text{CO}_2} V \phi E \quad (30.19)$$

where ρ_{CO_2} [ML⁻³] is the density of CO₂ in the aquifer, V [L³] is the volume of the aquifer, ϕ [-] is the porosity of the aquifer and E [-] is a dimensionless factor. The lower bound, a , upper bound, b , and maximum likelihood, c , for the four parameters are given in Table 30.6. A MATLAB function containing the model defined by Eq. (30.19) is given in Listing 30.3.

Listing 30.3 A MATLAB function containing the CO₂ storage capacity model, defined by Eq. (30.19).

```
function Mco2=CO2storageFun(X)
rhoCO2=X(1); %CO2 density (kg/m3)
V=X(2); %Aquifer volume (km3)
phi=X(3); %Porosity (-)
E=X(4); %Efficiency factor (-)
Mco2=rhoCO2*V*phi*E; %CO2 storage capacity (Mt)
```

The following MATLAB script uses the CO2storageFun, given in Listing 30.3, to perform the original deterministic analysis conducted for Problem 25.1 (a):

```
c=[650 56 0.25 0.02];
Mco2=CO2storageFun(c)
```

This results in a CO₂ storage capacity value of 182.0 Mt.

The MATLAB script below runs the CO2storageFun function (Listing 30.3), within a Monte Carlo simulation, using the MonteCarlo function (Listing 30.1), based on the parameter distributions defined in Table 30.6. The model results are

presented as a CDF. Parameter sensitivity is demonstrated through a tornado plot, generated using the `TornadoPlot` function (Listing 30.2).

```
FUN=@CO2storageFun; %Function containing model
Xnames{1}='CO_2 density (kg m^-^3)';
Xnames{2}='Aquifer volume (km^3)';
Xnames{3}='Porosity (-)';
Xnames{4}='Efficiency factor (-)';
abc=[600 30 0.15 0.005 %a parameters
700 80 0.3 0.025 %b paramaters
650 56 0.25 0.02]; %c paramaters
%Monte Carlo with uniform distribution
[PNE1,yi1,xj1,yj1]=MonteCarlo(FUN,abc(1:2,:),500);
%Monte Carlo with triangular distribution
[PNE2,yi2,xj2,yj2]=MonteCarlo(FUN,abc,500);
figure(1); clf
subplot(1,2,1)
plot(yi1,PNE1,'k-',yi2,PNE2,'r-')
xlabel('CO_2 storage capacity (Mt)')
ylabel('Probability of non-exceedance (%)')
legend('Uniform','Triangular')
title('a) CDF')
subplot(1,2,2)
TornadoPlot(xj2,yj2,Xnames)
title('b) Tornado plot')
```

Note that we have performed the Monte Carlo simulation twice, first with uniform parameter distributions then with triangular distributions. This has been done for comparison purposes and is not generally necessary. The tornado plot has only been generated using the results from the triangular distribution. The results are shown in Fig. 30.3.

30.2.6.1 Comparison of CDFs

The CDFs from the two Monte Carlo simulations are shown in Fig. 30.3a. The results using the uniform and triangular distributions are quite similar. However, the CDF from the triangular distributions is more narrow due to the additional constraint associated with the specification of maximum likelihood parameter values.

30.2.6.2 P10, P50 and P90 Values

A common method of abstracting data from a CDF is to determine P10, P50 and P90 results, which correspond to probabilities of non-exceedance of 10%, 50% and 90%. These can be obtained using the following additional code:

```
yiSTATS=interp1(PNE,yi,[10 50 90]);
```

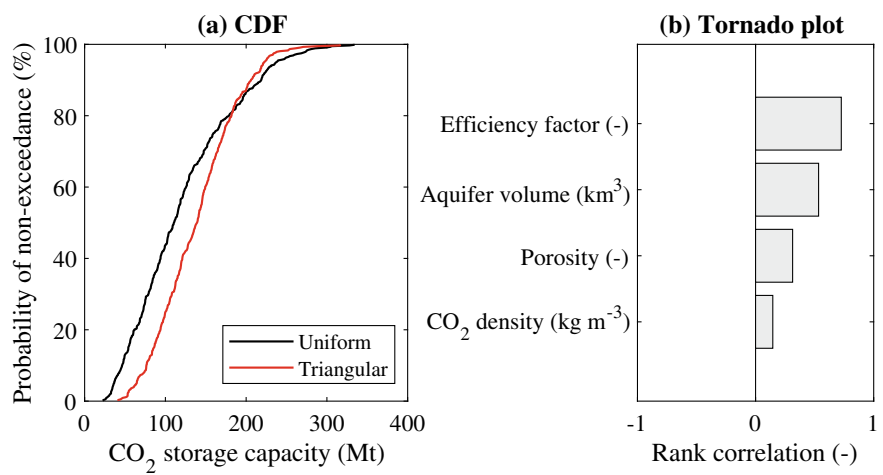


Fig. 30.3 **a** Cumulative distribution functions (CDF) resulting from the CO₂ storage capacity Monte Carlo simulations using uniform and triangular parameter distributions. **b** Corresponding tornado plot resulting from the Monte Carlo simulation with triangular parameter distributions

Table 30.7 P10, P50 and P90 results, interpolated from the CDFs shown in Fig. 30.3a

Distribution	P10	P50	P90
Uniform	45.4 Mt	102 Mt	212 Mt
Triangular	77.0 Mt	135 Mt	205 Mt

The MATLAB function, `interp1`, uses linear interpolation to interpolate the CDF to obtain values of y_i at 10, 50 and 90% PNE.

Results from Fig. 30.3a are shown in Table 30.7. The P10 and P90 values would be considered pessimistic and optimistic scenarios in this context. The P50 value is often interpreted as being a most likely value although the P50 corresponds to the median rather than the mode of the data.

Note that results from the triangular distributions yield quite different P10 and P50 values as compared to those derived using results from the uniform distributions. Providing we are confident about the robustness of our estimate of the maximum likelihood parameter values (i.e., the c values), we should consider the results from the triangular distribution to better reflect the reality of our understanding.

Results from the Monte Carlo simulation with triangular distributions could be explained to a lay person as follows:

- There is a 10% probability that the CO₂ storage capacity of the brine aquifer will not exceed 77.0 Mt.
- There is a 50% probability that the CO₂ storage capacity of the brine aquifer will not exceed 135 Mt.

- There is a 90% probability that the CO₂ storage capacity of the brine aquifer will not exceed 205 Mt.

30.2.6.3 Discussion About the Tornado Plot

Figure 30.3b shows a Tornado plot resulting from the Monte Carlo simulation with the triangular distributions. It can be seen that the rank correlation with CO₂ storage capacity is highest for the efficiency factor, E , then aquifer volume, then porosity. This would suggest that if we have additional resources to research the values of our model parameters we should first focus on constraining the efficiency factor, then aquifer volume and finally porosity. The very low rank correlation with CO₂ density suggests we already know enough about that parameter in this context.

Interestingly, if we look at the nature of Eq. (30.19) we should expect CO₂ storage capacity to have an equal sensitivity to each of the four parameters. However, the difference in rank correlation, shown in Fig. 30.3b, comes about due to the varying degrees of uncertainty about the parameters presented in Table 30.6.

In other cases, it is possible to have the same degree of uncertainty for each parameter with different rank correlations being observed due to different functional dependencies of a model output on a particular parameter. For example, if you were to have a function such as

$$y = x_1^2 x_2$$

the model output y would tend to be more sensitive to the value of x_1 than x_2 due to the fact that it has a squared dependency on x_1 but only a linear dependence on x_2 .

30.3 Problem Sheet

Problem 30.1 (see Worked Solution 30.1)

A farming cooperative is considering constructing a new irrigation system. The initial CapEx is expected to be £200,000 and the annual (current) OpEx is expected to be £2000. The irrigation system is expected to bring £22,000 per year in additional (current) revenues due to better crop production and has an anticipated operation life of 20 years. The expected inflation rate is 3%. Determine P10, P50 and P90 values for the real internal rate of return (IRR) assuming the expected values of the parameters are most likely but that there is a possibility they could all vary by $\pm 20\%$. Hint: This is a probabilistic extension of Problem 21.4.

Problem 30.2 (see Worked Solution 30.2)

A chimney is expected to emit NO_2 at a rate of 0.1099 kg s^{-1} . The effective stack height is expected to be 100 m. The wind speed is expected to be 5 m s^{-1} . The environmental temperature gradient is expected to be -10 K km^{-1} .

- (a) Plot a CDF for the maximum ground-level concentration assuming the expected values of the parameters are most likely but that there is a possibility they could all vary by $\pm 20\%$. Hint: This is a probabilistic extension of Problem 26.1 (b) (ii).
- (b) Construct an associated tornado plot and make a recommendation about which is the most important parameter requiring further research.

Problem 30.3 (see Worked Solution 30.3)

Trade effluent from the Bearpark dairy is discharged into the River Browney at an expected rate of $0.15 \text{ m}^3 \text{ s}^{-1}$. The effluent is expected to have a BOD_5 of 90 mg l^{-1} and a DO concentration of 2.3 mg l^{-1} . The river flow immediately upstream of the discharger is expected to be $0.9 \text{ m}^3 \text{ s}^{-1}$. The river water immediately upstream of the discharger is expected to have a BOD_5 of 2 mg l^{-1} and a DO concentration of 8 mg l^{-1} . The biodegradable matter aerobic consumption rate associated with the River Browney is expected to be 0.4 day^{-1} . The mean width of the river channel is expected to be 10 m. The mean water depth of the river channel is expected to be 1 m. The temperature of the river water is expected to be 10°C .

- (a) Plot a CDF for the minimum DO level expected in the river as a consequence of the discharger, assuming the expected values of the parameters are most likely but that there is a possibility they could all vary by $\pm 10\%$. Hint: This is a probabilistic extension of Problem 27.3 (e).
- (b) Construct an associated tornado plot and provide physical explanations for the top three most significant correlations.

30.4 Worked Solutions

Worked Solution 30.1 (see Problem 30.1)

See the worked solution for Problem 21.4 for a detailed explanation of the deterministic model. A MATLAB code for the deterministic part can take the form:

```
function iR=IRRFun(X)
I=X(1); %Initial CapEx (GBP)
A=X(2); %Annual OpEx (GBP)
B=X(3); %Annual benefits (GBP)
f=X(4); %Inflation rate (frac)
N=20; %Number of years
i0=0.02; %Initial guess for IRR
%Find current internal rate of return (IRR)
i=fzero(@(i) I+(A-B)*(1-(1+i)^-N)/i,i0);
iR=(1+i)/(1+f)-1; %Determine real IRR
```

A MATLAB code for the probabilistic part can take the form:

```
FUN=@IRRFun; %Function containing model
c=[200000 2000 22000 0.03]; %c parameters
%Incorporate plus or minus 20% uncertainty
abc=[c*0.8; c*1.2; c]; %a,b,c parameters
%Monte Carlo with triangular distribution
[PNE,yi,xj,yj]=MonteCarlo(FUN,abc,500);
%Determine P10, P50 and P90
yiSTATS=interp1(PNE,yi,[10 50 90]);
%Print results as a percentage
num2str(yiSTATS*100,3)
```

The MATLAB code for the MonteCarlo function is given in Listing 30.1. The P10, P50 and P90 values for the real IRR are found to be 2.57%, 4.53% and 6.98%, respectively. Note that the answers will vary slightly due to the random nature of the exercise.

Worked Solution 30.2 (see Problem 30.2)

See the worked solution for Problem 26.1 (b) (ii) for a detailed explanation of the deterministic model. A MATLAB code for the deterministic part can take the form:

```
function CMAX=MaxConcFun(X)
Mi0=X(1); %Emission rate (kg/s)
He=X(2); %Effective stack height (m)
u=X(3); %Wind speed (m/s)
dTdz=X(4); %Temperature gradient (K/km)
%Determine the location of maximum
%ground concentration, xMAX (m)
xMAXguess=1000; %Initial estimate of xMAX
FUN=@(x) -DispersionFun(Mi0,He,u,x,0,0,dTdz);
xMAX=fminsearch(FUN,xMAXguess);
%Determine the mass concentration at this location
```

```
CMAX=DispersionFun(Mi0,He,u,xMAX,0,0,dTdz);
%Convert to micro grams per m3
CMAX=CMAX*1e9;
```

The MATLAB code for the DispersionFun function is given in Listing 26.1.

A MATLAB code for the probabilistic part can take the form:

```
FUN=@MaxConcFun; %Function containing model
Xnames{1}='Emission rate (kg s-1)';
Xnames{2}='Effective stack height (m)';
Xnames{3}='Wind speed (m s-1)';
Xnames{4}='Temp. grad. (K km-1)';
c=[0.1099 100 5 -10]; %c parameters
%Incorporate plus or minus 20% uncertainty
abc=[c*0.8; c*1.2; c]; %a,b,c parameters
%Monte Carlo with triangular distribution
[PNE,yi,xj,yj]=MonteCarlo(FUN,abc,500);
figure(1); clf
subplot(1,2,1)
plot(yi,PNE,'k-')
xlabel('Maximum concentration (\mu g m-3)')
ylabel('Probability of non-exceedance (%)')
title('a) CDF')
subplot(1,2,2)
TornadoPlot(xj,yj,Xnames)
title('b) Tornado plot')
```

The MATLAB code for the MonteCarlo function is given in Listing 30.1. The MATLAB code for the TornadoPlot function is given in Listing 30.2.

The results are shown in Fig. 30.4. The Tornado plot tells us that the parameter that should be further researched first is the effective stack height. Note that ground surface concentration is negatively correlated with effective stack height and wind speed is a mitigating factor in this context. Temperature gradient seems not to have a significant bearing on the problem in this context.

Worked Solution 30.3 (see Problem 30.3)

See the solution for Problem 27.3 (e) for a detailed explanation of the deterministic model. A MATLAB code for the deterministic part can take the form:

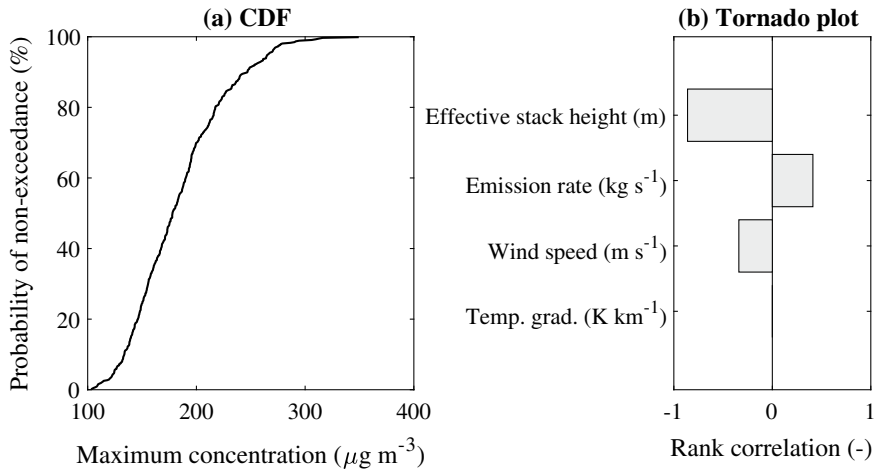


Fig. 30.4 Results for Problem 30.2 concerning maximum ground-level atmospheric NO_2 concentration, downstream of a polluting chimney stack. **a** Shows the cumulative distribution function (CDF) for the maximum ground-level concentration. **b** Shows a tornado plot illustrating the relative sensitivity of the different model parameters

```
function Umin=StreeterPhelpsFun(X)
Qe=X(1); %Effluent flow rate (m3/s)
BODe=X(2); %Effluent BOD_5 (mg/l)
Ue=X(3); %Effluent DO (mg/l)
Qu=X(4); %Upstream flow rate (m3/s)
BODu=X(5); %Upstream BOD_5 (mg/l)
Uu=X(6); %Upstream DO (mg/l)
kc=X(7); %Consumption rate (1/day)
W=X(8); %River channel width (m)
H=X(9); %Water depth (m)
Tc=X(10); %Water temperature (deg C)
%Determine ultimate BOD for effluent and upstream
Le=BODe/(1-exp(-5*kc));
Lu=BODu/(1-exp(-5*kc));
Q0=Qe+Qu; %Determine downstream flow rate
L0=(Qe*Le+Qu*Lu)/Q0; %Downstream BOD
U0=(Qe*Ue+Qu*Uu)/Q0; %Downstream DO
T=Tc+273.2; %Define temperature in Kelvin
%Define empirical coefficients
a=[-1.393441e2 1.575701e5 ...
-6.642308e7 1.243800e10 -8.621949e11];
%Determine the DO solubility limit, Us
Us=exp(sum(a./T.^[0:4]));
u=Q0/W/H; %Water velocity (m/s)
%Find reaeration rate (1/day) using Covar (1976)
if H<0.61
```



```

ka=5.32*u^0.67/H^1.85;%Owens et al. (1964)
elseif H>=0.61&H>3.45*u^2.5
ka=3.93*u^0.5/H^1.5;%O'Connor and Dobbins (1958)
else
ka=5.026*u^0.969/H^1.673;%Churchill et al. (1962)
end
G0=Us-U0; %Downstream DO deficit
u=u*24*60^2/1000; %Convert from m/s to km/day
%Determine distance to point of minimum DO
x=u/(ka-kc)*log(ka/kc*(1-G0/L0*(ka-kc)/kc));
%Determine DO deficit (mg/l)
G=kc*L0/(ka-kc)*(exp(-kc*x/u)-exp(-ka*x/u))...
+G0*exp(-ka*x/u);
%Determine DO concentration (mg/l)
Umin=Us-G;
if imag(Umin)~=0|Umin<0
Umin=0; %If <0 or complex then should be zero
end

```

A MATLAB code for the probabilistic part can take the form:

```

FUN=@StreeterPhelpsFun;
Xnames{1}='Effluent flow rate (m^3 s^-1)';
Xnames{2}='Effluent BOD_5 (mg l^-1)';
Xnames{3}='Effluent DO (mg l^-1)';
Xnames{4}='Upstream flow rate (m^3 s^-1)';
Xnames{5}='Upstream BOD_5 (mg l^-1)';
Xnames{6}='Upstream DO (mg l^-1)';
Xnames{7}='Consumption rate (day^-1)';
Xnames{8}='Width (m)';
Xnames{9}='Water depth (m)';
Xnames{10}='Water temperature (^oC)';
c=[0.15 90 2.3 0.9 2 8 0.4 10 1 10];
%Make incorporate plus or minus 10% uncertainty
abc=[c*0.9; c*1.1; c]; %a,b,c parameters
%Monte Carlo with triangular distribution
[PNE,yi,xj,yj]=MonteCarlo(FUN,abc,500);
figure(1); clf
subplot(1,2,1)
plot(yi,PNE,'k-')
xlabel('Minimum DO (mg l^-1)')
ylabel('Probability of non-exceedance (%)')
title('a) CDF')
subplot(1,2,2)
TornadoPlot(xj,yj,Xnames)
title('b) Tornado plot')

```

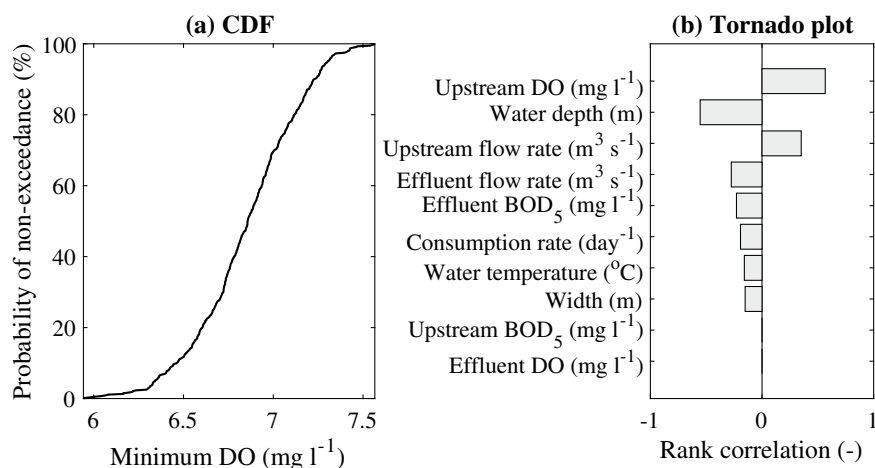


Fig. 30.5 Results for Problem 30.3 concerning dissolved oxygen (DO) concentration, downstream of a pollution discharger. **a** Shows the cumulative distribution function (CDF) for minimum DO concentration. **b** Shows a tornado plot illustrating the relative sensitivity of the different model parameters

The MATLAB code for the MonteCarlo function is given in Listing 30.1. The MATLAB code for the TornadoPlot function is given in Listing 30.2.

The results are shown in Fig. 30.5. Upstream DO concentration is positively correlated because the higher the upstream DO concentration the more DO there is provided to start with. Water depth is negatively correlated with minimum DO because the reaeration rate is inversely non-linearly proportional to water depth (Eq. 27.39). The upstream flow rate is positively correlated because the reaeration rate is non-linearly proportional to water velocity (Eq. 27.39). Zero rank correlations were reported for effluent DO concentration and upstream BOD₅ because these correlations failed their associated significance tests.

References

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