Industrial Mathematics

Case Studies in the Diffusion of Heat and Matter

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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).

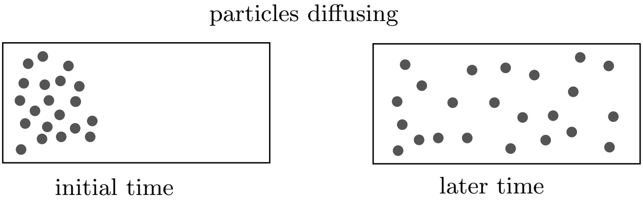

Fig. 1.1.1. The mechanism of diffusion — due to random motion of particles a high concentration redistributes towards a region of lower concentration.

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 $0\,\mathrm{K} = -273\,^\circ\mathrm{C}$. 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.

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 $[\mathit{energy}] = \mathtt{MLT}^{-2} \times \mathtt{L}$, *and* $[\mathit{area}] = \mathtt{L}^2$. *Hence*

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

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.

Diffusion in a tube

Consider a circular tube. Let A be the cross-sectional area of the hollow part of the tube. The hollow part is filled with a mixture containing a ***solute***. We assume the bulk mixture is ***not moving*** (but we consider this later in this section). However, if the solute concentration is higher at one end than at the other then the solute will diffuse towards the other end, as shown in Figure 1.5.1. We also assume the walls of the tube are impermeable to the solute.

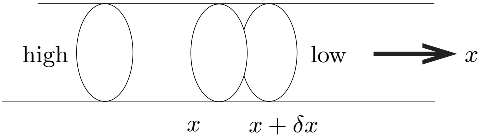

Fig. 1.5.1. Diffusion of a solute in a tube from high solute concentration to low solute concentration.

Let us define the concentration of the solute $C(x,t)$ as the ratio of the mass of the solute to the volume of the mixture. We can think of the concentration defined at a single point x by taking a small volume and then letting that volume tend to zero. Since the walls of the pipe are impermeable to the solute, the concentration of the solute will depend only on longitudinal position x and the time t.

We shall consider a small section x to $x+\delta x$ of the tube. As the solute diffuses through the tube the net change in the mass of the solute in the section is determined by the net difference in the mass of solute diffusing into and out of the tube. We can write this statement of conservation of mass as

$$\left\{\begin{matrix}\text{rate of}\\ \text{change of}\\ \text{solute mass}\end{matrix}\right\} = \left\{\begin{matrix}\text{net rate of}\\ \text{mass diffusing}\\ \text{in and out of section}\end{matrix}\right\}. \tag{1}$$

The term on the RHS refers to the net difference in rates of solute mass diffusing into the section and solute mass diffusing out of the section.

In terms of the concentration $C(x,t)$, the LHS of (1) can be written as the volume multiplied by the rate of change of concentration, evaluated at some internal point x_1, inside the section x to $x+\delta x$. Thus we write

$$\left\{\begin{matrix}\text{rate of}\\ \text{change of}\\ \text{solute mass}\end{matrix}\right\} = A\delta x \frac{\partial C}{\partial t}(x_1,t) \tag{2}$$

where $A\delta x$ is the volume of the section.

Let us define $J(x,t)$ to be the mass flux of the solute, defined as the net rate of mass of solute diffusing through a cross-section at x, per unit cross-section area, per unit time. We can now write the diffusion in terms of the mass flux J.

$$\left\{\begin{matrix}\text{net rate of}\\ \text{mass diffusing}\\ \text{in and out of section}\end{matrix}\right\} = J(x,t)A - J(x+\delta x,t)A.$$

Hence, the mass balance equation (1) now becomes

$$A\delta x\frac{\partial C}{\partial t}(x_1,t) = A\delta x[J(x,t) - J(x+\delta x,t)].$$

Dividing by $A\delta x$, we obtain

$$\frac{\partial C}{\partial t}(x_1,t) = -\left[\frac{J(x+\delta x,t) - J(x,t)}{\delta x}\right].$$

We now let $\delta x \to 0$ and we thus obtain

$$\frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x}, \tag{3}$$

using the definition of the partial derivative. Note that, as $\delta x \to 0$ we also have $x_1 \to x$, where $x < x_1 < x + \delta x$. Now ***all*** quantities are evaluated at the point x.

To relate the flux to the concentration we need a ***constitutive equation*** (an equation relating material variables, determined from experiments). The simplest one is ***Fick's law*** which states the mass flux is proportional to the concentration gradient. For 1-D diffusion, Fick's law can be written

$$J(x,t) = -D\frac{\partial C}{\partial x}(x,t) \tag{4}$$

where D is a positive constant known as the ***diffusivity***. Note the minus sign is included so that the solute diffuses in the direction of decreasing concentrations. Fick's law for diffusion is analogous to Fourier's law for heat conduction.

Substituting Fick's law (4) into the mass conservation equation (3) we obtain

$$\boxed{\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad (5)}$$

which is known as the 1-D diffusion equation.

Advection

Advection is where the solute is carried along with the bulk movement of the fluid. We can think of the mass flux J to be due to both diffusion and advection, so $J = J_d + J_a$. The mass flux at position x is the rate of movement of mass per unit time per unit area through the cross-section at x.

Let $v(x, t)$ denote the fluid velocity (of the mixture). In the absence of diffusion the solute particles move at the same speed as the mixture. The total mass of solute that is transported through the cross-section is the volume of mixture moving past the cross-section in a time δt multiplied by the concentration. This volume is $vA\delta t$. Thus the mass flux due solely to advection is given by

$$J_a(x, t) = v(x, t)C(x, t).$$

Using Fick's law for the mass flux due only to diffusion of solute particles relative to the mean flow of the mixture, the total mass flux is given by

$$J(x, t) = v(x, t)C(x, t) - D\frac{\partial C}{\partial x}.$$

Substituting this into the mass conservation equation (3) we obtain the partial differential equation for the concentration

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(v(x, t)C(x, t) - D\frac{\partial C}{\partial x}\right)$$

which may be written as

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(vC) = D\frac{\partial^2 C}{\partial x^2}. \tag{6}$$

If the moving mixture is an incompressible fluid then $v(x, t)$ is a constant. This follows from conservation of mass applied to the mixture — the mass flowing in $\rho A v$, where ρ is the density of the mixture, must be constant. The previous equation (6) then simplifies to

$$\frac{\partial C}{\partial t} + v\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}. \tag{7}$$

Turbulent diffusion

So far we have thought about diffusion as due to random motion of molecules of a solute. However, the diffusion equation can occur in a wider context. In many air flows, especially on environmental scales, the velocity is turbulent. This means the velocity has a random component. Thus air pollution, for example, can be advected with the mean flow while simultaneously mixing with the air due to the random component of the air flow. This type of diffusion is called ***turbulent diffusion***. In general this is a very complicated process that is not fully understood. In the simplest turbulent transport models, an eddy diffusivity is incorporated to relate turbulent flux to the gradient of mean concentration. (See Launder and Spalding (1972) for a more detailed discussion of the theory of eddy diffusivity. Wilcox (1994) and Weil (1988) give some extensions of this theory.) The value of the eddy diffusivity is usually several orders of magnitude larger than the diffusivity for molecular diffusion. In many problems it is typical for the diffusivity not to be constant. For example, the air becomes more turbulent with height from the ground.

For non-constant diffusivity, say $D(x)$ the governing equation for the concentration is not

$$\frac{\partial C}{\partial t} = D(x)\frac{\partial^2 C}{\partial x^2}.$$

A careful consideration of the derivation of the diffusion equation shows the appropriate form is

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial C}{\partial x}\right).$$

The generalised 1-D diffusion equation

We can consider the effects of advection, nonlinear diffusivity, and internal mass production. ***Nonlinear diffusivity*** occurs when the diffusivity depends on the concentration. ***Internal mass production*** is where the solute is created everywhere within the region of consideration (e.g. by some chemical reaction). Formulations of the modified diffusion equations for each of these phenomena are explored in the problems at the end of this chapter (see Question 6).

The results are summarised in the generalised 1-D diffusion equation

$$\boxed{\frac{\partial C}{\partial t}+\frac{\partial}{\partial x}(vC)=\frac{\partial}{\partial x}\left(D(C)\frac{\partial C}{\partial x}\right)+M. \qquad (8)}$$

Here v is the bulk velocity of fluid flowing through the tube and the term M is the rate of production of solute, per unit time per unit volume. When the fluid motion is incompressible (so that the velocity v is independent of x) then the generalised 1-D diffusion equation simplifies to

$$\frac{\partial C}{\partial t}+v\frac{\partial C}{\partial x}=\frac{\partial}{\partial x}\left(D(C)\frac{\partial C}{\partial x}\right)+M.$$

The 3-D diffusion equation

A similar type of argument for mass transport yields the 3-D diffusion equation for concentration $C(\mathbf{x},t)$,

$$\boxed{\frac{\partial C}{\partial t}=D\nabla^2 C \qquad \text{where} \quad \nabla^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2} \qquad (9)}$$

in cartesian coordinates (x,y,z).

For 3-D problems, the generalised diffusion equation is

$$\boxed{\frac{\partial C}{\partial t}+\boldsymbol{\nabla}\cdot(\mathbf{v}C)=\boldsymbol{\nabla}\cdot(D(C)\boldsymbol{\nabla}C)+M \qquad (10)}$$

where $D(C)$ is the concentration dependent diffusivity and M is the rate of production of mass of solute, per unit time per unit volume. For fluid flow which is incompressible ($\boldsymbol{\nabla}\cdot\mathbf{v}=0$) the 3-D generalised diffusion equation simplifies to

$$\boxed{\frac{\partial C}{\partial t}+\boldsymbol{\nabla}\cdot(\mathbf{v}C)=\mathbf{v}\cdot\boldsymbol{\nabla}C+M. \qquad (11)}$$

The reader who is familiar with fluid dynamics will recognise the advection term as coming from the ***material derivative*** (differentiation following the motion), see e.g. Acheson (1990).

1.6 Heat conduction equations

The fundamental equation describing heat conduction is a partial differential equation known as the ***heat conduction equation*** (or heat equation, for short). In this section we will see how to derive this equation for heat conduction along a long thin rod. The basic idea is that energy is conserved. We consider an infinitesimal section through the rod and account for the amount of heat energy entering and leaving the section. This rather simple approach can then be used on more complicated problems involving advection (heat carried along with a moving fluid), heat generation (e.g. by electrical resistance or chemical reaction), heterogeneity (different positions have different thermal properties) and nonlinearity (conductivity is temperature dependent).

Heat balance

Consider the heat flow in a ***solid*** rod with circular cross-section A. Assume that the surface of the rod is perfectly insulated so that no heat escapes radially. Thus the direction of heat flow is only in the longitudinal direction (along the axis of symmetry of the rod). Suppose that the rod is initially at a uniform low temperature. Then one end is suddenly raised to a higher temperature. Heat flows in the x-direction, from hot to cold, as shown in Figure 1.6.1.

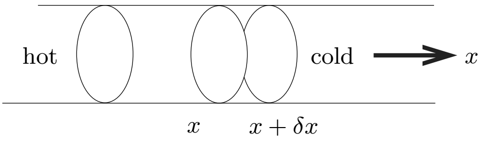

Fig. 1.6.1. Heat conduction in a rod.

Let δx be the thickness of a section through the rod located at the point x, where δx is taken to be very small compared to x. As the heat flows along the rod some of the heat will be absorbed by the rod as it raises the temperature of the rod. As a result of this, as heat flows into the cross-section at x a different amount of heat flows out at $x + \delta x$. We can write

$$\left\{\begin{array}{c}\text{rate of}\\ \text{change of}\\ \text{heat content}\end{array}\right\} = \left\{\begin{array}{c}\text{net rate of}\\ \text{heat conducted}\\ \text{in and out of section}\end{array}\right\} \tag{1}$$

by conservation of energy. This assumes that there is no heat production inside the rod or heat loss from the surface of the rod.

Formulating the equation

Let us now introduce some notation. Let $u(x,t)$ denote the temperature of the rod at position x at time t. Because there is no radial flow then the temperature will be constant over the cross-section provided it was constant initially.

Let us also define the ***heat flux*** $J(x,t)$ as the rate of heat passing through a cross-section, per unit area, per unit time. In terms of the heat flux, the term on the RHS of equation (1) becomes

$$\left\{\begin{array}{c}\text{net rate of}\\ \text{heat conducted}\\ \text{in and out of section}\end{array}\right\} = J(x,t)A - J(x+\delta x,t)A. \tag{2}$$

We now relate the LHS of equation (1) to the temperature. Some of the heat energy is absorbed by the rod and causes a change in the temperature of the rod. In a small time δt the temperature at x is changed by an amount $u(x,t+\delta t)-u(x,t)$ The amount of heat required to change the temperature of the entire mass of the section by this amount is proportional to both the mass of the section and the temperature difference. Thus

$$\left\{\begin{array}{c}\text{rate of}\\ \text{change of}\\ \text{heat content}\end{array}\right\} = c\rho A\delta x\,\frac{\partial u}{\partial t}(x_1,t) \tag{3}$$

where x_1 is some internal point $x < x_1 < x+\delta x$. Here $A\delta x$ is the volume of the section, ρ is the density and c is a proportionality factor called the specific heat. The specific heat is often taken to be constant, for a particular material, provided the temperature variation is not too great.

Substituting equations (3) and (2) into equation (1), and dividing by the product δx, we obtain

$$\rho cA\frac{\partial u}{\partial t} = -\frac{[J(x,t) - J(x+\delta x,t)]}{\delta x}A. \tag{4}$$

Letting δx tend to zero we obtain, in the limit, (alternatively, take Taylor series of each of the terms)

$$\rho c\frac{\partial u}{\partial t} = -\frac{\partial J}{\partial x}. \tag{5}$$

Note the minus sign on the RHS of equation (5). Equation (5) is the basic transport equation in one dimension. It needs to be supplemented by a constitutive equation which relates the heat flux J to the temperature u. For heat conduction we use Fourier's law.

Fourier's law

We now relate the RHS of equation (5) to the temperature. To a good approximation, for many solids, the heat flux is proportional to the temperature gradient. This is known as Fourier's law after the French mathematician and scientist, Fourier, who in 1822 published the first book on the mathematical theory of heat (and who is also famous for Fourier series and Fourier transforms).

Fourier's law may be written

$$J(x,t) = -k\frac{\partial u}{\partial x}(x,t) \tag{6}$$

where the proportionality factor k is known as the ***thermal conductivity***. In some heat flow problems k can be a function of u, x or t. However, it is usual in mathematical modelling to make the simplest assumption initially; $k =$ constant. Later, we might relax this assumption if necessary.

Substituting Fourier's law (6) into the energy conservation equation (5) we obtain

$$\rho c\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2},$$

taking the conductivity k to be constant.

This equation is often written in the form

$$\boxed{\frac{\partial u}{\partial t} = \alpha\frac{\partial^2 u}{\partial x^2}, \qquad \alpha = \frac{k}{\rho c}, \qquad (7)}$$

known as the ***heat equation***. Note the similarity in form to the diffusion equation from Section 1.5. Here the constant $\alpha = k/\rho c$ is called the ***heat diffusivity***. It characterises the ability of heat energy to diffuse through a given material. The heat equation (7) is a partial differential equation in two independent variables, time t, and position x.

Extensions of the heat equation

Modifications of the basic heat equation include heat sources, advection, and temperature dependent conductivity. A generalised heat equation, incorporating all of these is

$$\rho c\left(\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}(vu)\right)=\frac{\partial}{\partial x}\left(k(u)\frac{\partial u}{\partial x}\right)+Q \tag{8}$$

where $v(x,t)$ is the speed of a fluid, Q is the rate of heat produced internally in the fluid, per unit volume, per unit time and $k(u)$ is the temperature dependent conductivity. If the fluid flow is incompressible, then v is independent of x, and the generalised 1-D heat equation simplifies to

$$\rho c\left(\frac{\partial u}{\partial t}+v\frac{\partial u}{\partial x}\right)=\frac{\partial}{\partial x}\left(k(u)\frac{\partial u}{\partial x}\right)+Q.$$

A heat source can arise through an exothermic reaction within the material which generates heat at every point. It can also arise from an electric current which creates heat within the material as it experiences electrical resistance. Another way heat can be generated within a material is by nuclear fission in a nuclear fuel rod.

Advection is where heat is transported due to bulk movement of a fluid. This is sometimes referred to as convection in the context of heat. (See Section 1.5 for an explanation of advection for mass transport.) Suppose we have a fluid which is moving with velocity $v(x,t)$. In this case heat is transported both by conduction and by advection, due to bulk movement of material and also due to random movement of molecules. The term $\rho c\partial(vu)/\partial x$ in the above equation arises due to advection. When the movement of fluid is due to buoyancy (with hot fluid being less dense than cold fluid and therefore rising), the heat transport is known as convection.

The conductivity of a material will often vary with temperature, if the range of temperatures is large. The functional dependence of k on u will be determined experimentally. Note that, in equation (8), the term $k(u)$ must stay inside the $\partial/\partial x$ term, unless k is constant with respect to u.

The 3-D heat conduction equation

If the temperature depends on more than one spatial variable then we need to account for heat fluxes in different directions. This is accomplished by defining a vector valued heat flux.

We can define the vector heat flux $\mathbf{J}(\mathbf{x}, t)$. The direction of the vector is the direction of heat flow at the point $\mathbf{x}$, and its magnitude is the rate of heat flow per unit area, per unit time.

We must generalise Fourier's law to three dimensions. Recall that the 1-D version of Fourier's law stated that the heat flux was proportional to the temperature gradient. Thus in three dimensions

$$\mathbf{J}(\mathbf{x}, t) = -k\boldsymbol{\nabla} u \tag{9}$$

where k is the thermal conductivity. This gives the direction of heat flow as the direction of maximum rate of decrease of temperature (since from vector calculus the gradient gives the direction of maximum rate of increase). Also, we have assumed that the material is ***isotropic*** which means that there is no preferred direction of heat flow within the material itself. If a material were non-isotropic then (9) would need to be generalised to a linear combination of the partial derivatives of the temperature.

By assuming conservation of heat energy for an arbitrary region, and using the divergence theorem, it is possible to derive the 3-D heat equation (details are left to the exercises, see Question 8 for the mass diffusion case)

$$\rho c \frac{\partial u}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{J} = 0. \tag{10}$$

Substituting Fourier's law (9) into the transport equation (10) we obtain

$$\rho c \frac{\partial u}{\partial t} = k\nabla^2 u \qquad \text{where} \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$

Dividing by ρc gives

$$\boxed{\frac{\partial u}{\partial t} = \alpha \nabla^2 u, \qquad \text{where} \quad \alpha = \frac{k}{\rho c}. \qquad (11)}$$

This is the three-dimensional generalisation of the linear heat equation.