1
Preliminaries

In this chapter we set the scene by introducing the case studies of the following chapters. We also introduce the main physical concepts for diffusion and heat conduction, and show how to formulate the main partial differential equations that describe these physical processes. Finally, dimensionless variables are introduced and it is shown how to scale differential equations and boundary conditions to make them dimensionless.

1.1 Heat and diffusion — A bird's eye view

Here we give a basic physical description of mass transport and heat transport by diffusion. This provides the physical ideas needed to formulate an appropriate differential equation, which is done in the next chapter.

Diffusion

Diffusion is a physical phenomenon involving the mixing of two different substances. Some examples include salt in water, carbon in steel and pollution in the atmosphere.

A fundamental quantity is the ***concentration*** of one substance in another. This may be defined in several different ways. For example, the concentration can be measured as the ratio of the mass of one constituent to the total volume of the mixture (kilograms per litre). Another measure of concentration is the volume of one constituent to the total volume of the mixture.

Due to the random motion of constituent particles, concentrations tend to even out. Some molecules in a region of higher concentration move into a region of lower concentration. (See Figure 1.1.1).

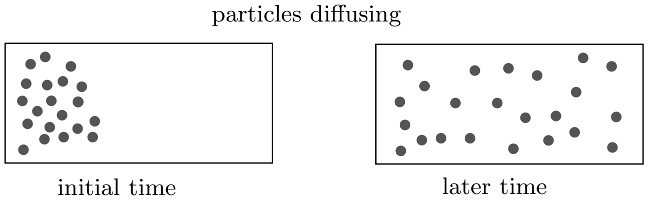

Fig. 1.1.1. The mechanism of diffusion — due to random motion of particles a high concentration redistributes towards a region of lower concentration.

Heat and temperature

An important thing to remember about modelling heat transport is that heat and temperature are ***not*** the same thing. Heat is a form of energy and may be measured in joules (the SI unit of energy). The heat energy of a rigid body is the kinetic energy due to the internal random motion of many vibrating constituent molecules. As heat is added to the body, energetic molecular collisions occur more frequently.

In the kinetic theory, temperature is interpreted as a measure of the average internal kinetic energy of constituent particles. The total heat energy is proportional to the temperature of an object and its mass; the latter being a measure of the number of particles. Temperature is a property that determines the ***rate*** at which heat is transferred to or from the object. Heat energy flows from hot (high temperature) to cold (low temperature). The temperature is defined according to a scale which depends on the expansion properties of certain materials. Temperature is usually measured in degrees Celsius (°C) or kelvin (K). Thus 10 °C means that mercury in a thermometer will rise to a given height, representing this temperature. Note that $0\,\mathrm{K} = -273\,°\mathrm{C}$. The Kelvin scale is designed to mean that 0 K corresponds to zero internal vibration (absolute zero).

This bird's eye view has deliberately been sketchy and incomplete. For more information on the kinetic theory of gases, the interested reader may consult almost any general introductory physics texts, such as Halliday and Resnick (1974). For the more general theory of thermodynamics, see for example (Feynman et al., 1977, Chapters 42–44).

1.2 Mathematics in industry

In this section we will briefly discuss general opportunities for applied mathematics in industry before focusing specifically on mathematical problems in heat and mass transport in the next section.

Opportunities for mathematicians

Mathematics is a subject that has been studied for several hundreds of years. Much new mathematics has been motivated by practical problems. On the other hand, mathematical models have also been used by industry to improve production, increase profits and generally improve understanding of complicated processes. There is a clear benefit to both mathematics and industry arising from the application of mathematics to industry.

In some countries (for example, Australia and New Zealand) industry puts less effort into research and development than do most other industrialised nations. However, this deficiency is now widely recognised in those countries and some remedial steps have been taken. Recent governments have provided various taxation incentives and assistance schemes for private companies to invest in their own research and development (although, more recently, this has unfortunately been cut back). This has opened up more employment opportunities for scientists, including applied mathematicians. Universities have made efforts to improve their level of collaboration with industry by setting up Industry Liaison Committees and forming consulting companies. Another source of contact between industry and academia throughout the world occurs through Mathematics and Industry Study Groups, pioneered at Oxford University in the United Kingdom. These bring together academics and representatives from industry to apply mathematics to industrially important problems in problem-solving workshops.

There are great benefits to be gained from employing applied mathematicians in industry. Optimisation skills are particularly important on the financial side. For engineering engineering many technical problems can be formulated as mathematical problems and thereby analysed and solved more efficiently. Mathematical models can be used to help understand the underlying physics, chemistry and biology of some processes. This understanding can then help to make the process more efficient. The financial savings can be considerable.

The applied mathematician working in an engineering or scientific environment must be a 'Jack' (or 'Jill') of all trades. That is, she or he must have good scientific general knowledge and also be skilled at formulating mathematical descriptions of practical problems. One advantage that an applied mathematician has is that because mathematics is a universal language he or she is able to communicate with other scientists from a wide variety of disciplines. The applied mathematician must be willing to be guided by other scientists in a team as to which physical variables are important and which directions the research should take once the initial mathematical model has been set up and validated.

Traditionally, applied mathematics students are taught mathematical methods and these are practised on standard problems which are already posed in mathematical form. It is more difficult to train someone to carry out the important first step of mathematical modelling, which is to take a practical problem and simplify or express it in a form which is amenable to mathematical analysis. Proficiency in formulating problems is usually obtained only after years of practice. However, there are some general principles which can be applied to some broad classes of problems, and these may be learnt. For example, heat and mass transport is based on the principle of conservation of energy and matter. As may be seen from reports of industrial study groups, there is considerable demand in industry for skills in this area.

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Glenn R. Fulford and Philip Broadbridge
Excerpt
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1.3 Overview of the case studies

In this book we will restrict ourselves to modelling those processes which involve transport of heat energy or mass. Industry provides many examples of the use of the standard equations of heat and mass transport and sometimes suggests interesting modifications to the basic theory.

Our primary aim is to study the industrial case studies that are described below. We will along the way, however, consider various other simpler industrial problems, as we develop sufficient physical and mathematical expertise with the phenomena of heat and mass transport. After developing skills for formulating appropriate partial differential equations we consider some analytical techniques for solving them.

Analytical techniques are useful for gaining physical insight. For very complex problems, numerical approaches are often used. It is often useful to start with a very simple model of a complex system whose equations yield an analytic solution. Then a more realistic model can be solved numerically. Together with the analytical results for the simpler models, the numerical results can yield maximum insight into the problem.

Continuous casting

One of the cases that we will study (Chapter 2) concerns a proposed technique of casting steel by pouring molten steel onto a cooled rotating drum. This is done to produce sheets of steel that are longer (and thinner) than those produced by pouring molten steel into moulds. The question we will try to answer is — under what circumstances will the process work? We will do this by predicting how fast the molten steel solidifies.

Water filtration

One method of extracting salt from water is to use a process called reverse osmosis. This involves water passing through a semi-permeable membrane and leaving the salt behind. In this process a major problem is that the salt accumulates at the semi-permeable membrane and restricts the passage of water through it. We will develop a simple diffusion model (Chapter 3) in an attempt to predict the salt buildup along the semi-permeable membrane. To do this we will introduce the method of stretching transformations as a method for solving the resulting diffusion equation.

Laser drilling

Another major case study we consider (Chapter 4) is where a high intensity laser or electron beam is focused on a sheet of metal. The laser drills a hole through the metal and we wish to predict how fast this occurs. This problem is of great interest in many industries where lasers are now being used for cutting and welding.

Factory fires

In another case study we will look at the previously unexplained sudden onset of fires in a New Zealand chipboard factory (Chapter 5) . The aim here is to determine if ignition can occur due to the heating of dust piling up on hot presses. Oxidation of the dust creates heat which may cause the dust to ignite. This is a situation that the factory must prevent from happening. Thus our aim is to use a mathematical model to determine for which thicknesses of dust layers ignition occurs.

Irrigation

An important part of primary industry is the production of food on farms. In arid regions (e.g. in many parts of Australia), irrigation is often used to provide water for crops. In the case study of Chapter 6 we investigate the optimal size for irrigation furrows. The mathematical content involves the solution of a partial differential equation for the unsaturated flow of water in soils by assuming an expansion in trigonometric functions to take advantage of the periodicity of the problem.

Mathematical modelling to help understand complex processes

These case study problems involve many processes happening at once. Mathematical modelling will be used to consider only the ***most important*** physical processes. This, in turn, will allow us to obtain sufficiently simple equations on which we can make good mathematical progress.

This leads to a much better understanding of the more complicated system.

The ability to recast real-world problems in mathematical form is a remarkable fact of history. For a clear account of the steps involved in the process of mathematical modelling, we refer to Fulford et al. (1997), Edwards and Hamson (1989) and Fowkes and Mahony (1994). For a philosophical consideration of the apparently unreasonable effectiveness of mathematics in the physical sciences, the interested reader is referred to the classic article Wigner (1960).

1.4 Units and dimensions

In the physical world measured quantities are determined relative to some standard measurements. It is important that equations developed as part of our modelling process are consistent no matter which units are the basis of our measurements. This is called dimensional consistency.

Units

Units of a physical quantity are the reference measurements to which we make comparisons. Some examples are metres, minutes, joules, miles, kilograms, etc. The same quantity can be measured in different units (e.g. 1 km = 1,000 m = 0.6214 miles). In this example, each unit (kilometre, metre or mile) refers to a quantity described by length.

We call length a ***primary quantity***. Some other primary quantities are mass, time and temperature. ***Secondary quantities*** are those which are combinations of more than one primary quantity. For example, in the SI system velocity is measured in metres per second, which is a secondary quantity.

A variable which measures length is said to have ***dimension*** length, denoted by the symbol $\mathtt{L}$. Thus a dimension $\mathtt{L}$ may take values of kilometre, metre or mile, depending on which system of units is adopted. Other dimensions, corresponding to some primary quantities, are mass, time and temperature, denoted by $\mathtt{M}$, $\mathtt{T}$ and Θ respectively. The four primary units relevant to this book are listed below in Table 1.4.1. For a primary or secondary quantity q, $[q]$ denotes the dimensions of the quantity represented by the symbol q. The value of $[q]$ is expressed in terms of $\mathtt{M}$, $\mathtt{L}$, $\mathtt{T}$ and Θ.

Table 1.4.1. *Fundamental units of primary quantities.*

Primary Quantity	Symbol	SI Unit	cgs Unit
mass	$\mathtt{M}$	kilogram, kg	gram, g
length	$\mathtt{L}$	metre, m	centimetre, cm
time	$\mathtt{T}$	second, s	second, s
temperature	Θ	kelvin, K	degree, °C

Other fundamental SI units include the ampere (A), the unit for electric current; the mole (mol), the unit for amount of a substance (i.e. the number of atoms or molecules); and the candela (cd), the unit for luminosity. All other units are derived from these base units and the ones in Table 1.4.1.

Rules for dimensions

Certain rules must be obeyed by a consistent set of units of measurement. They are mostly common sense. The rules are as follows:

(a) Two quantities may be ***added*** only if they have the ***same dimensions***. Quantities of different dimensions may be multiplied or divided.

(b) Index Laws. If $[f] = \mathtt{M}^{\alpha_1}\mathtt{L}^{\alpha_2}\mathtt{T}^{\alpha_3}\Theta^{\alpha_4}$ and $[g] = \mathtt{M}^{\beta_1}\mathtt{L}^{\beta_2}\mathtt{T}^{\beta_3}\Theta^{\beta_4}$ then $[fg] = \mathtt{M}^{\alpha_1+\beta_1}\mathtt{L}^{\alpha_2+\beta_2}\mathtt{T}^{\alpha_3+\beta_3}\Theta^{\alpha_4+\beta_4}$.

(c) Pure numbers are dimensionless, i.e. $[1] = 1$, $[2] = 1$, $[\pi] = 1$, $[0] = 1$. Thus multiplying by a pure number does not change the dimensions of a physical quantity, i.e. $[2m] = 1 \times \mathtt{M} = \mathtt{M}$.

(d) The dimensions of a derivative $\dfrac{\partial p}{\partial q}$ are $[p][q]^{-1}$. This is because a derivative is a limiting ratio of two quantities. Thus if u is temperature and x measures distance then $\left[\frac{\partial u}{\partial x}\right] = \Theta\mathtt{L}^{-1}$. Also $\left[\frac{\partial^2 u}{\partial x^2}\right] = \Theta L^{-2}$, and more generally,

$$\left[\frac{\partial^{m+n} u}{\partial x^m \partial t^n}\right] = \Theta\mathtt{L}^{-m}\mathtt{T}^{-n}.$$

(e) The dimensions of an integral $\int_a^b p\,dq$ are given by $[p][q]$.

(f) The arguments of functions having Taylor expansions (of more than one term) must be dimensionless. This is because this is the only way we can add different powers of a quantity. For example, for

$$e^{kt} = 1 + kt + \frac{1}{2!}k^2t^2 + \ldots$$

where t is time, then $[k] = \mathtt{T}^{-1}$ since kt must be dimensionless.

A useful way of checking equations is to check they are ***dimensionally homogeneous*** . This means that both sides of an equation must have the same dimensions. The following example illustrates this.

Example 1: *Newton's second law gives*

$$F = ma \tag{1}$$

where F is the force on a particle, m is its mass and a is the acceleration of the particle. Check that equation (1) is dimensionally homogeneous.

Solution: *Force is measured in newtons which are* $\mathrm{kg\,m\,s^{-2}}$. *Thus* $[LHS] = \mathtt{MLT}^{-2}$. *Now* $[m] = \mathtt{M}$ *and* $[a] = \mathtt{LT}^{-2}$. *Thus* $[RHS] = \mathtt{MLT}^{-2} = [LHS]$. *So (1) is dimensionally homogeneous.*

Checking equations

Dimensions of secondary quantities can easily be obtained from the above rules. The following example shows how to do this.

Example 2: *Fourier's law is an equation relating heat flux to temperature gradient (see Section 1.6),*

$$J = -k\frac{\partial u}{\partial x},$$

where J is the heat flux, u the temperature, x denotes distance and k is the conductivity. Hence determine $[k]$.

Solution: *The heat flux, J, is heat energy per unit area per unit time. So*

$$[J] = \frac{[\text{energy}]}{[\text{area}][\text{time}]}.$$

Now energy has the dimensions of work, which is force times distance, so $[energy] = \mathtt{MLT}^{-2} \times \mathtt{L}$, *and* $[area] = \mathtt{L}^2$. *Hence*

$$[J] = \frac{\mathtt{ML}^2\mathtt{T}^{-2}}{\mathtt{L}^2\mathtt{T}} = \mathtt{MT}^{-3}.$$

Now $[u] = \Theta$, *and* $[x] = \mathtt{L}$, *so*

$$\left[\frac{\partial u}{\partial x}\right] = \Theta \mathtt{L}^{-1}.$$

Since $[k] = [J] \times [\partial u/\partial x]^{-1}$ *then*

$$[k] = \mathtt{MLT}^{-3}\Theta^{-1}.$$

In SI units k is measured in $\mathrm{kg\,m\,s^{-3}\,K^{-1}}$. This is consistent with the above. For checking equations, Table 1.4.2 will be a useful reference.

Table 1.4.2. *Table of secondary quantities in mechanics and heat transport.*

Quantity	Dimensions	SI Units
density ρ	$\mathtt{ML}^{-3}$	$\mathrm{kg\,m^{-3}}$
velocity v	$\mathtt{LT}^{-1}$	$\mathrm{m\,s^{-1}}$
acceleration a	$\mathtt{LT}^{-2}$	$\mathrm{m\,s^{-2}}$
force F	$\mathtt{MLT}^{-2}$	newtons, N
pressure p	$\mathtt{ML}^{-1}\mathtt{T}^{-2}$	$\mathrm{N\,m^{-2}}$, pascal, Pa
energy E	$\mathtt{ML}^2\mathtt{T}^{-2}$	joule J
power $\dot{E}$	$\mathtt{ML}^2\mathtt{T}^{-3}$	watt W
heat flux J	$\mathtt{MT}^{-3}$	$\mathrm{W\,m^{-2}}$
heat conductivity k	$\mathtt{MLT}^{-3}\Theta^{-1}$	$\mathrm{W\,m^{-1}\,K^{-1}}$
specific heat c	$\mathtt{L}^2\mathtt{T}^{-2}\Theta^{-1}$	$\mathrm{J\,kg^{-1}\,K^{-1}}$
heat diffusivity α	$\mathtt{L}^2\mathtt{T}^{-1}$	$\mathrm{m^2\,s^{-1}}$
Newton cooling coefficient h	$\mathtt{MT}^{-3}\Theta^{-1}$	$\mathrm{W\,m^{-2}\,K^{-1}}$

1.5 Diffusion equations

The derivation of the one-dimensional diffusion equation is based on the idea of mass conservation. In this section we give a detailed formulation of the 1-D diffusion equation.