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John Dowden (Ed.)

The Theory of Laser Materials Processing

Heat and Mass Transfer in Modern Technology

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Preface

The use of lasers in materials processing has become widespread in recent years, so that an understanding of the nature of heat and mass transfer in this branch of modern technology is of increasing importance. The aim of the authors of this book is to concentrate on the physical processes; these can be developed from a mathematical point of view, or from direct experimentally-derived observation. The two approaches are complementary; each can provide insights and the synthesis of the two can lead to a very powerful understanding of the processes involved. Mathematical modelling of physical processes has had an important role to play in the development of technology over the centuries and particularly so in the last one hundred and fifty years or so. It can be argued that it is more important today than ever before since the availability of high-speed computers allows accurate numerical simulation of industrial processes at a fraction of the cost of the corresponding experiments. This is one aspect of mathematical modelling, high profile and much valued, but it is not the only one.

In the past mathematical modelling had to rely on qualitative investigation, very special analytical solutions, or inaccurate and time-consuming calculations performed with little in the way of tabulated or mechanical assistance. Log tables and slide rules are still remembered by people working today, though there are surely few who regret their disappearance.

The value and distinctive function of methods based on the analytical approach is now becoming much clearer, now that they are no longer expected to produce detailed imitations of what happens in real experiments of industrial processes, a function now fulfilled mostly by numerical methods, considered below. The emphasis today is on their ability to confirm and extend our understanding of the basic physical mechanisms involved in the processes of interest. These are essential for any intelligent use of numerical simulation.

The argument about the value of teaching people how to do arithmetic themselves without the aid of a calculator seems to be passing into history,

but it is an important one and provides a simple analogy. If someone does not have a feeling for numbers and the way arithmetic works, they will all too easily fail to spot an error produced by a machine. Computers are not infallible – and neither are those who build or program them. Computers are now taking on less mundane mathematical tasks and the same controversies are appearing in connection with algebraic manipulation. Equally, and with even greater penalties in terms of cost in the event of errors, the same considerations apply to numerical simulation of major industrial processes. Awareness of the analytical solutions can be invaluable in distinguishing the right from the wrong, i.e. for the practitioner to understand the basis of the work, and to have an idea of the kinds of outcomes that are plausible – and to recognise those which are not.

The phrase "mathematical modelling" is, however, ambiguous, perhaps more now than it has ever been. There is an enormous amount of work done today on simulation based on the use of very powerful computer programs, and it is quite correctly referred to as mathematical modelling. The programs are sometimes constructed in-house but are usually commercial packages. This is an entirely valid approach with specific (generally commercial) objectives. In general there are two uses. The dominant objective is numerical agreement with a particular experiment in the first instance, leading to predictive commercial use in the second instance. The second objective is the clarification of physical mechanisms, aimed at the generation of understanding of complex interconnected processes, rather than the exact reproduction of a particular experiment. It is sometimes overlooked that, with sufficient care, a numerical approach is equally valid in the investigation of physical fundamentals. Numerical simulation is not a central topic of this book, but because of its crucial importance to each of the two uses to which numerical modelling can be put, it is vital that the computational basis of the work should be completely sound. In addition, the level of process detail which can be considered by the numerical approach usually exceeds what is possible with the analytical approach significantly, leaving little choice but to revert to the numerical treatment when investigating the interconnections between processes. It is for these reasons that the book concludes with a chapter on comprehensive numerical simulation.

In many ways, the approach adopted here is complementary to the more phenomenological approach. It is always important in a field which has very direct industrial applications to bear in mind how techniques such as those described here will be used, but it is essential not to lose sight of the fundamentals. There are serious safety implications; there are cost implications; there are moral implications; there are considerations of the appropriateness of the technology to the application under consideration. A proper respect for all these requires an understanding of the fundamentals.

We are all too well aware that this book does little more than scratch the surface of the problems involved in a fundamental understanding of these phenomena. If we have provided ideas and information that cause others to

test them experimentally or intellectually, agree with them or dispute them vigorously, and develop them further, we will consider that we have achieved our aim.

Colchester
April, 2008 *John Dowden*

Contents

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Mathematics in Laser Processing

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Abstract. Methods by which physical laws can be converted into mathematical form as partial differential equations are discussed. Associated with these equations are boundary conditions, or the conditions to be applied at the interface between regions in which different regimes apply, represented by a discontinuity in some or all aspects of the variables describing the mathematical system. The manner in which the form of these conditions can be deduced is considered. The principles described are illustrated by application to some of the physical laws at the centre of laser technology.

1.1 Mathematics and its Application

The study of the theory of a technological discipline nearly always requires a return to its underlying physical principles. These in turn are usually expressed in their most general form in terms of standard language: the many different forms in which Newton's Laws of Motion are expressed provide a familiar example. All too often, however, the use of standard language proves to be far too cumbersome for the further investigation of technological processes and problems. In practice, *Mathematics* has been found to provide a convenient and concise tool for the purpose, as it has in science as a whole. The well-known assertion that "Mathematics is the Language of Science" is often attributed to Galileo (in his book, *The Assayer*) although it would be more accurately expressed, and closer to Galileo's original statement, to say that the language of science is mathematics.[1]

Mathematics is now proving to be an invaluable tool in the investigation of subjects which had not formerly been thought of as natural fields for its use. It is an intellectual discipline in its own right independently of science, as Galileo recognised, or from any other discipline in which it is used as a

[1] Indeed, Galileo went even further. The Assayer contains his well-known statement that mathematics is the language of God. (http://en.wikipedia.org/wiki/The_Assayer).

tool, but there has been a long history of beneficial interaction between it and its fields of application. Physics, engineering and modern technology are examples of the greatest importance.

Thus it is that the underlying physical principles of the theory of the applications of laser technology are well suited to expression in mathematical form, and their consequences investigated using mathematical techniques. Many of the laws of physics are expressed, either explicitly or implicitly, in terms of macroscopic objects or concepts. These are not necessarily the best starting point for mathematical investigation. In the past, it has been found helpful to convert them into other forms, in terms of concepts defined as abstractions; an example of such an abstraction is the mathematical process of differentiation. Similarly, numerical methods often resort to a kind of half-way house since digital computers are unable to deal with the true mathematical limit, a concept which rarely, if ever, has any real physical meaning; one only has to consider the concept of the density of an object at a point to realise that there are problems, when the atomic model of matter is called to mind.

This chapter therefore deals with the way in which some well-known physical laws can be converted into idealised mathematical forms expressed in terms of differential equations.

When attempts are made to solve differential equations, it rapidly becomes obvious that an important part of the statement of the mathematical problem consists of the boundary conditions, or, if there are surfaces at which discontinuities occur, the appropriate interface conditions. The derivations of these from the underlying principles are considered in the same way that the equations themselves are derived.

The language of mathematics is used freely in this book, in addition to the standard terminology of the fields of study of the individual chapters. On the whole, specialist (or relatively rare) terminology is not defined if it is standard in the field under discussion, and a reader who encounters a word that is unfamiliar is encouraged to look for its definition in the literature of the field; the World Wide Web will be found to be an invaluable resource in this connection – in doing so, the reader may also find a great deal of helpful additional material.

An exception is being made of the term "ansatz", which is current amongst theoretical physicists. One definition is given in the On-Line edition of the Oxford English Dictionary, but a much better one is provided by Wikipedia, which gives its meaning as

"In physics and mathematics, an **ansatz**... *is an educated guess that is verified later by its results. An* ansatz *is the establishment of the starting equation(s) describing a mathematical or physical problem. It can take into consideration boundary conditions. After an ansatz has been established, the equations are solved for the general function of interest. Typically, a word problem starts by writing down the* ansatz *with subsequent refinement leading to the solution of the problem."*

(http://en.wikipedia.org/wiki/Ansatz). There is no really satisfactory single word available in the less specialist mathematical literature, and it is used from time to time in this book in the sense described. As the Wikipedia definition says so well, it encapsulates one of the fundamental methods by which solutions to mathematical problems may be obtained. A colloquial alternative might be "inspired guess" – but it is an inspired guess that has to be rigorously justified.

The approach adopted here is in many ways complementary to that adopted in works such as those of Steen [1] and von Allmen and Blatter [2]. Steen's work, for example, is much more pragmatic. It must never be forgotten that laser technology is a rapidly evolving field with applications of the utmost importance, so it is essential to bear in mind the ways in which the theory will be used. Conversely, it is essential for the developer and indeed the end-user not to lose sight of the fundamentals; without understanding, there is always the danger of inadvertent error.

1.2 Formulation in Terms of Partial Differential Equations

1.2.1 Length Scales

Most laws in physics, at least at the macroscopic level, are statements about ideal objects; to be of interest they must nonetheless represent something with some kind of tangible reality. Examples are the "bodies" that appear in Newton's Laws of Motion and his Theory of Gravitation, electric charge, magnetic poles, and so on. Often these concepts are sufficient in themselves to solve important problems, but there are a great many circumstances where it is simply not practicable to deal with large numbers of these ideal objects. The behaviour of a moving liquid provides a familiar example, where the concept of an atom might be thought of as providing a point mass, but is really very little help at the basis for the analysis of weather forecasting, for example. The differences between the length and time scales of the basic entities and the subject of study are just too great. The problem is frequently tackled by re-phrasing the laws in such a way that they can cope with large numbers of the basic entities at once, and in that way statements are obtained which are usually best expressed in mathematical form with the use of integrals, often over an arbitrary surface, or volume in space. Some of the laws of electromagnetism, Faraday's law for example, are really integral statements in themselves and are therefore naturally expressed in mathematical form in this way.

Although the expression of physical laws as integrals is elegant, such a formulation has not, in the past at least, provided an easy way to solve problems since appropriate techniques did not exist. The traditional way round the problem was to convert the integral statements into differential equations. Since the days of Newton and Leibnitz a vast array of techniques have been developed to solve problems using the analytical techniques of differential

calculus. These have been applied very successfully, and were more or less the only resource available until the advent of high speed computers.

All the same there can be a philosophical problem with the approach since differential calculus has at its heart the use of the limiting process as some quantity tends to zero; it might be a length, or a time, or a volume... but whichever it is, there is a difficulty when one remembers that very often the formulation as an integral was used to avoid problems associated with small entities. The modelling approach behind calculus techniques assumes that there are properties (mass density, for example) that have a clear trend to their properties as the size of the volume (in the case of mass density) decreases; it is then assumed that the apparent trend can be extrapolated downwards to a vanishingly small size, even though such a process is impossible when thought of in terms of the more fundamental physical entities (atoms, for example). It is then possible to construct a value at a point, derivatives, etc. It is assumed that this *continuum approximation* can be used to deduce properties of the system that, on a large scale, are not inconsistent with the properties of the real system; the assumption is made even though the process of taking progressively smaller scales does not produce any kind of regularity in the limit in reality. The assumption itself is sometimes called the "continuum hypothesis" (not to be confused with Cantor's continuum hypothesis in set theory). See for example, Batchelor [3], §1.2. In the case of gases, the approximation can only be used if the *Knudsen number* is small. The Knudsen number, Kn, is the ratio of the molecular mean free path length to a characteristic physical length scale of the problem under consideration and is useful in the description of the flow of low-density gases. In particle dynamics, the mean free path (m) is

$$\frac{k_B T}{\pi \sigma^2 p \sqrt{2}}$$

where k_B (J K^{-1}) is Boltzmann's constant, σ (m) is the particle diameter and p (Pa) is the total pressure.

1.2.2 Conservation Equations and their Generalisations

A number of ideas of fundamental importance in the sciences take the form of conservation statements, a well-known example being the principle of conservation of energy. A very much larger class of fundamental ideas in physics however can be thought of as statements of the ways in which some quantity is not conserved; there may be processes whereby it is generated or destroyed or, equivalently, transferred into or out of another system that is analysed separately. The process by which such statements can be converted into partial differential equations is described in detail in Sect. 2.1.1 of [4]; it can be summarised as follows.

In the absence of generation or destruction terms, they are referred to as *conservation* equations. It is a not ideal terminology, not least because

the most famous conservation equation of all, the equation of conservation of energy for a single particle moving in a conservative field of force, is not of this form as usually stated. When generation or destruction terms are present, terminology for the resulting equations is not standard. Possibilities are to refer to them as *balance*, *generation* or *transfer* equations. The terminology that will be preferred here is to call them *generalised conservation equations* or, following [5], just *conservation equations*; both generation and destruction effects can then be included, distinguishing them only by the sign of the relevant term.

For many quantifiable physical properties Ω there is a relation between the way in which it increases (or decreases) in V and the manner in which Ω is introduced into V. Such a relationship can be summarised by saying that

- The net rate of increase of Ω in V is equal to the net rate of generation of Ω inside V and on its surface S, less its net rate of outward flow across S. (1.1)

The process of derivation of the mathematical form of such a statement can be summarised as follows.

First, in the case when all aspects of the physical process can be adequately described in terms of continuous functions, an assumption of sufficient differentiability will be made. The method will only be applied to properties that can be properly described in terms of scalars, vectors, or tensors of any order. When it is helpful to do so, the notation of rectangular Cartesian tensors will be employed, including the use of Einstein's summation convention with a comma separator to indicate differentiation. A vector $\mathbf{v}$, for example, has three components v_i $(i = 1 \ldots 3)$ and its divergence will be written

$$\nabla \cdot \mathbf{v}, \quad v_{j,j} \quad \text{or} \quad \frac{\partial v_j}{\partial x_j}.$$

Suppose Ω is defined at every point in some region of space V contained within the domain of investigation D, and that

- there is a density k_* units of Ω per unit volume at each point of V, where k_* is a tensor of order $r \geq 0$ with $_*$ indicating an appropriate set of r subscripts;
- there is a flow Q_{*i} defined at each point of D so that the direction of flow and magnitude of the quantity whose density is measured by k_* is Q_{*i} units of Ω per unit area per unit time;
- at an element with an outward unit normal $\mathbf{n}$ of the surface S of V, there is a rate of generation $G_{*j}n_j$ units of Ω per unit area of S per unit time.
- a net number q_* units of Ω are generated per unit volume per unit time.

In these statements the region V can be any region, big or small, contained within D, so that it and its bounding surface S can be conceptual rather than physically distinct entities, and S is a part of V. Again, they will be considered

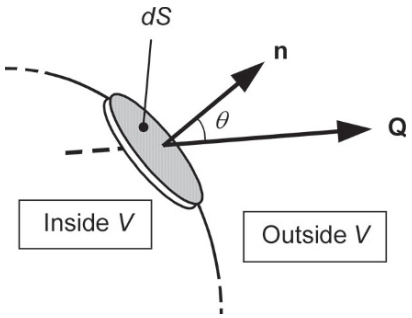

Fig. 1.1. Flow out of V across S in the case when the flow is a vector, $\mathbf{Q}$. The component of $\mathbf{Q}$ in the direction of $\mathbf{n}$ is $\mathbf{Q}\cos\theta$.

to be fixed in space for the moment, though that also is a condition which can be relaxed. The general configuration is shown in Fig. 1.1 for flow across S in the case when the flow is a vector, $\mathbf{Q}$. The same applies to the surface generation term except that in that case $\mathbf{G}$ cannot be considered as crossing the surface, but rather as being generated at it.

In the third property of the four properties of $\mathcal{Q}$, the discussion will be limited to the case where G_{*i} is independent of the orientation of the surface element. The third property is essentially the same as the second but the distinction is helpful when it comes to the physical origins of the respective terms; the two forms are usually thought of in quite different ways. The third is somewhat similar to Newton's Third Law of Motion, in that it shows how regions may be combined in the same way that the Third Law of Motion shows how bodies may be aggregated.

For a true conservation condition, G_{*i} and q_* are both identically zero.

Mathematically, the generalised conservation statement can be written

$$\frac{d}{dt}\int_V k_* dV = \int_V q_* dV - \int_S Q_{*j} n_j dS + \int_S G_{*j} n_j dS. \tag{1.2}$$

The two last terms in the equation correspond to the second and third of the properties above and are very similar in a formal sense; as already noted, they are worth distinguishing since they tend to arise for physically different reasons.

Since the region V is required to be fixed in space, the time derivative can be taken inside the integral. Suppose that $G_{*i} - Q_{*i}$ is a continuously differentiable field defined in a neighbourhood of V. Gauss's Theorem can be applied to the two surface integrals so that equation (1.2) can be written

$$\frac{1}{V}\int_V \left(\frac{\partial k_*}{\partial t} + \frac{\partial Q_{*j}}{\partial x_j} - \frac{\partial G_{*j}}{\partial x_j} - q_*\right) dV = 0. \tag{1.3}$$

This result is true whatever the size or shape of V provided only that it lies in D. If the volume V is taken to contain a particular point $\mathbf{x}$, and all points of V are within a distance d of it, the limit as d tends to zero of the left hand side has the value of the integrand at $\mathbf{x}$, provided that it is continuous. The argument can be applied at any point $\mathbf{x}$ of D and so (1.2) has the equivalent mathematical form

$$\frac{\partial k_*}{\partial t} + \frac{\partial Q_{*j}}{\partial x_j} = q_* + \frac{\partial G_{*j}}{\partial x_j}. \tag{1.4}$$

1.2.3 Governing Equations of Generalised Conservation Type

Table 1.1 provides some examples.

Comments in connection with some of these examples are necessary.

Flow of a Viscous Fluid

In the case of the Navier-Stokes equations (1.6) the bulk viscosity μ_B (also known as the volume viscosity) is also mentioned in Sect. 6.1.1. Formally at least, it can be incorporated into the pressure term if the context is such that no pressure values have absolute meaning; by contrast, that is not so in the case of atmospheric pressure for example, or the definition of pressure that follows (4.3). When an absolute definition of pressure is essential, the additional term involving μ_B should be included, but even so it is often left out. In incompressible flow, for which $u_{k,k} = 0$, it can in any case be ignored.

Viscous Heat Flow

As it stands, the form of the equation of heat conduction, (1.7), is appropriate to solids and liquids. In the case of gases, the heat flow is proportional to a pressure gradient as well as the temperature gradient [5, 6]; this additional contribution is known as the viscous heat flow. Although it is formally a second order effect in terms of its derivation in a kinetic theory description of gas flow and an expansion in powers of the Knudsen number, it can sometimes be comparable to the first order term, Fourier's law. The Knudsen number, Kn, is the ratio of the molecular mean free path length to a characteristic physical length scale and is useful in the description of the flow of low-density gases. For example, for the flow caused by a pressure gradient in a gas the viscous heat flow term is

$$\frac{\theta_4}{2}\frac{\mu}{\rho}\nabla p, \tag{1.10}$$

where, in the case of Maxwellian molecules, θ_4 has the value 3; see [3]; consequently it needs to be added to the Fourier's law term in the equation. Here, μ is the stress viscosity, ρ is the mass density and p is the pressure of the gas. Since the thermal conductivity λ and the viscosity μ are both proportional

Table 1.1. Some governing equations considered as examples of generalised conservation conditions. SI base units are assumed.

k_*	Q_{*j}	q_*	G_{*j}
	Dynamics of a Newtonian Fluid [3], ch 3		
Density, ρ	Mass flow rate, ρu_j	–	–
	Equation of conservation of mass: $\dfrac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$ (1.5)		
Momentum density, ρu_i	Momentum flow rate, $\rho u_i u_j$	Body forces, ρF_i	Stress, $\sigma_{ij} = -p\delta_{ij} + \mu_B u_{k,k}\delta_{ij} + d_{ij}$
Navier-Stokes equations:			
	$\dfrac{\partial \rho u_i}{\partial t} + (\rho u_i u_j)_{,j} = \rho F_i - p_{,i} + (\mu_B u_{j,j})_{,i} + \left\{ \mu \left(u_{i,j} + u_{j,i} - \dfrac{2}{3} u_{k,k}\delta_{i,j} \right) \right\}_{,j}$; (1.6)		
$\mathbf{u}$ is the velocity, μ is the coefficient of (dynamic) viscosity and p is the pressure; $d_{ij} = \mu \left(u_{i,j} + u_{j,i} - \frac{2}{3} u_{k,k}\delta_{i,j} \right)$ is the deviatoric stress tensor and μ_B the bulk viscosity.			
	Heat conduction in a moving medium [3], ch 3		
Internal energy per unit volume, ρE	Convection and Fourier's Law, $\rho E u_j - kT_{,j}$	Sources of thermal energy, q	–
	$\dfrac{\partial}{\partial t}(\rho E) + (\rho E u_j)_{,j} = q + (kT_{,j})_{,j}$ (1.7)		
T is the temperature and k the coefficient of thermal conductivity.			
	Electromagnetic Theory		
Net charge Density, ρ_{charge}	Current density, $\mathbf{j}$	–	–
	$\dfrac{\partial \rho_{charge}}{\partial t} + j_{k,k} = 0.$ (1.8)		
	Linear thermoelasticity in an isotropic medium at rest		
Momentum density, $\rho \dfrac{\partial \xi_i}{\partial t}$	–	Body forces, ρF_i	Stress (with strain relation and thermal expansion), $p_{ij} = \lambda e_{kk}\delta_{ij} + 2\mu e_{ij} - \frac{1}{3}\alpha(3\lambda + 2\mu)(T - T_0)\delta_{ij}$
	$\rho \dfrac{\partial^2 \xi_i}{\partial t^2} = \rho F_i + (\lambda + \mu)\xi_{j,ji} + \mu \xi_{i,jj} - \dfrac{1}{3}\alpha(3\lambda + 2\mu) T_{,i}$ (1.9)		
λ and μ are the Lamé constants, ξ the displacement, e_{ij} the strain tensor given by $e_{ij} = \frac{1}{2}(\xi_{i,j} + \xi_{j,i})$, T the temperature, and α the volume coefficient of expansion.			

to the molecular mean free path, this term, the viscous heat transfer, cannot be neglected in comparison with the Fourier's law term in the hydrodynamic limit (in which the Knudsen number tends to zero); see [6]. Under conditions in which the pressure is comparable to or greater than atmospheric pressure, so that the density of the gas is not low, the viscous heat flow term is likely to be small; for example, for air at standard temperature and pressure, the ratio of the viscous heat flow to the Fourier contribution is of the order of $10^{-3}\Delta p/\Delta T$, but it is clear from this that if the pressure differences are of the order of 1 bar, say, and the temperature differences on the same length scale are not too great, this ratio would indicated that the viscous heat flow was of importance. If conditions were near to a vacuum so that the gas density was small, the term might even become dominant.

Conservation of Electric Charge

The equation of conservation of net charge, (1.8) in the table, provides part of the theoretical justification for the existence of Maxwell's displacement current, an essential component of Maxwell's equations. They, like the field equation formulation of Newton's theory of gravitation, have their origins in the behaviour of an abstract test particle. The statements are then converted into differential form by a similar technique that is based on the use of Stokes's Theorem rather than Gauss's Theorem. The process is described briefly in §1.5.

Linear Thermo-Elasticity in a Moving Frame of Reference

It is sometimes helpful to use the equations of linear thermo-elasticity in a moving frame of reference. The linearisation depends only on the stress and strain tensors being small so, provided that the underlying motion of the entire work piece consists only of a combination of a velocity and a rotation, (1.9) in Table 1.1 can be used in a modified form. Suppose that there is a uniform, possibly time-dependent, velocity $\mathbf{U}(\mathrm{t})$ and a time-dependent angular velocity $\boldsymbol{\omega}(\tau)$ about a fixed point, $\mathbf{x}^0$ in the equivalent unstrained material. At the point $\mathbf{x}$ there is a small displacement $\boldsymbol{\xi}(\mathbf{x}, t)$ in the real material from the equivalent ideal unstrained material. Write

$$V_i = U_i\,(t) + \varepsilon_{ijk}\omega_j\,(t)\left(x_k - x_k^0\right);$$

$\mathbf{V}$ is thus the velocity of points in the ideal material, and is caused by a body force $\mathbf{F}^0$. An additional small body force $\mathbf{F}$ must be added to this to produce the small displacement $\vec{\boldsymbol{\xi}}$. $\mathbf{V}$ and $\mathbf{F}^0$ are related by

$$\rho\left\{\frac{\partial V_i}{\partial t} + \frac{\partial}{\partial x_j}\left(V_i V_j\right)\right\} = F_i^0.$$

This equation can be subtracted from the one which results from using the generalised conservation argument (for small displacements from the

undistorted motion) obtained by considering

$$k_i = \rho\left(V_i + \frac{\partial \xi_i}{\partial t} + V_k \frac{\partial \xi_i}{\partial x_k}\right),$$

$$Q_{ij} = k_i k_j/\rho, \quad q_i = \rho\left(F_i^0 + F_i\right) \text{ and } G_{ij} = p_{ij}$$

where p_{ij} is given in Table 1.1. Equation (1.4) then shows, to the small disturbance approximation, that the left-hand side of (1.9) in the table is replaced by

$$\rho\left\{\left(\frac{\partial}{\partial t} + V_j \frac{\partial}{\partial x_j}\right)^2 \xi_i + \frac{\partial}{\partial x_j}\left[V_i\left(\frac{\partial}{\partial t} + V_k \frac{\partial}{\partial x_k}\right)\xi_j\right]\right\}.$$

Note that $\nabla \cdot \mathbf{V} = 0$. The body-force term ρF_i on the right must be understood as any small force in addition to $\mathbf{F}^0$, the force that is necessary to account for the acceleration implied by the presence of the terms in $\mathbf{U}$ and $\boldsymbol{\omega}$. These last two quantities must not depend on position in space and the constitutive equation for the stress must depend only on the symmetric part of the displacement gradient (a consequence of the Principle of Material Frame-Indifference, a principle which is still a subject of some controversy, but seems unlikely to be found unsatisfactory in the context of macroscopic material processing involving solids and liquids.)

1.2.4 Gauss's Law

There are a number of physical laws whose mathematical form is very similar to generalised conservation equations, but which are not usually thought of as such, even though in some respects that is what they are. The reason is that the very existence of the underlying quantity, usually a scalar whose spatial density is q, itself produces effects that can be described in terms of a vector field $\mathbf{Q}$; it has the property that the flux of $\mathbf{Q}$ out of any volume V is proportional to the total amount of the quantity contained in V. They are thus generalised flux conservation laws. In the absence of q, it is then flux along a tube whose sides are parallel to $\mathbf{Q}$ which is conserved. It follows that

$$\int_S \mathbf{Q} \cdot \mathbf{n} dS = \alpha \int_V q \, dV.$$

It is always a part of the definition of $\mathbf{Q}$ that the constant of proportionality, α, depends only on the system of units chosen. The same mathematical arguments as those used above show that there is a corresponding differential form for these conditions, given by

$$\nabla \cdot \mathbf{Q} = \alpha q.$$

Table 1.2 gives some examples.

Table 1.2. Examples of generalised flux conservation laws.

q_*	Q_{*j}	α
	Newton's Theory of Gravitation	
Mass density, ρ	Gravitational field, $\mathbf{F}$	$-4\pi G$
	$\nabla \cdot \mathbf{F} = -4\pi G\rho$; G is the universal gravitational constant.	
	Electromagnetic Theory	
(Absence of monopoles) 0	Magnetic flux density, $\mathbf{B}$	–
	Gauss's law for magnetism: $\nabla \cdot \mathbf{B} = 0$ (1.11)	
Charge density, ρ_{charge}	Electric displacement field, $\mathbf{D}$	1
	Gauss's law: $\nabla \cdot \mathbf{D} = \rho_{charge}$ (1.12)	

1.3 Boundary and Interface Conditions

1.3.1 Generalised Conservation Conditions

A problem is described not only by the governing equations in the interior of the medium under consideration, but also by the initial conditions, the conditions at the external boundaries of the problem and any internal boundaries between regions with different properties. These initial and interface conditions are every bit as important as the governing equations [4], p56. Although the initial conditions quite often lapse into unimportance with the passage of time, the interface conditions must always be taken into account.

The form of the initial conditions to be imposed will depend on the structure of the governing equations and the kind of problem to be solved. To some extent they will always depend on previous history, though often in only very simple ways. The equation of heat conduction, for example, will normally only need to have the initial temperature distribution specified, but even in simple problems care must always be taken to ensure that assumptions made are justified and consistent with the mathematical model that it is proposed to use, as well as being a proper description of the physical processes involved.

Boundary and interface conditions must likewise be considered carefully; failure to do so can lead to many different problems. There might be no solution, many solutions when only one is expected or, most dangerously of all, a solution may be obtained that is in fact invalid but appears reasonable at a casual in glance.

Many interface conditions are based on the same ideas of conservation or lack of it that were considered in the previous section, and the appropriate

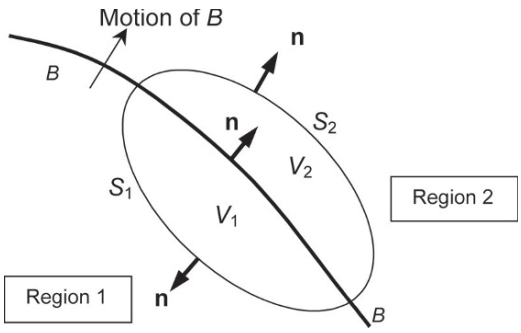

Fig. 1.2. The control volume V, whose surface S is divided into two sections S_1 and S_2 by the moving interface B. The figure shows the convention for the directions of the normals $\mathbf{n}$ on each of the surfaces B, S_1 and S_2; S_1 and S_2 are fixed.

mathematical form can be obtained in much the same way. The underlying statement is indeed identical and the initial starting-point in mathematical form is almost the same as (1.1). There is one important difference however and that is to the fourth of the properties listed. At a boundary or interface, B, there may be generation of Ω which occurs only there; suppose that it has a magnitude Δq_* per unit area of B. Perhaps the most familiar example is the release of latent heat as steam condenses to water.

The necessary interface condition can be found by considering a volume V with a fixed surface S which encloses the moving interface B separating region 1 from region 2 in the manner shown in figure 1.2. The property Ω is considered to be crossing B from V_1 to V_2 so that $V = V_1 \cup V_2$ and $S = S_1 \cup S_2$. Suppose that B is moving with a velocity $\dot{n}$ in the direction of its normal from V_1 into V_2; the unit normal $\mathbf{n}$ on B is likewise directed from V_1 to V_2.

The mathematical form of the generalised conservation statement (1.1) for the entire volume remains identical except that there is the additional term

$$\int_B \Delta q_* \, dS$$

on its right-hand side. V can now be split into its components V_1 and V_2 which are bounded by $S_1 \cup B$ and $S_2 \cup B$ respectively. Now notice that, for example,

$$\frac{d}{dt}\int_{V_1} k_* dV = \int_{V_1} \frac{\partial k_*}{\partial t} dV + \int_{V_1} k_* \frac{d}{dt}\,(dV) = \int_{V_1} \frac{\partial k_*}{\partial t} dV + \int_B [k_*]_1 \, \dot{n} \, dS. \tag{1.13}$$

In the case of V_2 the expression is similar except that the sign of the last term on the right is negative because of the convention adopted for the sign of $\dot{n}$.

The notation $[\ldots]_1$ is the value of the enclosed quantity in region 1 for example, and $[\ldots]_1^2$ is its value in region 2 minus its value in region 1. Equation (1.3) can be applied to V_1 and V_2 separately and both subtracted

from (1.13) to show that

$$\int_B [k_*]_1 \, \dot{n} \, dS - \int_B [k_*]_2 \, \dot{n} \, dS = \int_B [Q_{*j} - G_{*j}]_1 \, n_j dS - \int_B [Q_{*j} - G_{*j}]_2 \, n_j dS + \int_B \Delta q_* \, dS.$$

The whole equation can be written as a single integral over B, divided by its magnitude. Then so long as the integrand is continuous and the limit as the area of B tends to zero is taken in such a way that the distance of every point on B from an arbitrarily specified point on it tends to zero, the interface condition can be expressed as

$$[-k_* \dot{n} + (Q_{*j} - G_{*j}) \, n_j]_1^2 = \Delta q_*. \tag{1.14}$$

An alternative approach to the derivation of (1.14) can be found in [4]. It can often be convenient to express the normal in term of the gradient of an expression for the surface S. Suppose it is given by the equation $S(\mathbf{x}, t) = 0$, then

$$n_j = \pm \frac{S_{,j}}{\sqrt{S_{,k}^2}} \quad \text{and} \quad \dot{n} = \mp \frac{1}{\sqrt{S_{,k}^2}} \frac{\partial S}{\partial t}.$$

The choice of sign is necessary to ensure compatibility with the convention for the normal; $\dot{n}$ should be positive when the boundary is moving in the direction in which $\mathbf{n}$ points. A few examples of the use of (1.14) are shown in Table 1.3.

Characteristic interface conditions for Gauss's laws for gravitation, magnetism and electric fields in the absence of surface effects at the boundary are similarly

$$[\mathbf{F} \cdot \mathbf{n}]_1^2 = 0, \quad [\mathbf{B} \cdot \mathbf{n}]_1^2 = 0 \text{ and } [\mathbf{D} \cdot \mathbf{n}]_1^2 = 0.$$

They are easily modified by the addition of extra terms when surface effects are present.

1.3.2 The Kinematic Condition in Fluid Dynamics

At an interface between a fluid and another medium it is usual to specify that the tangential component of velocity is continuous across the separating surface, so that

$$[\mathbf{u} \cdot \mathbf{t}]_1^2 = 0 \tag{1.19}$$

where $\mathbf{u}$ is the velocity vector and $\mathbf{t}$ is any vector tangent to the surface. The background and reasons for such a condition are well presented in [3], p 149 and Sect. 1.9. In summary, at any discontinuity across a material

Table 1.3. Some interface conditions as examples of generalised conservation conditions; the notation is the same as that used in Table 1.1.

Dynamics of a Newtonian Fluid [3]
$\Delta q_* = 0,$
Mass conservation: $\left[\rho\left(u_j n_j - \dot{n}\right)\right]_1^2 = 0.$ (1.15)
$\Delta q_* = n_i\left(\gamma n_{j,j} + n_j\gamma_{,j}\right) - \gamma_{,i}$ where γ is the coefficient of surface tension.
Momentum transfer: $\left[\rho u_i\left(u_j n_j - \dot{n}\right) + p n_i - d_{ij} n_j\right]_1^2$ $= n_i\left(\gamma n_{j,j} + n_j\gamma_{,j}\right) - \gamma_{,i}.$ (1.16)
The normal and tangential components of this condition simplify to $\left[\dot{m} n_i u_i + p - n_i d_{ij} n_j\right]_1^2 = \gamma n_{j,j}$ if $\dot{m} = \left[\rho\left(u_j n_j - \dot{n}\right)\right]_1 = \left[\rho\left(u_j n_j - \dot{n}\right)\right]_2$, $\left[t_i d_{ij} n_j\right]_1^2 = t_i\gamma_{,i}$ where use is made of (1.15) and (1.19); t_i is the ith component of a unit tangential vector.
Heat conduction in a moving medium [3]
$\Delta q_* = -\dot{m} L_1^2.$
The Stefan condition: $\left[k n_j T_{,j}\right]_1^2 = \dot{m} L_1^2$ (1.17)
where $\dot{m}$ is $\left[\rho\left(u_j n_j - \dot{n}\right)\right]_1 = \left[\rho\left(u_j n_j - \dot{n}\right)\right]_2$ and L_1^2 is the latent heat of transition from phase 1 to phase 2 (i.e. in the direction of the normal $\mathbf{n}$).
Electromagnetic Theory
When $\Delta q_* = 0$:
$\left[\rho_{charge}\dot{n} - j_k n_k\right]_1^2 = 0.$ (1.18)

surface, molecular transport would rapidly give rise to a very large stress at the surface, whose effect would be to tend to eliminate the relative velocity. In the case of a boundary separating a fluid and a solid, the condition that the tangential component of velocity should be continuous is known as the *no-slip condition.*

The same argument can be used to support (1.19) in the case of two different substances, and of a single substance in different phases, including the case when matter crosses the phase boundary, but it is then less satisfactory. The validity of the no-slip condition between a solid and a fluid was discussed at length in the nineteenth century, but the result has been adequately confirmed by experiment, and its practical success. It cannot be regarded as having the same firm theoretical foundations as the other conditions and there are circumstances where it may not apply, either for pragmatic reasons, of because it has been found to be false. An example of the first occurs when the inviscid fluid model is used as an approximation, in which case (1.19) cannot be employed. The inviscid model of fluid flow at normal temperatures ignores the region very close to the boundary in which normal molecular

interactions occur, so that the arguments supporting the no-slip condition still apply, but are supposed to have no influence beyond a short distance from the interface.

The inviscid model is an example where (1.19) applies but is ignored for compatibility with a useful approximation in the solution procedure for the problem under consideration. A circumstance in which it does not necessarily apply, however, occurs in the case of low-density gases, where the mean velocity of a molecule can vary significantly in distances comparable with the mean free path. In this case there can be a non-zero change in velocity and a temperature difference between the gas and the solid or liquid adjacent to it [5,6]. The question is considered further in §4.3.1 in connection with the Knudsen layer.

1.4 Fick's Laws

The heat conduction equation (1.7) is an example of a diffusive process. Suppose $\mathcal{Q}$ is some quantifiable substance which is conserved. Examples might be thermal energy, particles diffusing through some medium, or a contaminating chemical. If it has a concentration C and $\mathcal{Q}$ is conserved, then its flow rate $\mathbf{q}_c$ is related to C by *Fick's First Law*,

$$\mathbf{q}_c = -D\nabla C \tag{1.20}$$

relative to the underlying medium, which is normally assumed to be at rest. In (1.20) D is a diffusion coefficient. Conservation of $\mathcal{Q}$, by (1.4) in the absence of any generation processes, gives

$$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{q}_c.$$

If this equation is combined with (1.20), *Fick's Second Law* is obtained,

$$\frac{\partial C}{\partial t} = D\nabla^2 C, \tag{1.21}$$

provided the diffusion constant D can be regarded as a constant.

1.5 Electromagnetism

1.5.1 Maxwell's Equations

A number of physical laws are usually stated in the form that no work is done when a unit test particle acted on by a force field $\mathbf{F}$ is moved round any closed path in space. Another way of stating the result is to say that $\mathbf{F}$ is

conservative. Such a statement can be expressed in mathematical form as

$$\int_C \mathbf{F} \cdot \mathbf{dr} = 0$$

where C is such a path. It can be converted into the form of a differential equation as follows. Suppose that C is simple and smooth but otherwise arbitrary in size, orientation and location, and that it can be spanned by a surface at every point of which $\mathbf{F}$ is differentiable. In that case Stokes' Theorem shows that

$$\int_S \nabla \times \mathbf{F} \cdot \mathbf{n}\, dS = 0 \tag{1.22}$$

where $\mathbf{n}$ is the unit normal to S. Then consider a particular point in space and construct a circular path of radius a about the point in a plane with a fixed (but otherwise arbitrary) normal. Divide (1.22) by the area of the circle and take the limit as a tends to zero, to show that the integrand must vanish. Since the direction of the normal is arbitrary it follows that

$$\nabla \times \mathbf{F} = \mathbf{0} \tag{1.23}$$

everywhere in the domain in which $\mathbf{F}$ has the required properties. Consequently, $\mathbf{F}$ can be expressed as the gradient of a scalar. It is a standard result for conservative fields that is sometimes taken as their definition, although the more usual definition is that they are expressible as the gradient of some scalar field, usually referred to as the potential (conventions vary on the sign of the potential however). The terminology is independent of the physical interpretation of these scalar and vector fields.

If, by extension, a finite amount of work is done equal to the flux of a second field, $\mathbf{Q}$ say, across a surface spanning the path C and lying in the domain of definition of $\mathbf{F}$, and the flux is otherwise independent of the choice of S, then

$$\int_C \mathbf{F} \cdot \mathbf{dr} = \int_C \mathbf{Q} \cdot \mathbf{n}\, dS.$$

Stokes' theorem can be applied in the same way as before to show that

$$\nabla \times \mathbf{F} = \mathbf{Q} \tag{1.24}$$

in the domain of definition of $\mathbf{F}$ and $\mathbf{Q}$. The divergence of a vector field which is the curl of another vector field is identically zero; necessarily, therefore,

$$\nabla \cdot \mathbf{Q} = 0. \tag{1.25}$$

A vector field that satisfies such a condition is said to be solenoidal, and again the terminology is used irrespective of the physical interpretation.

Comparison with the ideas of §1.2.2 shows that it might sometimes be helpful to think of $\mathbf{Q}$ as a rate of flow of some conserved quantity in a steady state, or when the density of the conserved quantity is constant in time.

The field theory formulation of Newton's theory of gravitation is of this type. The work done by a gravitational field $\mathbf{F}$ on a particle moving in a closed path C is zero, and so the argument just given shows that

$$\nabla \times \mathbf{F} = \mathbf{0}.$$

There therefore exists a gravitational potential, and as a result of Gauss's law for the gravitational field (see Table 1.1), it satisfies Poisson's equation. The classical form for the law of Conservation of Energy for a single particle moving under the action of a gravitational field only is then a consequence of Newton's Second Law of Motion.

The application of the idea to electromagnetism is rather more involved. Faraday's law states that the induced electromotive force in a closed loop is proportional to the rate of change of the magnetic flux through it. It is supplemented by Lenz's law which adds that the polarity of the induced electromotive force induces a current whose magnetic field opposes the change which produced it. These laws can be summarised by saying that if $\mathbf{F}$ (above) is taken as the electric field $\mathbf{E}$, $\mathbf{B}$ is the magnetic flux vector, and $\mathbf{Q}$ is proportional to $\partial\mathbf{B}/\partial t$, then the latter is proportional to $\nabla \times \mathbf{E}$. Lenz's law means that the sign of the constant is negative and in SI base units its magnitude is one, so that

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}. \tag{1.26}$$

In the case of the magnetic field $\mathbf{H}$ the starting point is Ampère's Circuit Law which says that in a steady state the circulating magnetic field $\mathbf{H}$ in a closed path C is proportional to the total electric current $\mathbf{J}$ linked with C. Thus, in the same way as for Faraday's law, take $\mathbf{F}$ to be $\mathbf{H}$ and $\mathbf{Q}$ to be $\mathbf{j}$. In SI base units, the constant of proportionality is one (and is positive) so that

$$\nabla \times \mathbf{H} = \mathbf{j}.$$

The result is clearly unsatisfactory when conditions are changing with time, since the form of the law implies that $\nabla \cdot \mathbf{j} = 0$ contrary to (1.8) in Table 1.1. Maxwell saw, however, that the difficulty could be resolved by the addition of an extra term to the equation; suppose it is the vector $\mathbf{X}$, and appears on the right of the equation. Then necessarily $\nabla \cdot \mathbf{X} = -\nabla \cdot \mathbf{j}$ and so from (1.8) and Gauss's law, (1.12),

$$\nabla \cdot \left\{ \mathbf{X} - \frac{\partial \mathbf{D}}{\partial t} \right\} = 0.$$

Thus $\mathbf{X} = \partial\mathbf{D}/\partial t$ to which could in principle be added a solenoidal field which necessarily vanishes whenever conditions are steady, but it is not required. Maxwell's extension to Ampère's law therefore results in the equation

$$\nabla \times \mathbf{H} = \mathbf{j} + \frac{\partial \mathbf{D}}{\partial t}. \tag{1.27}$$