ISSN 0103-2509

Industrial mathematics: heat and mass transfer

MCKEE, S.

nº 5

São Carlos (SP)
1990

Industrial Mathematics: Heat and Mass Transfer

The objective of this course is:

to teach mathematical modelling of real industrial problems in the area of heat and mass transfer through a series of case studies. Emphasis will be placed on the concept of units, nondimensionalisation and nondimensional parameters. The case studies will also bring out solution techniques. Thus separation of variables, Laplace transform techniques, perturbation methods and some aspects of numerical analysis will be exemplified. This course will require the active participation of the 'audience' to complete the solution of these problems generally using NAG; computing support to help the student in these endeavours is seen as an important part of the course.

1. The diffusion equation

Diffusion is the process by which matter is transported from one part of a system to another as a result of random molecular motions.

Consider a tall cylindrical vessel with its lower part filled with iodine solution. A column of clear water is poured on top, slowly and carefully, so that no convection currents are set up. After some time a colour gradient appears with the colour getting fainter towards the top. Eventually the whole column becomes uniformly coloured. This is an example of molecular diffusion.

If in the example above we let c(x,t) be the concentration of the iodine (usually in moles/c.c. or gram moles/c.c.) then c(x,t) satisfies

$$\frac{\partial c}{\partial t} = D\left[\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right] \qquad (1.1)$$

where D, assumed constant, is the diffusion coefficient (with dimensions L^2T^{-1} e.g. cm^2/sec). The space coordinate is x and t is time. Note: c has dimensions L^{-3}.

If D is dependent on the spatial variables (1.1) becomes

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left[D\frac{\partial c}{\partial x}\right] + \frac{\partial}{\partial y}\left[D\frac{\partial c}{\partial y}\right] + \frac{\partial}{\partial z}\left[D\frac{\partial c}{\partial t}\right] \qquad (1.2$$

1.2 Diffusion in a cylinder or sphere

cylinder

$$\frac{\partial c}{\partial t} = \frac{1}{r}\left\{\frac{\partial}{\partial r}\left[rD\frac{\partial c}{\partial r}\right] + \frac{\partial}{\partial \theta}\left[\frac{D}{r}\frac{\partial c}{\partial \theta}\right] + \frac{\partial}{\partial z}\left[rD\frac{\partial c}{\partial z}\right]\right\}$$

sphere

$$\frac{\partial c}{\partial t} = \frac{1}{r^2}\left\{\frac{\partial}{\partial r}\left[Dr^2\frac{\partial c}{\partial r}\right] + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[D\sin\theta\frac{\partial c}{\partial\theta}\right] + \frac{D}{\sin^2\theta}\frac{\partial^2 c}{\partial\phi^2}\right\}$$

In the nomenclature of vector analysis

$$\frac{\partial c}{\partial t} = \text{div}(D \text{ grad } c) = \underline{\nabla}.(D\underline{\nabla}c).$$

1.3 Heat conduction equation

Diffusion theory is based on Fick's two equations

$$F = -D\frac{\partial c}{\partial x} \quad \text{and} \quad \frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \qquad (1.3a,b)$$

where F denotes the rate of transfer per unit area. (If c is measured in moles/c.c. then the dimensions of F are $L^{-2}T^{-1}$.)

The two corresponding equations in heat flow are

$$F = -K\frac{\partial\theta}{\partial x} \quad \text{and} \quad \frac{\partial\theta}{\partial t} = \left[\frac{K}{c\rho}\right]\frac{\partial^2\theta}{\partial x^2} \qquad (1.4a,b)$$

where θ is the temperature (e.g. ^{o}K), K is the heat conductivity (e.g. W/mK), ρ is the density (e.g. Kg/m^3) and c is the specific heat (e.g. J/KgK), so that ρc is the heat capacity per unit volume.

In (1.4a) F is the amount of heat flowing in the direction x per unit time through unit area of a section which is normal to x.

In order that the two sets of equations should correspond we may identify concentration c with temperature θ, and take D = K in (1.3a) and (1.4a) and $D = K/(c\rho)$ in (1.3b) and (1.4b). The two together imply $c\rho = 1$. This is a consequence of our having identified c with θ. The 'diffusing substance' in heat flow is heat not temperature. The factor $c\rho$ is needed to convert temperature to the amount of heat per unit volume. Note, it is usual to write $K/c\rho = k$, the heat diffusivity (e.g. Wm^2/J).

1.4 Boundary conditions

1.4.1 $T = T_a$

Prescribed surface temperature corresponds to prescribed concentration just within the surface.

1.4.2 Heat flux

Prescribed heat flux corresponds to flux of the diffusant and we have

$$-K \frac{\partial \theta}{\partial x} = F(t), \quad \text{in heat} \tag{1.5a}$$

$$-D \frac{\partial c}{\partial x} = F(t), \quad \text{in diffusion} \tag{1.5b}$$

where F is in general a known function of time or a constant.

1.4.3 Insulated surface

A heat-insulated surface corresponds to an impermeable surface and is a special case of (1.5a,b) with $F = 0$ i.e.

$$\frac{\partial c}{\partial x} = \frac{\partial \theta}{\partial x} = 0.$$

1.4.4 Radiation boundary condition

What is usually referred to as a 'radiation boundary condition' in heat flow usually means that the heat flux across unit area of the surface is proportional to the difference between the surface temperature θ_s and the temperature θ_o of the outside medium i.e. is given by $H(\theta_s - \theta_o)$.

But the rate of loss of heat from unit area of surface is $-K \frac{\partial \theta}{\partial n}$ in the direction of the normal $\underline{n}$, measured away from the surface, so that the boundary condition is

$$K \frac{\partial \theta}{\partial n} + H(\theta_s - \theta_o) = 0$$

i.e.
$$\frac{\partial \theta}{\partial n} + h(\theta_s - \theta_o) = 0$$

where $h = H/K$, is called the heat transfer coefficient. This corresponds to surface evaporation in diffusion, and we have

$$\frac{\partial c}{\partial n} + \alpha(c_s - c_o) = 0.$$

If the surface is perpendicular to the x-direction then $\frac{\partial c}{\partial n} = \frac{\partial c}{\partial x}$ if n is along the direction of increasing x, but $\frac{\partial c}{\partial n} = -\frac{\partial c}{\partial x}$ if along x decreasing. Thus for a slab between 0 and 1 we have

$$\frac{\partial c}{\partial x} + \alpha(c_s - c_o) = 0, \qquad x = 1$$

but

$$-\frac{\partial c}{\partial x} + \alpha(c_s - c_o) = 0, \quad x = 0.$$

1.4.5 A perfect heat conducting 'surface' with finite volume

A perfect conductor of heat is always at a uniform temperature and so is equivalent in this respect to a well-stirred fluid. Thus, a boundary condition describing thermal contact with a perfect conductor also describes diffusion of solute from a well-stirred solution or vapour. Conservation of heat from a well-stirred fluid of fixed volume V and uniform temperature θ_s, a function of time, gives us a boundary condition on the surface $x = 0$ of a medium, $x > 0$, in contact with the fluid

$$c\rho \frac{\partial \theta_s}{\partial t} = K \frac{\partial \theta}{\partial x}, \qquad x = 0.$$

Correspondingly, for diffusion we have

$$V \frac{\partial c_s}{\partial t} = D \frac{\partial c}{\partial x}, \qquad x = 0.$$

1.4.6 Interface

The conservation principle applied at the interface between two media of different properties leads immediately to boundary conditions

$$\theta_1 = \theta_2, \quad K_1 \frac{\partial \theta_1}{\partial x} = K_2 \frac{\partial \theta_2}{\partial x}$$

in heat flow and

$$c_1 = Pc_2 + Q, \quad D_1 \frac{\partial c_1}{\partial x} = D_2 \frac{\partial c_2}{\partial x}$$

in diffusion, where the suffices 1 and 2 denote the two media and P and Q are constant.

1.4.7 Heat source

If heat is produced in a medium, e.g. as a result of an exothermic reaction, at a rate A per unit volume, then the heat conduction equation takes the form

$$c\rho \frac{\partial \theta}{\partial t} = K \frac{\partial^2 \theta}{\partial x^2} + A.$$

The diffusion equation must be similarly modified if the diffusing substance is created or removed as diffusion proceeds. We identify A as the rate of creation per unit volume and put $c\rho = 1$, $K = D$ as usual.

2.1 Method of Separation of Variables

We assume the variables are separable and seek a solution

$$c(x,t) = X(x)\,T(t). \tag{2.1}$$

Substitution in (1.36) yields

$$X\frac{dT}{dt} = DT\frac{d^2X}{dx^2} \tag{2.2}$$

which may be written as

$$\frac{1}{T}\frac{dT}{dt} = \frac{D}{X}\frac{d^2X}{dx^2} \tag{2.3}$$

so that we have on the left-hand side an expression depending on t only, while the right-hand side depends on x only. Both sides therefore must be equal to the same constant which, for the sake of the subsequent algebra, is conveniently taken as $-\lambda^2 D$. We have therefore two ordinary differential equations

$$\frac{1}{T}\frac{dT}{dt} = -\lambda^2 D \quad \text{and} \quad \frac{1}{X}\frac{d^2X}{dx^2} = -\lambda^2 \tag{2.4a,b}$$

with solutions

$$T = e^{-\lambda^2 Dt} \quad \text{and} \quad X = A\sin\lambda x + B\cos\lambda x. \tag{2.5a,b}$$

Thus

$$c(x,t) = (A\sin\lambda x + B\cos\lambda x)\exp(-\lambda^2 Dt) \tag{2.6}$$

where A and B are constants of integration.

Since (1.3b) is a linear equation, the most general solution is obtained by summing solutions of type (2.6) so that we have

$$c(x,t) = \sum_{m=1}^{\infty}(A_m\sin\lambda_m x + B_m\cos\lambda_m x)\exp(-\lambda_m Dt) \tag{2.7}$$

where A_m, B_m, λ_m are determined by the initial and boundary conditions for any particular problem.

Thus if we are interested in diffusion out of a plane sheet of thickness ℓ, through which the diffusing substance is initially uniformly distributed and the surfaces are kept at zero concentration, the conditions are

$$c = c_o, \quad 0 < x < \ell, \quad t = 0 \tag{2.8}$$

$$c = 0, \quad x = 0, \ell, \quad t > 0. \tag{2.9}$$

The boundary conditions (2.9) demand that

$$B_m = 0, \quad \lambda_m = m\pi/\ell \tag{2.10}$$

and hence the initial condition (2.8) becomes

$$c_o = \sum_{m=1}^{\infty} A_m \sin(m\pi x/\ell), \quad 0 < x < 1. \tag{2.11}$$

By multiplying both sides of (2.11) by $\sin(p\pi x/\ell)$ and integrating from 0 to ℓ using the relationships

$$\int_0^{\ell} \sin\left[\frac{p\pi x}{\ell}\right] \sin\left[\frac{m\pi x}{\ell}\right] dx = \begin{cases} 0 & m \neq p \\ \frac{1}{2}\ell & m = p \end{cases}$$

we find that terms for which m is even vanish, and

$$A_m = 4c_o/m\pi, \quad m = 1,3,5,\ldots .$$

The final solution is

$$c(x,t) = \frac{4c_o}{\pi} \sum_{n=0}^{\infty} \frac{1}{2n+1} \exp(-D(2n+1)^2\pi^2 t/\ell^2) \sin\frac{(2n+1)\pi x}{\ell} .$$

For moderate and large times this series converges satisfactorily and can be used for numerical evaluation by truncating the series (after, say, 10 terms).

Equation (1.3b) could have been solved directly by the Fourier sine transform (see, e.g. Kreyszig (1988)).

3.1 Method of Laplace Transform

Suppose $f(t)$ is a known function of t for positive values of t. Then the Laplace transform $\bar{f}(p)$ of $f(t)$ is defined as

$$\bar{f}(p) = \int_0^{\infty} e^{-pt} f(t)dt \tag{3.1}$$

where p is a number sufficiently large to make the integral (3.1) converge. For example, if $f(t) = e^{2t}$, p must exceed 2.

Laplace transforms of common functions can be computed directly:

$$f(t) = 1, \qquad \bar{f}(p) = \int_0^\infty e^{-pt}dt = 1/p$$

$$f(t) = e^{at}, \qquad \bar{f}(p) = \int_0^\infty e^{-pt+at}dt = \frac{1}{p-a}$$

$$f(t) = \sin \omega t, \quad \bar{f}(p) = \int_0^\infty e^{-pt}\sin \omega t \, dt = \frac{\omega}{p^2+\omega^2}.$$

A short table of transforms is given in Annex 1, and this may be used to evaluate the inverse function. For those functions whose Laplace transform is not included within this table the inverse formula must be used (or more extensive tables found):

$$f(t) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} \bar{f}(z)e^{itz}dz. \tag{3.2}$$

Contour integration (see e.g. Copson (1966)) is required. Not infrequently this integral cannot be evaluated analytically and it is necessary to resort to a numerical method in which case the method proposed by Talbot (1979) is to be recommended.

3.2 Semi-infinite medium

Consider the problem of diffusion in a semi-infinite medium, $x > 0$, when the boundary is kept at a constant concentration c_o, the initial concentration being zero throughout the medium.

We require to solve

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{3.3}$$

subject to the boundary condition

$$c = c_o, \quad x = 0, \quad t > 0 \tag{3.4}$$

and the initial condition

$$c = 0, \quad x > 0, \quad t = 0. \tag{3.5}$$

On multiplying both sides of (3.3) by e^{-pt} and integrating with respect to t from 0 to ∞ we obtain

$$\int_0^\infty e^{-pt}\frac{\partial^2 c}{\partial x^2}dt - \frac{1}{D}\int_0^\infty e^{-pt}\frac{\partial c}{\partial t}dt = 0.$$

If we assume that the orders of integration and differentiation can be interchanged, and this can be justified for the functions in which we are interested, then

$$\int_0^\infty e^{-pt} \frac{\partial^2 c}{\partial x^2} dt = \frac{\partial^2}{\partial x^2} \int_0^\infty c e^{-pt} dt = \frac{\partial^2 \bar{c}}{\partial x^2} .$$

Also by integrating by parts

$$\int_0^\infty e^{-pt} \frac{\partial c}{\partial t} dt = [c e^{-pt}]_0^\infty + p\int_0^\infty c e^{-pt} dt = p\bar{c}$$

since the term in the square bracket vanishes at $t = 0$ by virtue of the initial condition (3.5) and at $t = \infty$ through the exponential factor. Thus (3.3) reduces to

$$D \frac{\partial^2 \bar{c}}{\partial x^2} = p\bar{c}. \qquad (3.6)$$

By treating the boundary condition (3.4) in the same way we obtain

$$\bar{c} = \int_0^\infty c_o e^{-pt} dt = \frac{c_o}{p}, \quad x = 0. \qquad (3.7)$$

Thus the Laplace transform reduces the partial differential equation (3.3) to the ordinary differential equation (3.6). The solution of (3.6) satisfying (3.7), and for which $\bar{c}$ remains finite as x approaches infinity is

$$\bar{c}(x,p) = \frac{c_o}{p} e^{-qx}$$

where $q = p/D$. Reference to the table of Annex 1 gives

$$c(x,t) = c_o \operatorname{erfc}\left[\frac{x}{2\sqrt{Dt}}\right]$$

where

$$\operatorname{erfc}(z) = 1-\operatorname{erf}(z) = 1 - \frac{1}{\sqrt{\pi}} \int_0^z e^{-t^2} dt.$$

4. The General Transport Equations and Nondimensionalisation

Conservation of mass, momentum and energy (see, e.g. Landau and Lifshitz (1963)) leads to the (2-D) equations:

$$\nabla . \underline{q} = 0 \tag{4.1}$$

$$\rho\left[\frac{\partial \underline{q}}{\partial t} + (\underline{q}.\nabla)\underline{q}\right] = -\nabla p + \mu\nabla^2\underline{q} + \rho\underline{F} \tag{4.2}$$

$$\rho c\left[\frac{\partial T}{\partial t} + (\underline{q}.\nabla)T\right] = K\nabla^2 T \tag{4.3}$$

Here the velocity $\underline{q} = (u,v)^T$ and the pressure p are the unknown dependent variables. The constants involved are the density ρ, the coefficient of viscosity μ, the specific heat c, the conductivity K, and if the body force $\underline{F}$ is due to gravity, the gravitational acceleration g. Equations (4.1,2) are often called the Navier-Stokes equations. In equation (4.2) the physical effects modelled are inertia, viscous forces, and gravity; in equation (4.3) they are heat convection, and heat conduction.

To see if any of these effects may be neglected (i.e. corresponding terms neglected), it is usual to perform a nondimensionalisation. To do this we require reference or scale values. These are usually obtained from the boundary conditions without which equations (4.1-3) would be ill-posed i.e. not have a unique solution.

Suppose we have the following scaling:

U for $\underline{q}$, L for $\underline{x}$, L/U for t

and $T_1 - T_o$ for T where T_o is usually the ambient temperature and T_1 is some typical temperature.

Define the nondimensional variables by

$$\underline{x}' = \frac{\underline{x}}{L}, \quad \underline{q}' = \frac{\underline{q}}{U}, \quad t' = \frac{tU}{L}, \quad p' = \frac{p}{\rho U^2},$$

$$\text{and} \quad T' = \frac{T}{T_1 - T_o}.$$

The equations (4.1-3) become

$$\nabla \cdot \underline{q}' = 0$$

$$\frac{\partial \underline{q}'}{\partial t} + (\underline{q}' \cdot \nabla)\underline{q}' = -\nabla p + \frac{1}{Re} \nabla^2 \underline{q}' - \frac{1}{Fr} \underline{k}$$

$$Re \left[\frac{\partial T'}{\partial t} + (\underline{q}' \cdot \nabla)T' \right] = \frac{1}{Pr} \nabla^2 T'$$

where ∇ is with respect to the $\underline{x}'$ variables and $\underline{k}$ is the unit normal in upward vertical direction.

Three nondimensional parameters are required. We have the Reynolds number $Re = \rho UL/\mu$, which compares the effects of inertia and viscosity, the Froude number $Fr = U^2/Lg$, which compares inertia and gravity and the Prandtl number, $Pr = \mu c/K$, which compares the viscous time scale with that of heat conduction. Another commonly used parameter is the Peclet number, $Pe = RePr = \frac{\rho cUL}{K}$. Nondimensionalisation provides a mathematical (rather than, say, physical) means of saying what terms may or may not be neglected in equations (4.1-3). For example, for large Froude number the effect of gravity may be neglected. It only appears in a single term with a small coefficient.

The scaling here is not unique. How one chooses the correct scaling is an art which has to be learned from experience.

5. Medical Product Design and Calibration

5.1 The Mathematical Model

Unilever Research recently developed a pregnancy testing kit under the brand-name Clear Blue. This is based on antibody-antigen technology. When a woman is pregnant antibodies are automatically produced and these show up in the urine. The product is essentially a small container with a dip stick which has

antigen on its surface. If a reaction takes place the colour blue shows up much in the same way as with litmus paper. Let X denote the antibody concentration and Y denote the antigen concentration. The reaction is given as:

$$X + Y \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} XY$$

where k_1 and k_{-1} are the forward and backward reaction rates. It is vital to know how long this reaction takes and the concentration of $\theta(t)$ of the complex XY as a function of time. To quantify this information requires a mathematical model.

Let

$[X] \equiv$ concentration of X (in moles/m^3)

$[Y] \equiv$ concentration of Y (in moles/m^2)

$[XY] \equiv$ concentration of XY (in moles/m^2).

We require the following constants:

a_o : initial Y concentration (moles/m^2)

c_o : initial X concentration at the reaction side wall (moles/m^3)

d : edge of vessel to surface - vessel is assumed to be 2d

D : diffusion coefficient of X (in m^2/s).

Now clearly [X] satisfies the diffusion equation

$$\frac{\partial [X]}{\partial t} = D \frac{\partial^2 [X]}{\partial x^2} . \tag{5.1}$$

Also

$$\left.\frac{\partial [X]}{\partial x}\right|_{x=0} = 0. \tag{5.2}$$

Further

$$[X]_{t=0} = c_o \text{ (since concentration is assumed uniform initially).} \tag{5.3}$$

We need however the boundary condition at $\left.\frac{\partial [X]}{\partial x}\right|_{x=d}$.

To facilitate the discussion let us introduce the notation:

$u(x,t) \equiv$ conc. of X i.e [X]

$\theta(t)$ = conc. of XY i.e. [XY].

Now the law of mass action states

$$D \left.\frac{\partial u}{\partial x}(x,t)\right|_{x=d} = k_{-1}\theta(t) - k_1 u(d,t)\,[Y]$$

NB. - we are assuming that one molecule of X and one of Y combine to give one of the complex XY.

The initial concentration of Y is a_o; this will be depleted by the amount of X used up in the reaction. Therefore

$$[Y](t) = a_o - (c_o d - \int_0^d u(x,t)dx).$$

Thus

$$\frac{\partial u}{\partial x}(x,t)\Big|_{x=d} = k_{-1}\theta(t) - k_1 u(d,t)\left\{a_o - c_o d + \int_0^d u(x,t)dx\right\}. \tag{5.4}$$

In addition, there is the conservation of total number of species X, either in solution or bound in the complex XY. This is given by

$$\int_0^d u(x,t)dx + \theta(t) = c_o d. \tag{5.5}$$

The equations (5.4) and (5.5) together imply

$$D\frac{\partial u}{\partial x}(x,t)\Big|_{x=d} = k_{-1}\theta(t) - k_1 u(d,t)\left\{a_o - \theta(t)\right\}. \tag{5.6}$$

Summarising, we have the well-posed problem:

$$\frac{\partial u}{\partial t}(x,t) = D\frac{\partial^2 u}{\partial x^2}(x,t) \tag{5.7}$$

subject to the initial condition

$$u(x,0) = c_o \tag{5.8}$$

and the boundary conditions

$$\frac{\partial u}{\partial x}(x,t)\Big|_{x=0} = 0 \tag{5.9}$$

$$D\frac{\partial u}{\partial x}(x,t)\Big|_{x=d} = k_{-1}\theta(t) - k_1 u(d,t)(a_o - \theta(t)). \tag{5.10}$$

5.2 Non-dimensionalisation

Introduce the nondimensional variables

$$x' = x/d, \quad t' = (D/d^2)t$$

and scale the dependent variables

$$u'(x',t') = u(x,t)/c_o; \quad \theta'(t') = \theta(t)/a_o$$

and note that

$$\frac{\partial}{\partial x} \equiv \frac{\partial x'}{\partial x} \cdot \frac{\partial}{\partial x'} \equiv \frac{1}{d} \cdot \frac{\partial}{\partial x'}$$

and

$$\frac{\partial}{\partial t} \equiv \frac{\partial t'}{\partial t} \frac{\partial}{\partial t'} \equiv \frac{D}{d^2} \frac{\partial}{\partial t'} .$$

Equation (5.7) reduces to

$$\frac{\partial u'}{\partial t'}(x',t') = \frac{\partial^2 u'}{\partial x'^2}(x',t')$$

(5.8) to $u'(x',0) = 1$

and (5.9) to $\left.\frac{\partial u'}{\partial x'}(x',t')\right|_{x'=1} = 0.$

We shall consider (5.10) in a little more detail.

$$\frac{Dc_o}{d} \left.\frac{\partial u'}{\partial x'}(x',t')\right|_{x'=1} = k_{-1}a_o\theta'(t') - k_1c_ou'(1,t')(a_o - a_o\theta'(t'))$$

$$\therefore \left.\frac{\partial u'}{\partial x'}(x',t')\right|_{x'=1} = \frac{da_o}{Dc_o}\left\{k_{-1}\theta'(t') - k_1c_ou'(1,t')(1-\theta'(t'))\right\}$$

$$= \frac{k_1da_o}{D}\left\{\frac{k_{-1}}{k_1c_o}\theta'(t') - u'(1,t')(1-\theta'(t'))\right\} \qquad (5.11)$$

It is now convenient to define:

(a) the molar ratio $m = \frac{a_o}{c_o d}$

(b) the reaction time scale ratio $L = \frac{k_{-1}}{k_1c_o}$

(c) the diffusion reaction time scale $E = \frac{(k_1c_o+k_{-1})d^2}{D}$

so that (5.11) becomes

$$\left.\frac{\partial u'}{\partial x'}(x',t')\right|_{x'=1} = \frac{Em}{1+L}\,(L\theta'(t') - (1-\theta'(t'))u'(1,t')).$$

Note

$$\frac{Em}{1+L} = \frac{(k_1c_o+k_{-1})d^2}{k_{-1}\left(1+\frac{}{k_1c_o}\right)D}\cdot\frac{a_o}{c_o d}$$

$$= \frac{da_o k_1}{D}\,.$$

Dropping the 'primes' results in the nondimensionalised problem:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{5.12a}$$

subject to

$$u(x,0) = 1 \tag{5.12b}$$

and

$$\frac{\partial u}{\partial x}(0,t) = 0 \tag{5.12c}$$

and

$$\frac{\partial u}{\partial x}(1,t) = \frac{Em}{1+L}\,(L\theta(t) - (1-\theta(t))u(1,t) \tag{5.12d}$$

together with

$$m\theta(t) + \int_0^1 u(x,t)dx = 1. \tag{5.12e}$$

5.3 Integro-differential Derivation

The characteristics of the solution are particularly dependent upon the order of magnitude of the parameter E, which physically represents how fast the reaction at the 'wall' occurs compared with the diffusion adjustment within the vessel. Of particular interest are the two extreme cases $E \ll 1$ and $E \gg 1$. In the case $E \ll 1$ (reaction limited systems) the reaction is slow compared to the diffusion response, and consequently the X concentration gradient will be small. If $E \gg 1$ (diffusion limited systems) the diffusion response is slow compared to the reaction, and it is expected that at the reaction side wall u will decrease quickly before diffusion causes it to rise to the equilibrium value.

In general the initial boundary-value problem (5.12) cannot be solved analytically. Using Laplace transforms it is possible, however, to reduce it to a nonlinear Volterra integro-differential equation for $\theta(t)$. We shall require the convolution theorem for Laplace transforms and therefore state it now:

Define the convolution function $h = f*g$ of the functions f and g by

$$h(t) = (f*g)(t) = \int_0^t f(t-u)g(u)du.$$

The convolution theorem states:

Theorem

If $h(t) = (f*g)(t)$ then $\bar{h}(p) = \bar{f}(p)\bar{g}(p)$.

Differentiate (5.12e) with respect to time:

$$m\frac{d\theta}{dt}(t) + \int_0^1 \frac{\partial u}{\partial t}(x,t)\,dx = 0.$$

From (5.12a) it follows that

$$-m\frac{d\theta}{dt}(t) = \int_0^1 \frac{\partial^2 u}{\partial x^2}(x,t)dx = \frac{\partial u}{\partial x}(x,t)\Big|_0^1$$

$$\text{or} \quad -m\frac{d\theta}{dt}(t) = \frac{\partial u}{\partial x}(x,t)\Big|_{x=1} \tag{5.13}$$

using (5.12c).

Denote the Laplace transform of u in time by $\bar{u}$ where

$$\bar{u}(x,p) = \int_0^\infty u(x,t)e^{-pt}dt.$$

Taking Laplace transforms of equation (5.12a) and using the initial condition (5.12b) results in

$$\frac{d^2\bar{u}}{dx^2}(x,p) = p\bar{u}(x,p) - 1$$

The general solution is

$$\bar{u}(x,p) = \frac{1}{p} + A(p)\cosh(\sqrt{p}x) + B(p)\sinh(\sqrt{p}x). \tag{5.14}$$

Differentiating with respect to x,

$$\frac{d\bar{u}}{dx}(x,p) = A(p)\sqrt{p}\sinh(\sqrt{p}x) + B(p)\sqrt{p}\cosh(\sqrt{p}x)$$

and the boundary condition (5.12c) at $x = 0$ implies $B(p) = 0$.

Therefore

$$A(p) = \frac{\left.\frac{d\bar{u}}{dx}(x,p)\right|_{x=1}}{\sqrt{p}\sinh\sqrt{p}}$$

and it follows from (5.14) that

$$\bar{u}(1,p) = \frac{1}{p} + \bar{u}_x(1,p)\,\bar{k}(p)$$

where

$$\bar{u}_x(1,p) = \left.\frac{d\bar{u}}{dx}(x,p)\right|_{x=1}$$

and $\bar{k}(p) = \dfrac{\cot\sinh\sqrt{p}}{\sqrt{p}}$.

Inverting using the convolution theorem it follows that

$$u(1,t) = 1 + \int_0^t \frac{du}{dx}(1,s)\,k(t-s)ds$$

where

$$k(t) = (\pi t)^{-1/2}\left(1+2\sum_{n=1}^{x}\exp(-n^2/t)\right). \qquad (5.15)$$

Note that $\mathcal{L}^{-1}(1/p) = 1$ and, from tables, we discover that $\mathcal{L}^{-1}(\bar{k}(p)) = k(t)$ above.

From the convolution theorem, we then identify

$$\bar{f}(p) = \frac{d\bar{u}}{dx}(1,p) \quad \text{and} \quad \bar{g}(p) = \bar{k}(p)$$

before applying the convolution theorem.

Hence using (5.13)

$$u(1,t) = 1-m \int_0^t \frac{d\theta}{ds}(s)\, k(t-s)ds. \tag{5.16}$$

Once θ is known equation (5.16) may be used to determine u on the boundary $x = 1$.

By (5.13) and (5.16) the condition (5.12d) becomes

$$-\frac{d\theta}{dt} = \frac{E}{1+L}\left\{L\theta(t) - (1-\theta(t))(1-m\int_0^t \frac{d\theta}{ds}(s)\, k(t-s)ds)\right\}. \tag{5.17}$$

This is a nonlinear Volterra integro-differential equation for θ, with initial condition $\theta(0) = 0$. The kernel k is given by (5.15); it is weakly singular, that is, k possesses an integrable singularity within the range of singularity.

5.4 Numerical Method

The equations to be solved are

$$\theta'(t) = C - E\theta(t) - Cm(1-\theta(t)) \int_0^t k(t-s)\, \theta'(s)ds \tag{5.18}$$

with $\theta(0) = 0$ and

$$u(1,t) = 1 - m \int_0^t k(t-s)\theta'(s)ds \tag{5.19}$$

with the kernel k(t) defined by

$$k(t) = (\pi t)^{-1/2} (1+2 \sum_{n=1}^{\infty} \exp(-n^2/t)). \tag{5.20}$$

Here $\theta'(t)$ denotes differentiation with respect to time and $C = E/(1+L)$.

Firstly, it is of interest to note that an asymptotic result exists for small t,

$$\theta(t) \sim Ct - 4/3\, C^2 m\pi^{-2/3}\, t^{3/2} + O(t^{5/2}).$$

Before we can obtain a numerical method it is first necessary to truncate the infinite series in (5.20).

Let $k_\ell(t)$ denote the kernel truncated after ℓ terms, that is,

$$k_\ell(t) = (\pi t)^{-1/2}(1+2 \sum_{n=1}^{\ell} \exp(-n^2/t)).$$

Given T, $\xi > 0$, ℓ is chosen so that

$$|k(t) - k_\ell(t)| < \xi, \text{ for all } t \in [0,T]. \tag{5.21}$$

Now

$$|k(t) - k_\ell(t)| = 2(\pi t)^{-1/2} \sum_{n=\ell+1}^{\infty} \exp(-n^2/t)$$

$$< 2(\pi t)^{-1/2} \int_\ell^\infty \exp(-n^2/t)dn$$

$$= \left[\frac{2}{\pi}\right]^{1/2} \int_{(2/t)^{1/2}\ell}^\infty \exp(-x^2/2)dx$$

$$= 1 - \phi((2/t)^{1/2}\ell)$$

where

$$\phi(z) = \left[\frac{2}{\pi}\right]^{1/2} \int_0^z \exp(-t^2/2)dt$$

is a normal distribution; tables of $\phi(z)$ may be found in any statistical reference textbook.

It follows that (5.21) is satisfied if ℓ is chosen so that

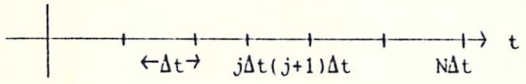
$$\phi((2/\pi)^{1/2}\ell) > 1 - \xi.$$

We shall derive an explicit product integration method, the product Euler method. The idea of product integration is: given two functions $f(t)$ and $g(t)$, we write

$$\int_0^1 f(t)g(t)dx = \sum_{j=0}^{N-1} \int_{t_j}^{t_{j+1}} f(t)g(t)dx \simeq \sum_{j=0}^{N-1} \int_{t_j}^{t_{j+1}} p_n(t)g(t)dx$$

where $t_{j+1} = t_j + \Delta t$ and $N\Delta t = T$ and where, for $t \in [t_j, t_{j+1})$, we approximate $f(t)$ by the n degree polynomial $p_n(t)$.

Let $\Delta t > 0$ denote the time step size and let $t_i = i\Delta t$, $i = 0(1)N$, $N\Delta t = T$.



In the following discussion θ_i and u_i will denote approximations to $\theta(t_i)$ and $u(1,t_i)$ respectively.

Replacing $k(t)$ by $k_\ell(t)$ in (5.18) gives

$$\theta'(t_i) = C - E\theta(t_i) - Cm(1-\theta(t_i)) \sum_{j=0}^{i-1} \int_{t_j}^{t_{j+1}} k_\ell(t_i-s)\theta'(S)ds.$$

For $t \in [t_j, t_{j+1}]$ approximate $\theta(t)$ by the linear Lagrange polynomial

$$\frac{1}{\Delta t}\left[(t-t_j)\theta(t_{j+1}) - (t-t_{j+1})\theta(t_j)\right]. \tag{5.22}$$

Then using the approximation

$$\int_{t_j}^{t_{j+1}} \exp\left[-\frac{n^2}{t_i-s}\right] \frac{1}{(t_i-s)^{1/2}}\, ds \simeq \exp\left[-\frac{n^2}{t_i-t_j}\right] \int_{t_j}^{t_{j+1}} \frac{ds}{(t_i-s)^{1/2}}$$

leads to the scheme

$$\theta_o = 0$$

$$\frac{\theta_i-\theta_{i-1}}{\Delta t} = C - E\theta_i - Cm\pi^{-1/2}(1-\theta_i)\Delta t \sum_{j=0}^{i-1} \gamma(i-j) \frac{(\theta_{j+1}-\theta_j)}{\Delta t}, \qquad i = 1(1)N \tag{5.23}$$

where the quadrature weights $\gamma(i-j)$ are given by

$$\gamma(i-j) = \frac{1}{\Delta t}\left[1+2 \sum_{n=1}^{\prime} \exp\left[-\frac{n^2}{t_i-t_j}\right]\right] \int_{t_j}^{t_{j+1}} \frac{ds}{(t_i-s)^{1/2}}$$

$$j = 0(1)i-1, \quad i = 1(1)N.$$

This scheme is implicit since the right hand side of (5.23) involves a term in θ_i^2, so that at each time step a nonlinear equation must be solved.

On rearranging (5.23) takes the form

$$\theta_i = g_{i-1} + F(\theta_i) \tag{5.24}$$

where g_{i-1} contains known (and previously calculated values) and $F(\theta_i)$ involves θ_i^2. The nonlinear equation (5.24) may be solved iteratively using

$$\theta_i^{(0)} = \theta_{i-1}$$

$$\theta_i^{(n)} = g_{i-1} + F(\theta_i^{(n-1)}), \quad n = 1,2,\ldots .$$

In practice, only one or two iterations are required.

Having found θ_i, the approximation u_i to $u(1,t_i)$ is given by the corresponding discretization of (5.19), namely

$$u_o = 1$$

$$u_i = 1 - m\pi^{-1/2} \sum_{j=0}^{i-1} \gamma(i-j)(\theta_{j+1} - \theta_j), \quad i = 1(1)N.$$

Note that in evaluating θ_i the summation

$$a_i = \gamma(1)\theta_{i-1} - \sum_{j=0}^{i-2} \gamma(i-j)(\theta_{j+1} - \theta_j)$$

has already been computed and u_i is then determined by

$$u_i = 1 - M\pi^{-1/2} (\gamma(1)\theta_i - a_i).$$

Figure 5.1 and 5.2 show $\theta(t)$ and $u(1,t)$ as a function of time for different parameter values. Note for E = 100 ($\gg$ 1) $u(1,t)$ decreases rapidly before then returning to its equilibrium level. This is an example of a diffusion limited system.

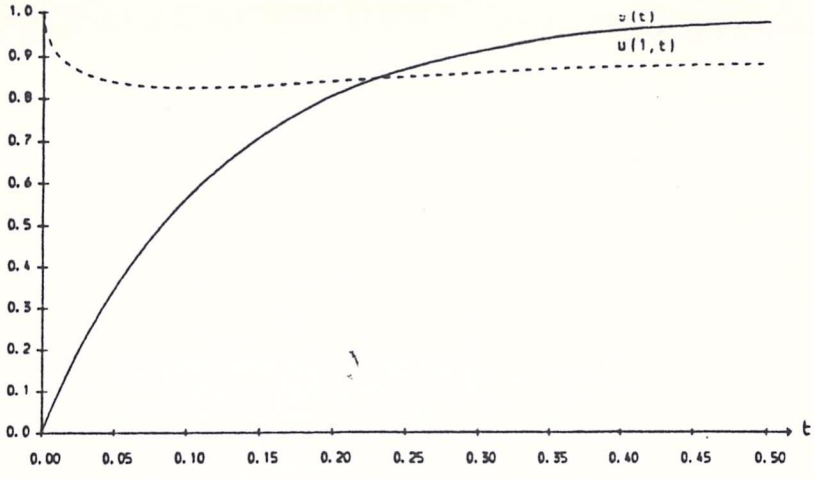


Figure 1 E = 10, L = 0.001, m = 0.1

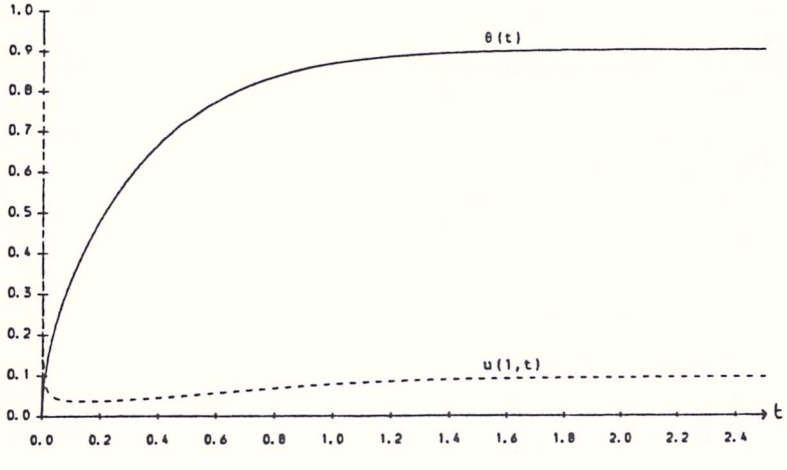


Figure 2 E = 100, L = 0.01, m =1.0

6. Smoke Dispersion from a High Chimney

6.1 The Mathematical Model

Consider smoke, that is a mixture of gases and particles, diffusing from a tall chimney of height h into the atmosphere and convected by the prevailing wind. It is important to know the concentration and, in particular, the maximum concentration on the ground. This is especially so if the dust cloud is radioactive like for instance Chernobyl, but it is also important for any pollutant. The equations governing the transport of smoke are equations (4.1-3) where T is to be interpreted as the concentration of particulate matter. These particles are generally small (1 μm) and the effects of gravity can be neglected (the Froude number based on wind speed and chimney height is large), and there is an inversion layer in the lower atmosphere at a height d through which there is no transport of smoke. At the ground the smoke will be deposited at a rate λ which depends on the terrain and the local concentration, and this rate is usually determined experimentally. In general both the wind speed and the diffusion coefficient will vary from point to point in a random manner, but we shall, for simplicity, consider the problem in the two dimensional plane of the prevailing wind. Further, we shall assume that U and D change only with height, that is $D = D(z)$, $U = U(z)$. The steady-state convective diffusion equation for the concentration c with diffusion coefficient D is, from equations (4.1-3),

$$(\underline{q}.\nabla)c = \mathrm{div}(D\ \mathrm{grad}\ c) \qquad (6.1)$$

where $\underline{q} = (U,0)^T$ is the mean wind speed (which is in the direction x), and z is measured vertically upwards so that U and D are in general functions of z (see Fig. 6.1)

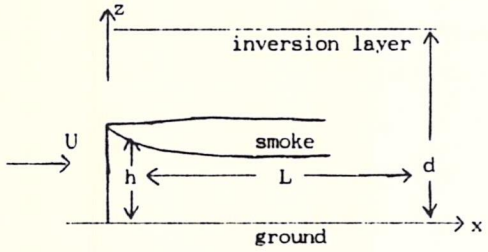


Figure 6.1

Consider (6.1) in cartesian coordinates

$$U(z)\ \frac{\partial c}{\partial x} = \frac{\partial}{\partial x}\left[D(z)\ \frac{\partial c}{\partial x}\right] + \frac{\partial}{\partial z}\left[D(z)\ \frac{\partial c}{\partial z}\right]. \qquad (6.2)$$

The boundary conditions on c are

$$z = 0,\ D\ \frac{\partial c}{\partial z} = \lambda; \qquad z = d,\ \frac{\partial c}{\partial z} = 0$$

together with

$$x = 0,\ c = Q\ \delta(z-h); \quad x \to \infty,\ c \to 0,$$

where Q is the source strength emanating from the chimney.

Consider $x' = x/(Uh^2/D)$ and $z' = z/h$. For simplicity consider $U(z) = U$, $D(z) = D$

$$\therefore \quad U\left[\frac{D}{Uh^2}\right]\frac{\partial c}{\partial x'} = D\left[\left[\frac{D}{Uh^2}\right]^2\frac{\partial^2 c}{\partial x'^2}\right] + D\cdot\frac{1}{h^2}\frac{\partial^2 c}{\partial z'^2}$$

$$\underline{\text{or}} \quad \frac{\partial c}{\partial x'} = \left[\frac{D}{Uh}\right]^2\frac{\partial^2 c}{\partial x'^2} + \frac{\partial^2 c}{\partial z'^2}\cdot$$

Thus if $\frac{D}{Uh} \ll 1$ then the term $\frac{\partial^2 c}{\partial x'^2}$ can be neglected.

For the problem to remain well-posed it is necessary also to omit the boundary condition $c \to 0$ as $x \to \infty$. In the original variables the equation (6.2) reduces to

$$U(z)\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}\left[D(z)\frac{\partial c}{\partial z}\right]. \tag{6.3}$$

To be able to proceed further analytically we further assume

(a) $\lambda = 0$

(b) $U(z) = U$, $D(z) = D$ i.e. $U(z)$ and $D(z)$ are assumed independent of z.

We introduce the nondimensional variables and scaling:

$$x' = x\Big/\left[\frac{Uh^2}{D}\right]; \quad z' = z/h; \quad c' = c/Q$$

so that (6.3) (with $D(z) = D$, $U(z) = U$) becomes

$$UQ\cdot\frac{D}{Uh^2}\frac{\partial c'}{\partial x'} = Q\frac{D}{h^2}\frac{\partial^2 c'}{\partial z'^2}$$

$$\underline{\text{or}} \quad \frac{\partial c'}{\partial x'} = \frac{\partial^2 c'}{\partial z'^2} \tag{6.4}$$

subject to

$$z' = 0, \quad \frac{\partial c'}{\partial z'} = 0; \quad z' \to \infty, \quad \frac{\partial c'}{\partial z'} = 0; \tag{6.4a,b}$$

$$x = 0, \quad c' = \delta(z' - 1) \tag{6.4c}$$

(For clarity we now drop the superscripts.)

6.3 Laplace transform solution

Define a Laplace transform

$$\bar{c}(p,z) = \int_0^\infty e^{-px} c(x,z)dx$$

so that

$$\frac{d^2\bar{c}}{dz^2}(p,z) - p\bar{c}(p,z) = -\delta(z-1) \tag{6.5}$$

with $\frac{\partial \bar{c}}{\partial z} = 0$ on $z = 0$ and $z \to \infty$.

The solution is

$$\bar{c}(p,z) = Ae^{-z/\sqrt{p}}, \qquad z > 1 \tag{6.6a}$$

$$= B(e^{z/\sqrt{p}} + e^{-z/\sqrt{p}}), \quad z < 1 \tag{6.6b}$$

where

$$A = B(e^{2\sqrt{p}} + 1) \quad \text{and} \tag{6.7a}$$

$$[-Ae^{-\sqrt{p}} - B(e^{\sqrt{p}} - e^{-\sqrt{p}})]\sqrt{p} = -1. \tag{6.7b}$$

It is easily checked that the solution (6.6) satisfies the differential equation (6.5) and the two boundary conditions above. Condition (6.7a) arises from the requirement for continuity of the solution across $z = 1$. Condition (6.7b) results from integrating equation (6.5) with respect to z. Thus

$$\frac{d\bar{c}}{dz}(p,z)\bigg|_{z=1^-} - \frac{d\bar{c}}{dz}(p,z)\bigg|_{z=1^+} - p\int_0^\infty \bar{c}(p,z)dz = -\int_0^\infty \delta(z-1)dz = -1.$$

Note that the term

$$\int_0^\infty \bar{c}(p,z)dz$$

vanishes when (6.7a) is employed and (6.7b) is obtained.

Now the concentration at the ground $\bar{c}(p,o)$ (in transform space) is

$$\bar{c}(p,o) = 2B$$

$$= \frac{e^{-\sqrt{p}}}{\sqrt{p}} .$$

This Laplace transform can be inverted from look-up tables (Spiegel, Shaum series p.250) or directly by contour integration

$$c(x,o) = \frac{1}{2\pi i} \int_{\Gamma} \frac{e^{px-\sqrt{p}}}{\sqrt{p}} \, dp$$

noting the branch point at $p = 0$.

Either way we obtain

$$c(x,o) = \frac{1}{\sqrt{\pi x}} \exp(-1/4x),$$

which has a maximum value of $(2/\pi e)^{1/2}$ at $x = \frac{1}{4}$.

In dimensional variables the ground concentration is $(Q/U)(2/\pi e)^{1/2}$ at a distance $Uh^2/2D$ from the chimney. This of course depends upon the assumption that $Uh/D \gg 1$.

Thus provided $Uh/D \gg 1$ this analysis has given us a ball-park indication as to the likely concentration of pollutant and where it is likely to be a maximum.

An alternative means of obtaining $\bar{c}(p,z)$ is to further take Laplace transforms of (6.5) with respect to z:

$$\frac{d^2\bar{c}}{dz^2}(p,z) - p\bar{c}(p,z) = -\delta(z-1).$$

Define

$$\bar{\bar{c}}(p,q) = \int_0^{\infty} e^{-qz} \, \bar{c}(p,z) dz$$

NB. $$\int_0^\infty e^{-qz}\frac{d^2\bar{c}}{dz^2}\,.\,dz = \frac{d\bar{c}}{dz}\,.\,e^{-qz}\Big|_o^\infty + q\int_0^\infty e^{-qz}\frac{d\bar{c}}{dz}\,dz$$

$$= \left[\frac{d\bar{c}}{dz}\right]e^{-qz}\Big|_o^\infty + q\bar{c}\,e^{-qz}\Big|_o^\infty + q^2\int_0^\infty e^{-qz}\bar{c}\,dz$$

$$= -q\bar{c}(p,o) + q^2\bar{\bar{c}}$$

$$\therefore\quad -q\bar{c}(p,o) + q^2\bar{\bar{c}}(p,q) - p\bar{\bar{c}}(p,q) = -\int_0^\infty e^{-qz}\,\delta(z-1)dz = -e^{-q}$$

$$\therefore\quad \bar{\bar{c}}(p,q) = \frac{q\bar{c}(p,o)-e^{-q}}{q^2-p}$$

$$= \frac{q}{q^2-p}\,\bar{c}(p,o) - \frac{1}{q^2-p}\,e^{-q}$$

$$\therefore\quad \bar{c}(p,z) = \cosh\sqrt{p}z.\bar{c}(p,o) - \int_0^z \frac{\sinh\sqrt{p}(z-u)}{\sqrt{p}}\,\delta(u-1)du.$$

Thus

$$\bar{c}(p,z) = \cosh\sqrt{p}z\;\bar{c}(p,o) \quad \text{if} \quad z < 1$$

$$= \cosh\sqrt{p}z\;\bar{c}(p,o) - \frac{\sinh\sqrt{p}(z-1)}{\sqrt{p}} \quad \text{if} \quad z > 1.$$

But the boundary condition

$$\lim_{z\to\infty}\frac{\partial\bar{c}}{\partial z}(p,z) = 0$$

has not yet been utilised.

Now

$$\frac{\partial\bar{c}}{\partial z}(p,z) = \sqrt{p}\sinh\sqrt{p}z\;\bar{c}(0,p) - \cosh\sqrt{p}(z-1) \text{ for } z > 1$$

$$\therefore \quad \bar{c}(p,0) = \lim_{z\to\infty} \frac{\cosh\sqrt{p}(z-1)}{\sqrt{p}\sinh\sqrt{p}z}$$

$$= \lim_{z\to\infty} \frac{e^{\sqrt{p}(z-1)} + e^{-\sqrt{p}(z-1)}}{\sqrt{p}(e^{\sqrt{p}z} - e^{-\sqrt{p}z})}$$

$$= \lim_{z\to\infty} \frac{e^{-\sqrt{p}} + e^{\sqrt{p}-2\sqrt{p}z}}{\sqrt{p}(1-e^{-2\sqrt{p}z})}$$

$$= \frac{e^{-\sqrt{p}}}{\sqrt{p}} .$$

6.4 A Numerical Solution

To obtain more detailed results for the general problem it would be necessary to resort to a numerical method. It is known that U(z) is a parabola (to a good approximation) in z and D(z) probably increases slightly with increasing z. From a numerical point of view it is probably more effective to treat the problem as time dependent and seek the steady state solution as $t \to \infty$. Thus we seek a solution to the following problem:

$$\frac{\partial c}{\partial t} = D(z) \frac{\partial^2 c}{\partial x^2} - U(z) \frac{\partial c}{\partial x} + \frac{\partial}{\partial z}\left[D(z) \frac{\partial c}{\partial z}\right]$$

subject to the initial condition

$$c(x,z,0) = 0$$

and boundary conditions

$$c(0,z,t) = \delta(z-h)$$

$$D \frac{\partial c}{\partial z}(x,0,t) = \lambda$$

$$\frac{\partial c}{\partial z}(x,d,t) = 0$$

$$\lim_{x\to\infty} c(x,z,t) = 0.$$

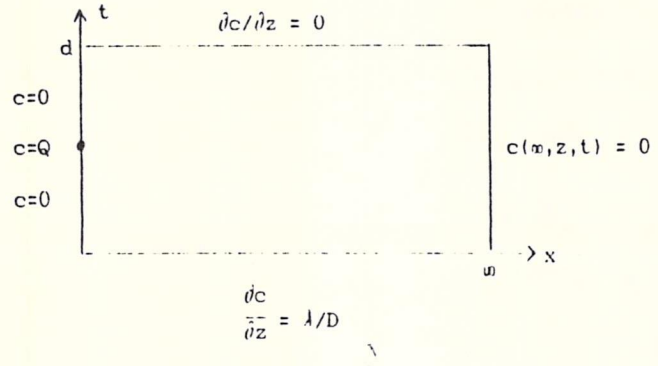


Figure 6.2

Figure 6.2 indicates the region in which we wish a solution and the boundary conditions.

One method of solution is Alternating Direction Implicit Methods or ADI methods. We shall illustrate their use on the somewhat simpler problem, while reserving the problem at hand for an exercise.

Consider

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

subject to $u(x,y,0) = f(x,y)$

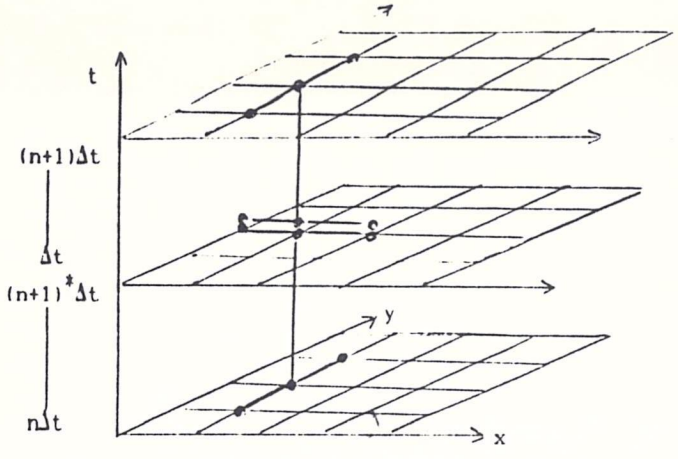
and $u(0,y,t) = 0$

$u(1,y,t) = 0$

$u(x,0,t) = 0$

$u(x,1,t) = 0.$

Define $\Delta x = \Delta y = h$ so that $(N+1)h = 1$



Consider the Peaceman-Rachford method

$$(1-r\delta^2_x)U^{n+1^*}_{i,j} = (1+r\delta^2_y)U^n_{i,j}$$

$$(1-r\delta^2_y)U^{n+1}_{i,j} = (1+r\delta^2_x)U^{n+1^*}_{i,j}$$

where

$$\delta^2_x U^n_{i,j} = U^n_{i+1,j} - 2U^n_{i,j} + U^n_{i-1,j}$$

and $r = \Delta t/h^2$ and $U^n_{i,j}$ is an approximation to $U(i\Delta x, j\Delta y, n\Delta t)$.

Note that these equations require the solution of N tridiagonal systems of equations per half time step (see Mitchell and Griffith (1980)).

7. Furnace Reaction Rate

This problem is essentially an inverse problem: that is given some experimental data can we determine a model which will allow us to 'fit' some unknown sample property parameters.

This chapter is an exercise in nondimensional scaling and the use of a regular perturbation expansion.

One technique of analysing the properties of a given chemical sample is to heat it continuously in a furnace to a temperature at which a reaction takes place, and to compare the temperature profile in the sample with that in the furnace.

7.1 The Physical Model

For simplicity consider a one dimensional model, that is the sample is an infinite block of width 2L, heated from both sides with no heat transfer parallel to its sides (see Fig. 7.1)

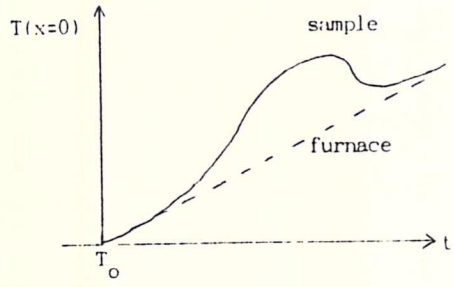


Figure 7.1

The temperature of the furnace T_F[K] can be regulated. We consider a problem in which the furnace is heated at a uniform (and known) rate β[Ks^{-1}] so that

$$T_F(t) = T_o + \beta t \qquad (7.1)$$

where T_o[K] is the temperature of the environment.

If the y-dimensions are much larger than L we need only consider a one-dimensional model, that is the temperature only depends on x and t

$$T = T(x,t).$$

Thus we seek a solution in the region portrayed by Fig. 7.2.

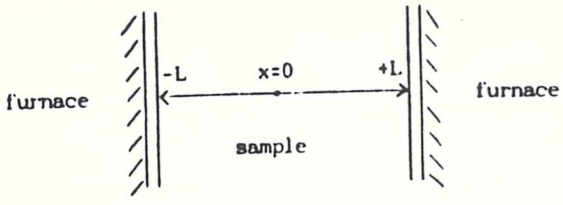


Figure 7.2

A thermocouple is placed at the centre of the sample (x = 0) to measure the temperature T(0,t). The problem is to determine the constants which describe the reaction, namely the heat of reaction λ, the activation energy E, and the rate constant A^* given the experimental observation (see Fig. 7.3)

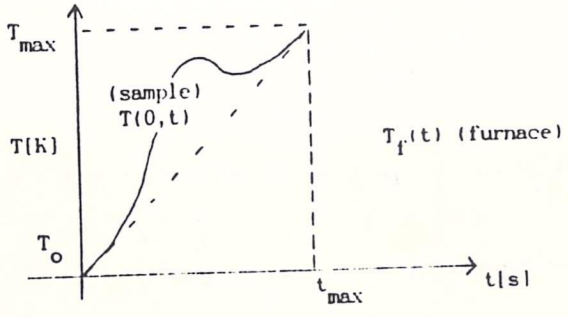


Figure 7.3

In Fig. 7.3 above t_{max}, T_{max} and the area Q between the curves T(0,t) and $T_F(t)$ can easily be measured from experimental evidence.

7.2 A mathematical model

If $\alpha(x,t)$ is the mass fraction of active material then from the (classical) Arrhenius law

$$\frac{\partial \alpha}{\partial t} = -A\alpha \exp(-E/RT) \qquad (7.2)$$

where E is the activation energy needed to get the reaction started [J kg^{-1}]

and R is the universal gas constant per unit of mass [J $kg^{-1}K^{-1}$].

Note $\alpha = \alpha(x,t)$ - hence the partial derivative.

In the sample heat transfer is governed by conduction - hence

$$\rho c \frac{\partial T}{\partial t} = K \frac{\partial^2 T}{\partial x^2} - \rho\lambda \frac{\partial \alpha}{\partial t} \qquad (7.3)$$

where $-\rho\lambda \frac{\partial \sigma}{\partial t}$ should be regarded as a source term; the chemical reaction is assumed to be exothermic and it generates heat in the sample. Here we have

ρ : density $[kg\ m^{-3}]$

c : specific heat $[Jkg^{-1}K^{-1}]$

K : thermal conductivity $[Wm^{-1}K^{-1}]$ or equivalently $[Jm^{-1}s^{-1}K^{-1}]$

$Q(= -\rho\lambda \frac{\partial \sigma}{\partial t})$: production of heat per unit volume and time, due to the chemical reaction $[Jm^{-3}s^{-1}]$

λ : heat of the reaction $[Jkg^{-1}]$

T : absolute temperature [K] (i.e. degrees Kelvin).

The initial/boundary conditions are that no reaction takes place at t = 0 so that $\sigma = 1$ and $\sigma \geq 0$ for all t.

Also $T = T_o$ at t = 0 and symmetry at x = 0 implies $\frac{\partial T}{\partial x} = 0$.

For heating due to the furnace at x = L, a simple model is to assume that a heat transfer coefficient h from the furnace to the sample is known so that

$$K \frac{\partial T}{\partial x} = h(T_F(t) - T). \qquad (7.4)$$

The units of h are $[Jm^{-2}s^{-1}K^{-1}]$.

(Note there should be no confusion between the thermal conductivity K and degrees Kelvin [K].)

7.3 The scaled model

We now nondimensionalise the problem using the scaled variables

$x' = x/L$; $t' = t/(L^2/(K/\rho c))$ (conduction time scale); $T' = (T-T_o)/(\lambda/c)$.

Recall that

$$\frac{\partial}{\partial x} \equiv \frac{1}{L}\frac{\partial}{\partial x'}, \quad \frac{\partial}{\partial t} \equiv \frac{k}{L^2}\frac{\partial}{\partial t'}$$

where k is the thermal diffusivity $= K/\rho c [m^2s^{-1}]$. (Thermal diffusivity is the analogue of diffusion coefficient.)

Thus

$$\frac{k}{L^2}\frac{\partial^2 T}{\partial x'^2} = \rho c \frac{k}{L^2}\frac{\partial T}{\partial t'} + \rho\lambda \frac{k}{L^2}\frac{\partial a}{\partial t'},$$

or $$\frac{\partial^2 T}{\partial x'^2} = \frac{\partial T}{\partial t'} + (\lambda/c)\frac{\partial a}{\partial t'}.$$

Now $T' = (T-T_o)/(\lambda/c)$ or $T = \left[\frac{\lambda}{c}\right] T' + T_o$

$$\therefore \left[\frac{\lambda}{c}\right]\frac{\partial^2 T'}{\partial x'^2} = \left[\frac{\lambda}{c}\right]\frac{\partial T'}{\partial t'} + \left[\frac{\lambda}{c}\right]\frac{\partial a}{\partial t'},$$

yielding

$$\frac{\partial^2 T'}{\partial x'^2} = \frac{\partial T'}{\partial t'} + \frac{\partial a}{\partial t'}, \qquad 0 < x < 1. \tag{7.5}$$

Equation (7.2) can be similarly nondimensionalised:

$$-\frac{k}{L^2}\frac{\partial a}{\partial t'} = Aa \exp\left[\frac{-1}{(R/E)((\lambda/c)T'+T_o)}\right]$$

$$\therefore -\frac{\partial a}{\partial t'} = \frac{L^2 A}{k} a \exp\left[\frac{-1}{(RT_o/E)\left[1 + \left[\frac{\lambda}{cT_o}\right]T'\right]}\right]$$

$$= A^* a \exp\left[\frac{-1}{\epsilon(1+\delta T')}\right] \tag{7.6}$$

with

$$A^* = \frac{AL^2}{k}, \quad \epsilon = \frac{RT_o}{E} \text{ and } \delta = \frac{\lambda}{cT_o}.$$

The boundary conditions become

$$x' = 0, \quad \frac{\partial T'}{\partial x'} = 0$$

$$x' = 1, \quad \frac{K}{L} \cdot \frac{\lambda}{c} \cdot \frac{\partial T'}{\partial x'} = h(T_o + \beta t - T)$$

$$= h\left[T_o + \beta \frac{L^2 \rho c}{K} t' - \left\{\left[\frac{\lambda}{c}\right] T' + T_o\right\}\right]$$

$$\underline{\text{or}} \quad \frac{\partial T'}{\partial x'} = -h^*(T' - \omega t') \qquad (7.7)$$

where $h^* = hL/K$ and $\omega = \dfrac{\rho c^2 L^2 \beta}{\lambda K}$.

The initial conditions are

$$\theta = 1 \quad \text{at } t' = 0$$

and $T' = 0$ at $t' = 0$.

There are five nondimensional parameters, three of which are unknown constants, h (which is given) and ω which is not known but can be varied. We summarise:

$$A^* = \frac{L^2 \rho c A}{K} \quad \left(= \frac{L^2 A}{k} \right)$$

$$\epsilon = \frac{RT_o}{E}$$

$$\delta = \frac{\lambda}{cT_o}$$

$$h^* = \frac{hL}{K}$$

$$\omega = \frac{\rho c^2 L^2 \beta}{\lambda K} \quad \left[= \frac{cL^2 \beta}{\lambda k} \right].$$

Note we have reduced the problem from 11 dimensional parameters $\rho, c, K, \lambda, A, E, R, h, \beta, T_o$ and L to 5 nondimensional parameters.

If all are O(1) the problem is very hard and would require a numerical solution; and fitting A^*, E, λ from numerical results is non-trivial. To make (analytic) progress, therefore, consider $\omega \ll 1$, that is the temperature is increased slowly. However, as $\omega \to 0$ the furnace heating term will disappear. This tells us that we must rescale time. Write

$\tau = \omega t'$ and note $\dfrac{\partial}{\partial t'} \equiv \dfrac{\omega \partial}{\partial \tau}$

so that equation (7.5) becomes

$$\frac{\partial^2 T'}{\partial x'^2} = \omega \frac{\partial T'}{\partial \tau} + \omega \frac{\partial a}{\partial \tau} = \omega \left[\frac{\partial T'}{\partial \tau} + \frac{\partial a}{\partial \tau} \right] \tag{7.8}$$

and equation (7.6) becomes

$$- \frac{\partial a}{\partial \tau} = \tilde{A} a \exp\left[\frac{-1}{\epsilon (1 + \delta T')} \right] \tag{7.9}$$

with $\tilde{A} = A^*/\omega$.

Boundary and initial conditions become

$$x' = 0, \quad \frac{\partial T'}{\partial x'} = 0; \quad x' = 1, \quad \frac{\partial T'}{\partial x'} = -h^*(T' - \tau)$$

$$\tau = 0, \quad a = 1 \quad \text{and} \quad T' = 0.$$

7.4 Regular perturbation analysis

We require to solve for small ω ($\ll 1$)

$$\frac{\partial^2 T}{\partial x^2} = \omega \left[\frac{\partial T}{\partial \tau} + \frac{\partial a}{\partial \tau} \right] \tag{7.10a}$$

and

$$- \frac{\partial a}{\partial \tau} = A a \exp\left[\frac{-1}{\epsilon (1 + \delta T)} \right] \tag{7.10b}$$

subject to

$$x = 0, \quad \frac{\partial T}{\partial x} = 0; \quad x = 1, \quad \frac{\partial T}{\partial x} = -h(T - \tau) \tag{7.10c,d}$$

$$\tau = 0, \quad a = 1 \quad \text{and} \quad T = 0. \tag{7.10e,f}$$

Note superscripts ($'$ and *) have been dropped from now on for clarity.

We seek a regular expansion in powers of ω:

$$T = T^{(0)} + \omega T^{(1)} + O(\omega^2)$$

$$a = a^{(0)} + \omega a^{(1)} + O(\omega^2).$$

Equation (7.10a) becomes

$$\frac{\partial^2}{\partial x^2}\left(T^{(o)} + O(\omega)\right) = \omega\left[\frac{\partial T^{(o)}}{\partial \tau} + \frac{\partial \theta^{(o)}}{\partial \tau} + O(\omega)\right]$$

$$\Rightarrow \quad \frac{\partial^2 T^{(o)}}{\partial x^2} = 0, \quad \text{on equating terms independent of } \omega$$

$$\therefore \quad T^{(o)} = A+Bx \quad \text{(where A and B could be functions of } \tau\text{. A should not be confused with the A of (7.10b)).}$$

The boundary conditions then imply

$$\frac{\partial T^{(o)}}{\partial x} = 0 \quad \text{i.e.} \quad B = 0, \quad \text{thus } T^{(o)} = A.$$

But

$$\frac{\partial T^{(o)}}{\partial x} = -h(T^{(o)} - \tau) \text{ and so } T^{(o)} = \tau.$$

Therefore

$$T = \tau + \omega T^{(1)}(x,\tau) + O(\omega^2). \tag{7.11}$$

Using $\theta = \theta^{(o)} + \omega\theta^{(1)} + O(\omega^2)$ and substituting (7.11) into (7.10b) results in

$$-\left[\frac{\partial \theta^{(o)}}{\partial \tau} + O(\omega)\right] = A(\theta^{(o)} + O(\omega))\exp\left[\frac{-1}{\epsilon(1+\delta(\tau+O(\omega)))}\right]$$

or

$$-\frac{\partial \theta^{(o)}}{\partial \tau} = A\theta^{(o)}\exp\left[\frac{-1}{\epsilon(1+\delta\tau)}\right]$$

equating terms independent of ω.

Therefore

$$\ln \theta^{(o)}(\tau) - \ln \theta^{(o)}(0) = -A\int_0^{\tau} \exp\left[\frac{-1}{\epsilon(1+\delta\tau')}\right]d\tau'$$

$$\therefore \quad \theta^{(o)}(\tau) = \exp\left[-A\int_0^{\tau} \exp\left[\frac{-1}{\epsilon(1+\delta\tau')}\right]d\tau'\right]$$

$$\therefore \quad a(\tau) = a^{(o)}(\tau) + \omega a^{(1)}(\tau) + O(\omega^2) \tag{7.12}$$

with $a^{(o)}(\tau)$ as above.

NB. $a^{(o)}(\tau)$ is a function of τ only, but we cannot assume that $a^{(1)}$ is also independent of x.

Substitute (7.11) and (7.12) into (7.10a) to obtain

$$\omega \frac{\partial^2 T^{(1)}}{\partial x^2} + O(\omega^2) = \omega\left\{\frac{\partial a^{(o)}}{\partial \tau} + \omega \frac{\partial a^{(1)}}{\partial \tau} + O(\omega^2)\right\}$$

$$+ \omega\left\{\frac{\partial T^{(o)}}{\partial \tau} + \omega \frac{\partial T^{(1)}}{\partial \tau} + O(\omega^2)\right\}$$

and, equating powers of ω, gives

$$\frac{\partial^2 T^{(1)}}{\partial x^2} = \frac{\partial a^{(o)}}{\partial \tau} + \frac{\partial T^{(o)}}{\partial \tau} = \dot{a}^{(o)} + 1 \tag{7.13}$$

with boundary conditions

$$x = 0, \quad \frac{\partial T^{(1)}}{\partial x} = 0 \quad \text{and} \quad x = 1, \quad \frac{\partial T^{(1)}}{\partial x} = -hT^{(1)}.$$

From (7.13) we obtain

$$T^{(1)} = (1 + \dot{a}^{(o)}) \frac{x^2}{2} + Cx + D.$$

But

$$\left.\frac{\partial T^{(1)}}{\partial x}\right|_{x=0} = 0 \quad \text{implies} \quad C = 0.$$

Further

$$\frac{\partial T^{(1)}}{\partial x} = -hT^{(1)} \quad \text{implies} \quad D = -(1+\dot{a}^{(o)})\left[\frac{1}{2} + \frac{1}{h}\right].$$

Thus

$$T^{(1)} = (1+\dot{a}^{(o)})\left[\frac{x^2-1}{2} - \frac{1}{h}\right]$$

and so

$$T = \tau + \omega(1 + \delta^{(0)})\left[\frac{x^2-1}{2} - \frac{1}{h}\right] + O(\omega^2)$$

is a consistent expansion for T if the constants involved are all of order 1, except near $\tau = 0$ where the initial condition T = 0 has not been satisfied. However, for small τ the reaction will hardly have started and so this is not of great interest.

The principal question of interest for us is: Does this expansion for T (evaluated at x = 0) give the form displayed in Figure 7.3, that is can constants A, ϵ and δ be chosen so that the observed results can be fitted by

$$T_{x=0} = \tau + \omega\left[\frac{1}{2} + \frac{1}{h}\right]\left\{A \exp\left[\frac{-1}{\epsilon(1+\delta\tau)}\right]\left[-A\int_0^\tau \exp\left[\frac{-1}{\epsilon(1+\delta\tau')}\right] d\tau'\right] - 1\right\}. \quad (7.14)$$

Given the experimental measurements

$$\hat{T}(0,t_j), \quad j = 1,2,\ldots,N$$

the parameters A, ϵ and δ may be fitted by a a least squares technique.

8. The classical Stefan problem

8.1 Single phase: melting ice or the gin and tonic problem

A simple version of a Stefan problem is the melting of a semi-infinite sheet of ice, initially at the melting temperature, taken to be zero, the surface of which is raised at time t = 0 to a temperature above zero, at which it is subsequently maintained. A boundary surface or interface on which melting occurs, moves from the surface into the sheet and separates a region of water from one of ice at zero temperature as in Figure 8.1

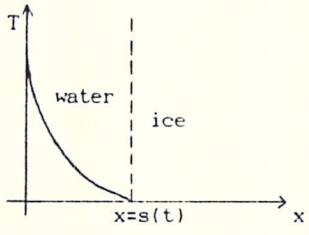
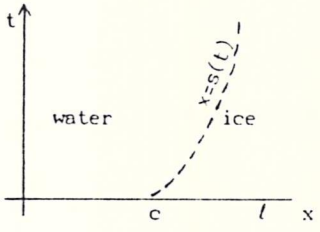


Fig. 8.1



path of melting interface

Fig. 8.2

The path of the melting interface, s(t), in the x-t plane is shown in Figure 8.2, where s(t) denotes the thickness of the water phase at time t and x is the space coordinate measured from the outer surface of the sheet, x = 0.

If T(x,t) denotes the temperature distribution in the water at time t, the problem is to find the pair of unknowns T(x,t) and S(t) by solving the heat-flow equation

$$c\rho \frac{\partial T}{\partial t} = K \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < s(t), \quad t > 0 \tag{8.1a}$$

subject to a fixed boundary condition

$$T = T_o, \quad x = 0, \quad t > 0 \tag{8.1b}$$

where T_o is the constant surface temperature, and initial conditions

$$T = 0, \quad x > 0, \quad t = 0 \tag{8.1c}$$

$$s(0) = 0. \tag{8.1d}$$

In equation (8.1a) the specific heat c, density ρ, and heat conductivity K are assumed to be constants. Two further conditions are required on the moving surface, one to provide the second boundary condition necessary for the solution of the second order equation (8.1a) and the other to determine the position of the interface itself. In this problem they are

$$T = 0 \tag{8.1e}$$

$$-K \frac{\partial T}{\partial x} = L\rho \frac{ds}{dt} \quad \text{at } x = s(t), \quad t > 0 \tag{8.1f}$$

where L [Jkg^{-1}] is the latent heat required to melt the ice.

Equation (8.1f) is known as the 'Stefan condition' and it expresses the heat balance on the interface (see section 8.3).

8.2 Two phases

If the ice is initially at a temperature below the melting temperature, heat flow occurs in both the water and ice phases. This two-phase problem is to find the triple $[T_1(x,t), T_2(x,t), s(t)]$, where T_1 and T_2 denote the temperatures in the water and ice phases respectively. A typical example is a finite sheet of ice occupying the space $0 \leq s(t) \leq x \leq l$, where

$$c_i \rho_i \frac{\partial T_i}{\partial t} = K_i \frac{\partial^2 T_i}{\partial x^2}, \quad i = 1,2 \tag{8.2a}$$

where l is as given in Figure 8.2.

The Stefan conditions

$$\left.\begin{aligned} T_1 = T_2 = 0 \qquad & (8.2b) \\ K_2 \frac{\partial T_2}{\partial x} - K_1 \frac{\partial T_1}{\partial x} = L\rho \frac{\partial s}{\partial t} \qquad & (8.2c) \end{aligned}\right\} \quad x = s(t)$$

and for the time being volume changes on melting are assumed negligible i.e. ice and water have the same density ρ, so that $\rho_1 = \rho_2 = \rho$.

8.3 The Stefan condition

The Stefan condition (8.2c) is easily derived by referring to Figure 8.3 which shows the boundary moving a distance δx in time δt.

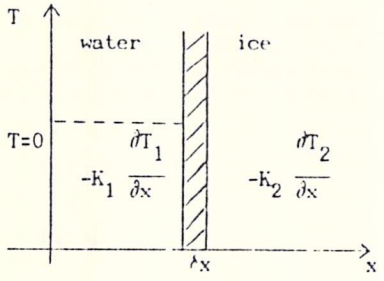


Fig. 8.3

In order to melt the ice contained per unit area perpendicular to x in the shaded region an amount of heat $L\rho\delta x$ is required. An amount of heat $-K_1 \delta t \frac{\partial T_1}{\partial x}$ enters the shaded element from the water phase and $-K_2 \delta t \frac{\partial T_2}{\partial x}$ escapes into the ice. Assuming there are no heat sources on the interface the heat balance of the shaded element requires that

$$-K_1 \frac{\partial T_1}{\partial x} + K_2 \frac{\partial T_2}{\partial x} = L\rho \frac{\delta x}{\delta t}$$

which in the limit gives (8.2c) with $\frac{dx}{dt} = \frac{ds}{dt}$ on the interface.

8.4 Nondimensional Form of the Stefan Problem

Equations (8.1) can be reduced to non-dimensional form using the scaling

$$x' = x/\ell, \quad t' = \left[\frac{K}{c\rho\ell^2}\right]t, \quad u = T/T_o, \quad s' = s/\ell$$

where ℓ is some standard length. Equation (8.1a) becomes

$$c\rho\left[\frac{K}{c\rho\ell^2}\right]T_o \cdot \frac{\partial u}{\partial t'} = K\left[\frac{T_o}{\ell^2}\right]\frac{\partial^2 u}{\partial x'^2}$$

$$\text{or} \quad \frac{\partial u}{\partial t'} = \frac{\partial^2 u}{\partial x'^2}, \qquad 0 < x < s'(t'), \quad t' > 0. \tag{8.3a}$$

Further

$$u = 1, \quad x' = 0, \quad t' > 0 \tag{8.3b}$$

$$u = 0, \quad x' > 0, \quad t' = 0 \tag{8.3c}$$

$$s'(0) = 0$$

and

$$\left.\begin{aligned} u &= 0 \\ -K \cdot \frac{T_o}{\ell}\frac{\partial u}{\partial x'} &= L\rho\ell\left[\frac{K}{c\rho\ell^2}\right]\frac{\partial s'}{\partial t'} \end{aligned}\right\} \quad \text{at } x' = s'(t'), \quad t' > 0.$$

The last two conditions on the free surface give

$$\left.\begin{aligned} u &= 0 \\ -\frac{\partial u}{\partial x'} &= \lambda\frac{\partial s'}{\partial t'} \end{aligned}\right\} \quad \text{at } x' = s'(t'), \quad t' > 0 \tag{8.3d,e}$$

where $\lambda = (L/cT_o)$ is a dimensionless 'latent heat' and $1/\lambda$ is the Stefan number. For a given (non-dimensional) heat flux $\frac{\partial u}{\partial x'}$, if $\lambda << 1$ (i.e. $L << cT_o$) then $\frac{\partial s'}{\partial t'} >> 1$, that is if the latent heat required to change the phase is small then the phase change will occur rapidly or equivalently the moving boundary will move rapidly.

The two phase system of Section 8.2 can similarly be expressed in non-dimensional variables:

$$x' = x/\ell, \quad t' = \frac{K_o}{c_o\rho\ell^2}t, \quad u_i = T_i/T_o, \quad s' = s/\ell$$

where T_o, K_o and c_o are any typical values of temperature, thermal conductivity and specific heat respectively. This results in the non-dimensional equations

$$\frac{\partial u_i}{\partial t'} = \kappa_i \frac{\partial^2 u_i}{\partial x'^2}, \qquad i = 1,2, \tag{8.4a}$$

where $\kappa_i = (K_i/K_o)(c_o/c_i)$ and

$$\left.\begin{aligned} u_1 &= u_2 = 0 \\ \gamma_2 \frac{\partial u_2}{\partial x'} &- \gamma_1 \frac{\partial u_1}{\partial x'} = \frac{\partial s'}{\partial t'} \end{aligned}\right\} \quad x' = s'(t') \tag{8.4b,c}$$

where

$$\gamma_i = K_i/(\lambda K_o).$$

8.5 Numerical Methods

A great deal of work has been done in this field over the last 10-15 years. The two most relevant recent books are that by Crank (1987) and Elliott and Ockendon (1982). We shall not here discuss front tracking methods or the enthalpy method, but shall consider the introduction of "immobilization variables" which will have the effect of fixing the moving boundary and incorporating it within the differential equation itself.

Consider equation (8.3)

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad 0 < x < s(t), \quad t > 0 \tag{8.5a}$$

$$u = 1, \quad x = 0, \quad t > 0 \tag{8.5b}$$

$$u = 0, \quad x > 0, \quad t = 0 \tag{8.5c}$$

$$s(0) = 0 \tag{8.5d}$$

together with

$$\left.\begin{aligned} u &= 0 \qquad (8.5e) \\ -\frac{\partial u}{\partial x} &= \lambda \frac{\partial s}{\partial t} \qquad (8.5f) \end{aligned}\right\} \quad \text{at } x = s(t), \quad t > 0$$

where the ' have been dropped for clarity.

Now consider the transformation $\xi = x/s(t)$ which fixes the melting boundary at $\xi = 1$ for all t.

We thus obtain

$$\frac{\partial u}{\partial x} = \frac{1}{s(t)} \frac{\partial u}{\partial \xi}, \quad \frac{\partial^2 u}{\partial x^2} = \left[\frac{1}{s(t)}\right]^2 \frac{\partial^2 u}{\partial \xi^2}$$

and $$\frac{\partial u}{\partial t} = -\frac{x}{(s(t))^2} \frac{ds}{dt} \frac{\partial u}{\partial \xi} + \frac{\partial u}{\partial t} \tag{8.6}$$

so that (8.5a) and (8.5f) become respectively

$$\frac{\partial^2 u}{\partial \xi^2} = s^2 \frac{\partial u}{\partial t} - s\xi \frac{ds}{dt} \frac{\partial u}{\partial \xi}, \quad 0 < \xi < 1, \quad t > 0 \tag{8.7}$$

and

$$-\frac{1}{s} \frac{\partial u}{\partial \xi} = \lambda \frac{ds}{dt}, \quad \xi = 1, \quad t > 0. \tag{8.8}$$

NB: to obtain (8.6) we consider the change of variables $\tau = f(x,t) = t$ and $\xi = g(x,t) = x/s(t)$ and use the chain rule. Thus

$$\frac{\partial u}{\partial t} = \frac{\partial \tau}{\partial t} \cdot \frac{\partial u}{\partial \tau} + \frac{\partial \xi}{\partial t} \cdot \frac{\partial u}{\partial \xi}$$

$$= \frac{\partial f}{\partial t} \cdot \frac{\partial u}{\partial \tau} + \frac{\partial g}{\partial t} \cdot \frac{\partial u}{\partial \xi}$$

$$= 1 \cdot \frac{\partial u}{\partial \tau} + (-x(s(t))^{-2} s'(t)) \frac{\partial u}{\partial \xi} \quad \text{etc.}$$

Thus the problem has now been reduced to:

$$s^2 \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial \xi^2} + s\xi \frac{ds}{dt} \frac{\partial u}{\partial \xi}, \quad 0 < \xi < 1, \quad t > 0 \tag{8.9a}$$

with initial conditions

$$u = 0, \quad \xi > 0, \quad t = 0 \tag{8.9b}$$

and $$s(0) = 0 \tag{8.9c}$$

and fixed boundary conditions

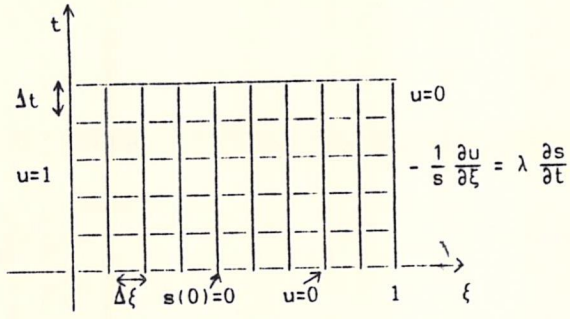
$$u = 1, \quad \xi = 0, \quad t > 0 \tag{8.9d}$$

and

$$u = 0$$

$$-\frac{1}{s} \frac{\partial u}{\partial \xi} = \lambda \frac{ds}{dt} \qquad \text{at } \xi = 1, \quad t > 0. \tag{8.9e,f}$$

To solve this problem numerically consider the grid



A Crank-Nicolson type finite difference scheme gives

$$\left[\frac{s^n+s^{n-1}}{2}\right]^2\left[\frac{u_i^n-u_i^{n-1}}{\Delta t}\right] = \frac{1}{2}\left[(u_{i+1}^n - 2u_i^n + u_{i-1}^n) + (u_{i+1}^{n-1} - 2u_i^{n-1} + u_{i-1}^{n-1})\right]/(\Delta\xi)^2$$

$$+ \left[\frac{s^n+s^{n-1}}{2}\right]\xi_i\left[\frac{s^n-s^{n-1}}{\Delta t}\right]\left[\frac{u_{i+1}^n-u_{i-1}^n}{2\Delta\xi}\right] \quad i=1,2,\ldots,N \text{ and } n=1,2,\ldots \qquad (8.10a)$$

with

$$u_i^o = 0 \qquad i = 1,2,\ldots,N+1 \qquad (8.10b)$$

$$s^o = 0 \qquad (8.10c)$$

and

$$u_o^n = 1, \qquad n = 0,1,2,\ldots \qquad (8.10d)$$

$$u_{N+1}^n = 0, \qquad n = 0,1,2,\ldots \qquad (8.10e)$$

$$-\frac{1}{s^n}\left[\frac{u_{N+2}^n-u_N^n}{2\Delta\xi}\right] = \lambda\left[\frac{s^n-s^{n-1}}{\Delta t}\right], \qquad n = 1,2,\ldots \quad . \qquad (8.10f)$$

Here $\xi_i = i\Delta\xi$ and $\xi_i = \xi_{i-1} + \Delta\xi$

$t_n = n\Delta t$ and $t_n = t_{n-1} + \Delta t$

U_i^n denotes the finite difference approximation $u(i\Delta x, n\Delta t)$

S^n denotes $s(n\Delta t)$.

Clearly to solve (8.10) requires the solution of a nonlinear set of equations at each time step.

This approach dates back to 1957 and there are arguably better methods (e.g. enthalpy etc.) now in existence. However, for real problems as opposed to model problems (see Section 9) this direct approach still has a lot to recommend it.

9. Deicing helicopter blades

Helicopter rotors are extremely sensitive to icing conditions. The relatively small size and high subsonic speeds achieved by rotors make them efficient collectors of ice which very quickly deforms the aerofoil profile and results in damaging effects to both the aerodynamic and dynamic characteristics of the rotor. One of the most viable means of providing rotor protection, due to low energy requirements, appears to be an electrothermal deicing system. This consists of an electrical heating element embedded in the blade near the surface to be deiced.

This chapter will be involved in building a mathematical model to predict the best on/off switching strategy and the electrical power required.

9.1 The physical model

The heater is placed (typically) 0.5 mm from the upper slab boundary or blade surface. The heater when energised is capable of producing a heating intensity of 20-27W/square inch (31-42 KW/m^2). The ice adhering to the blade surface is assumed to have a uniform thickness in the range 5-10 mm; physical properties of ice are displayed in Table 1. It is assumed that the upper surface of the ice radiates into an air environment at $-20^{\circ}C$ by Newton cooling: the heat transfer coefficient at the ice/air interface is in the range 500-1000 W/m^2K. Furthermore it is assumed that the above blade/ice system is initially at the external environmental temperature of $-20^{\circ}C$ (prior to energising the heater mat). When the heater mat is switched on, the blade and ice will warm up by transient conduction. The production of heat as a result of passing a current through a wire (or in this case a wire mat) is usually called Joule heating. Finally, so as to simulate the small convective heat transfer from the blade (which is made of reinforced glass fibre) to the air within the blade cavity, the lower boundary of the slab is assumed to be insulated.

		Blade	Water	Ice
Latent heat of fusion	L(J/kg)			3.25×10^5
Fusion temperature	T_f(K)			273
Density	ρ(kg m^3)	1800	998	916
Specific heat	c_p(J/kgK)	879	4174	2106
Thermal conductivity	K(W/mK)	0.34	0.554	2.3
Thickness of blade	D(mm)	5		
Initial thickness of ice	H(mm)			5-10
Initial and environmental temperature	T_i(K)			253
Air ice heat transfer coefficient	h(W/m^{2}K)			500-1000
Heater input	q (W/sq ins, kW/m^2)			(20-27, 30-42)

Table 1

9.2 The mathematical model

The model is constructed in two stages associated with the warm-up period and the melting regime.

9.2a The warm-up period

Let z measure the distance normal to the lower blade surface and let the blade/ice interface be located at z = D. The heater mat is located at $z = D^{*} (< D)$; let z^{*} measure the normal distance from the blade/ice interface into the ice-layer and let the ice/air interface be located at $z^{*} = H$.

In the blade $z \in [0,D]$, $t > 0$

$$k_b \frac{\partial^2 T_b}{\partial z^2} = \frac{\partial T_b}{\partial t} \tag{9.1a}$$

where T_b is the blade temperature, $k_b = K_b/\rho_b c_{p_b}$ is the thermal diffusivity and t is the time.

In the ice layer $z^{*} \in [0,H]$, $t > 0$

$$k_I \frac{\partial^2 T_I}{\partial z^{*2}} = \frac{\partial T_I}{\partial t} \tag{9.1b}$$

where T_I is the ice temperature and $k_I = K_I/\rho_I c_{p_I}$ is its thermal diffusivity.

The boundary conditions for $t > 0$ are as follows:

$$\frac{\partial T_b}{\partial z} = 0, \quad z = 0 \tag{9.1c}$$

$$K_b \left[\left[\frac{\partial T_b}{\partial z} \right]_{z=D^{*}+} - \left[\frac{\partial T_b}{\partial z} \right]_{z=D^{*}-} \right] = -q(t), \quad z = D^{*}; \tag{9.1d}$$

(Joule heating)

$$T_I = T_b, \quad K_I \frac{\partial T_I}{\partial z^{*}} = K_b \frac{\partial T_b}{\partial z} \quad \text{at} \quad z = D \text{ and } z^{*} = 0; \tag{9.1e,f}$$

and finally

$$K_I \frac{\partial T_I}{\partial z^{*}} = -h(T_I - T_i), \quad z^{*} = H. \tag{9.1g}$$

The initial conditions are

$$T_I = T_b = T_i \quad \text{at} \quad t = 0 \quad \text{for} \quad z \in [0,D] \text{ and } z^{*} \in [0,H]. \tag{9.1h,i}$$

Figure 9.1 illustrates the situation.

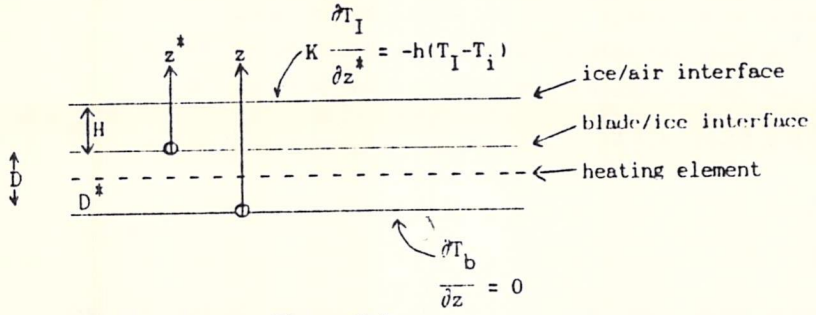


Figure 9.1

In the above T_i denotes the initial temperature taken to be the ice/air environmental temperature, h is the ice/air convective heat transfer coefficient and q is the heat flux produced by the heater when switched on. In general q will be a function of t to allow for switched on-off heater simulations.

An alternative formulation of the blade system (9.1a-d) is to write these equations as a single equation

$$K_b \frac{\partial^2 T_b}{\partial z^2} = \rho_b c_{P_b} \frac{\partial T_b}{\partial t} - q(t)\delta(z-D^*), \quad \text{for } t > 0,\ z \in [0,D], \tag{9.2}$$

where the Dirac delta function

$$\delta(z-D^*) = 0 \quad \text{for} \quad z \neq D^*$$

and

$$\int_{D^*-\epsilon}^{D^*+\epsilon} \delta(z-D^*)dz = 1,$$

These formulations are identical.

The simplest transient response to investigate is that due to

$$q(t) = q, \quad \text{a constant for } t > 0. \tag{9.3}$$

The warm-up period for the blade and ice will proceed for $t \leq t_m$, where t_m is the time taken for the ice/blade interface to reach the ice fusion temperature T_F, and t_m is determined from solving the transcendental equation

$$T_I(0,t_m) = T_b(D,t_m) = T_F. \tag{9.4}$$

For $t \geq t_m$ it is necessary to investigate the melting regime.

9.2b The melting regime

At time $t > t_m$ assume that the melt has penetrated a distance E(t) into the ice region. Let the suffix w denote the water properties.

For $t > t_m$ the governing equations for the blade/water/ice system are as follows:

$$\text{for } z \in [0,D] \qquad k_b \frac{\partial^2 T_b}{\partial z^2} = \frac{\partial T_b}{\partial t} \; ; \tag{9.5a}$$

$$\text{for } z^* \in [0, E(t)] \qquad k_w \frac{\partial^2 T_w}{\partial z^{*2}} = \frac{\partial T_w}{\partial t} \; ; \tag{9.5b}$$

$$\text{for } z^* \in [E(t),H] \qquad k_I \frac{\partial^2 T_I}{\partial z^{*2}} = \frac{\partial T_I}{\partial t} \; . \tag{9.5c}$$

The boundary conditions are:

$$z = 0, \quad \frac{\partial T_b}{\partial z} = 0; \tag{9.5d}$$

$$z = D^*, \quad K_b \left\{ \left[\frac{\partial T_b}{\partial z} \right]_{z=D^{*+}} - \left[\frac{\partial T_b}{\partial z} \right]_{z=D^{*-}} \right\} = -q \tag{9.5e}$$

$$z^* = 0, \quad T_w = T_b, \quad K_w \frac{\partial T_w}{\partial z^*} = K_b \frac{\partial T_b}{\partial z} \tag{9.5f}$$

(z=D)

$$z^* = E, \quad T_I = T_w = T_F \tag{9.5g}$$

$$z^* = E, \quad K_I \frac{\partial T_I}{\partial z^*} - K_w \frac{\partial T_w}{\partial z^*} = \rho_I L \frac{dE}{dt} \tag{9.5h}$$

$$z^* = H, \quad K_I \frac{\partial T_I}{\partial z^*} = -h(T_I - T_i) \tag{9.5i}$$

Note that in equation (9.5h) the change in the volume in the ice and water at phase change has been neglected.

At $t = t_m$ the initial conditions are

$$z \in [0,D], \quad T_b(z,t) = T_b(z,t_m) \tag{9.5j}$$

$$z^* \in [0,H), \quad T_I(z^*,t) = T_I(z^*,t_m) \tag{9.5k}$$

$$E(t_m) = 0. \tag{9.5l}$$

Note that the mathematical model has been formulated under the assumption that there is no vaporization of the water layer. The criteria for this, and other delineating situations, are readily deduced on seeking asymptotic solutions of the governing equations for large t.

Firstly it is easy to establish that if

$$q < q_1 = h(T_F - T_i)/(1+hH/k_I)$$

there can never be any melting since the asymptotic solution predicts that all the heat liberated by the mat is conducted away across the ice and that the blade/ice temperature always remains below T_F. Secondly there is a value of the heater strength q_2 above which all the ice will be removed if the heater is energised for long enough. It is not surprising that $q_2 = h(T_F - T_i)$ and that its value is independent of the ice thickness.

The third value for heater strength of interest is that which would, if the heater were left on long enough, raise the temperature of the water adjacent to the blade to its boiling temperature. The value of this is assessed by firstly assuming the ice layer does not totally melt, in which case the maximum temperature at the blade surface is the asymptotic value appropriate to linear temperature profiles. Under this assumption

$$q_3 = h(T_F - T_i)\,\frac{1}{(1+hH/K_I)}\left[1 + \frac{K_w(T_B - T_F)}{K_I(T_F - T_i)}\right]$$

where T_B is the boiling temperature.

Therefore if $q_3 < q < q_2$ there will be some vaporization of the water layer for the specified value of H, while if $q_3 < q_2$ and $q < q_2$ it is less obvious what happens because without detailed information about the rate of melting it is not clear whether the complete ice layer melts before the blade surface reaches temperature T_B. It is, however, possible to make an estimate of this by assuming the temperature profile across the water layer is linear at the time the ice is completely melted (this is only an approximation because the system is transient in this case), and since the temperature gradient is now given, both q and

$$K\left[\frac{\partial T}{\partial z^*}\right]_{z^*=0}$$

are known, which yields

$$q = \frac{K_w(T(0,t) - T_F)}{H} .$$

Thus if the temperature just reaches the boiling point T_B, the corresponding value of q, denoted by q_4, is

$$q_4 = \frac{K_w(T_B - T_F)}{H} .$$

The values of q_1, q_2, q_3 and q_4 are listed in Table 2 for a range of values of the heat transfer coefficient h and ice thickness H for properties given in Table 1.

h (W/m²K)	H (mm)	q_1 (kW/m²)	q_2 (kW/m²)	q_3 (kW/m²)	q_4 (kW/m²)
500.00	1	8.21	10	18.10	55.40
500.00	5	4.79	10	10.56	11.08
500.00	10	3.15	10	6.94	5.54
500.00	15	2.35	10	5.17	3.69
500.00	20	1.86	10	4.12	2.77
500.00	25	1.55	10	3.42	2.21
500.00	50	0.84	10	1.85	1.11
500.00	100	0.44	10	0.96	0.55
∞	1	46.00	∞	101.39	55.40
∞	5	9.20	∞	20.27	11.08
∞	10	4.60	∞	10.14	5.54
∞	15	3.07	∞	6.76	3.69
∞	20	2.30	∞	5.07	2.77
∞	25	1.84	∞	4.05	2.22
∞	50	0.92	∞	2.02	1.11
∞	100	0.46	∞	1.01	0.55

Table 2

9.3 Nondimensionalisation

For the warm-up period introduce the following dimensionless variables:

Blade

$$z' = z/D, \quad t' = k_I t/H^2, \quad \theta(z',t') = -\frac{K_b(T_F - T_b)}{K_I(T_F - T_i)} \qquad (9.6a,b)$$

Ice layer

$$z^{*'} = z^{*}/H,\ t' = k_I t/H^2,\ \phi(z^{*'},t') = -\frac{(T_F - T_I)}{(T_F - T_i)}\ .$$

The governing equations now transform to the following dimensionless form.

In the blade $z' \in [0,1]$, $t' > 0$

$$\frac{\partial^2\theta}{\partial z'^2} = a\,\frac{\partial\theta}{\partial t'}\ , \tag{9.7}$$

and in the ice layer $z^{*'} \in [0,1]$, $t' > 0$

$$\frac{\partial^2\phi}{\partial z^{*'2}} = \frac{\partial\phi}{\partial t'}\ . \tag{9.8}$$

The boundary conditions for $t > 0$ are as follows:

$$z' = 0,\quad \frac{\partial\theta}{\partial z'} = 0 \tag{9.9a}$$

$$z' = z'_o\ ,\quad \left[\frac{\partial\theta}{\partial z'}\right]_{z'=z'_o{}^+} - \left[\frac{\partial\theta}{\partial z'}\right]_{z'=z'_o{}^-} = -Q \tag{9.9b}$$

$$z' = 1,\ z^{*'} = 0,\quad \theta = b\phi,\quad \frac{\partial\theta}{\partial z'} = a\,\frac{\partial\phi}{\partial z^{*'}} \tag{9.9c}$$

and finally

$$z^{*'} = 1,\quad \frac{\partial\phi}{\partial z^{*'}} = B_i(1+\phi). \tag{9.9d}$$

The initial conditions for $t' = 0$ are

$$z' \in [0,1],\quad \theta = -b$$

$$z^{*'} \in [0,1],\quad \phi = -1 \tag{9.9e,f}$$

In the above the following dimensionless constants have been introduced.

$$a = D/H,\quad z'_o = D^{*}/D,\quad b = K_b/K_I,$$

$$Q = \frac{qD}{K_I(T_F - T_i)} \quad\text{and}\quad a = \frac{D^2 k_I}{H^2 k_b}\ , \tag{9.10a,b}$$

together with the dimensionless Biot number

$$B_i = \frac{hH}{K_I} . \tag{9.10c}$$

Once again if the heater mat flux is kept constant for $t > 0$, namely,

Q = constant,

then the dimensionless time t'_m taken for the blade/ice interface to reach fusion temperature is determined on solving the transcendental equation

$$\theta(1,t'_m) = \psi(0,t'_m) = 0.$$

For the melting regime $t' > t'_m$ the governing equations are nondimensionalised in a similar fashion.

Blade

$$z' = z/D,\ t' = K_I t/H^2,\ \theta(z',t') = -\frac{K_b(T_F - T_b)}{K_I(T_F - T_i)} \tag{9.11a}$$

Water layer

$$z^{*'} = z^*/H,\ t' = k_I t/H^2,\ \psi(z^{*'},t') = -\frac{K_w(T_F - T_w)}{K_I(T_F - T_i)} \tag{9.11b}$$

Ice layer

$$z^{*'} = z^*/H,\ t' = k_I t/H^2,\ \psi(z^{*'},t') = -\frac{(T_F - T_I)}{(T_F - T_i)} \tag{9.11c}$$

The governing equations then become:

Blade $z' \in [0,1],\ t' > t'_m$

$$\frac{\partial^2\theta}{\partial z'^2} = \alpha \frac{\partial\theta}{\partial t'}, \tag{9.12}$$

Water $z^{*'} \in [0,S(t')],\ t' > t'_m$

$$\frac{\partial^2\phi}{\partial z^{*'2}} = \beta \frac{\partial\phi}{\partial t'}, \tag{9.13}$$

Ice $\quad z^{*'} \in [S(t'),1], \quad t' > t'_m$

$$\frac{\partial^2 \psi}{\partial z^{*'2}} = \frac{\partial \psi}{\partial t'} \,. \tag{9.14}$$

In (9.13) and (9.14) the ice/water interface is located at

$$S(t') = E(t)/H \tag{9.15}$$

and

$$\beta = k_I/k_w. \tag{9.16}$$

The boundary conditions are:

$$z' = 0, \quad \frac{\partial \theta}{\partial z'} = 0 \tag{9.17a}$$

$$z' = z'_o, \quad \left[\frac{\partial \theta}{\partial z'}\right]_{z'=z'_o{}^+} - \left[\frac{\partial \theta}{\partial z'}\right]_{z'=z'_o{}^-} = -Q \tag{9.17b}$$

$$z' = 1, \; z^{*'} = 0, \; \theta = c\phi, \; \frac{\partial \theta}{\partial z'} = a \frac{\partial \phi}{\partial z^{*'}} \tag{9.17c}$$

$$z^{*'} = S(t'), \; \phi = \psi = 0, \; \frac{dS}{dt'} = \epsilon \left\{ \frac{\partial \psi}{\partial z^{*'}} - \frac{\partial \phi}{\partial z^{*'}} \right\} \tag{9.17d}$$

$$z^{*'} = 1, \quad \frac{\partial \psi}{\partial z^{*'}} = -B_i(1+\psi). \tag{9.17e}$$

The 'initial' conditions at $t' = t'_m$ are:

$$S(t'_m) = 0 \tag{9.18a}$$

$$z' \in [0,1], \; \theta(z',t') = \theta(z',t'_m) \tag{9.18b}$$

$$z^{*'} \in [0,1], \quad \psi(z^{*'},t') = \psi(z^{*'},t'_m) \tag{9.18c}$$

and finally

$$\theta(1,t'_m) = \psi(0,t'_m) = 0. \tag{9.18d}$$

In equation (9.17c)

$$c = K_b/K_w \tag{9.19}$$

and in the latent heat condition (9.17d) the Stefan number ϵ is defined by

$$\epsilon = \frac{c_{p_w}(T_F - T_i)}{L} . \tag{9.20}$$

9.4 Immobilization variables for the melting regime

The idea here is the introduction of variables which immobilize the moving interface and transfers the nonlinear interface transients into the diffusion equations.

The immobilization variables are:

Blade

$$\xi = z', \quad \tau = \epsilon t', \quad \theta = \theta \tag{9.21a}$$

Water layer

$$\eta = z^{*'}/S(\tau), \quad \tau = \epsilon t', \quad \phi = \phi \tag{9.21b}$$

Ice layer

$$\zeta = \frac{z^{*'} - S(\tau)}{1-S(\tau)}, \quad \tau = \epsilon t', \quad \psi = \psi. \tag{9.21c}$$

Equations (9.11) to (9.18) now transform to the following:

Blade $\tau > \tau_m$, $\xi \in [0,1]$

$$\frac{\partial^2 \theta}{\partial \xi^2} = \epsilon a \frac{\partial \theta}{\partial \tau} \tag{9.21d}$$

Water $\tau > \tau_m$, $\eta \in [0,1]$

$$\frac{\partial^2 \phi}{\partial \eta^2} = a\beta\left[S^2 \frac{\partial \phi}{\partial \tau} - S \frac{dS}{d\tau} \eta \frac{\partial \phi}{\partial \eta}\right] \tag{9.21e}$$

Ice $\tau > \tau_m$, $\zeta \in [0,1]$

$$\frac{\partial^2 \psi}{\partial \zeta^2} = \epsilon\left[(1-S)^2 \frac{\partial \psi}{\partial \tau} - (1-S) \frac{dS}{d\tau} (1-\zeta) \frac{\partial \psi}{\partial \zeta}\right]. \tag{9.21f}$$

The boundary conditions for $\tau > \tau_m$ are:

$$\xi = 0, \quad \frac{\partial \theta}{\partial \xi} = 0 \tag{9.21g}$$

$$\xi = z_o', \quad \left[\frac{\partial \theta}{\partial \xi}\right]_{\xi=z_o'^+} - \left[\frac{\partial \theta}{\partial \xi}\right]_{\xi=z_o'^-} = -Q \tag{9.21h}$$

$$\xi = 1, \ \eta = 0, \ \theta = c\phi, \ S(\tau) \quad \frac{\partial \theta}{\partial \xi} = a \frac{\partial \phi}{\partial \eta} \tag{9.21i}$$

$$\eta = 1, \ \zeta = 0, \ \theta = \psi = 0, \ S \frac{\partial \psi}{\partial \zeta} - (1-S) \frac{\partial \phi}{\partial \eta} = S(1-S) \frac{dS}{d\tau} \tag{9.21j}$$

and finally

$$\psi = -1, \quad \zeta = 1. \tag{9.21k}$$

(NB: This condition comes about by making the simplifying assumption that $B_i \to \infty$.)

The initial conditions at $\tau = \tau_m$ are

$$S(\tau_m) = 0 \tag{9.21l}$$

$$\xi \in [0,1], \ \theta(\xi,\tau) = \theta(z', \tau_m) \tag{9.21m}$$

$$\zeta \in [0,1], \ \psi(\zeta,\tau) = \theta(z^{*'}, \tau_m). \tag{9.21n}$$

These equations can now in principle be solved numerically by a Crank-Nicolson type approach similar to that outlined in Section 8.5.

10. Nuclear Waste Disposal

One way of disposing of nuclear waste is to melt and solidify glass adding the waste to the glass in its molten stage. The glass blocks are then disposed of by some means or other.

Another motivation for studying the melting of glass is that this is necessary for the manufacture of glass products.

Consider a vessel containing glass chips which is heated at the side walls. As the glass melts further glass chips are added - see Fig. 10.1.

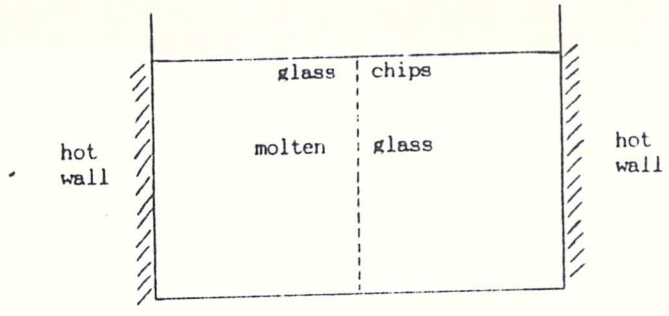


Figure 10.1

Mathematically, from symmetry we consider the region as given in Figure 10.2.

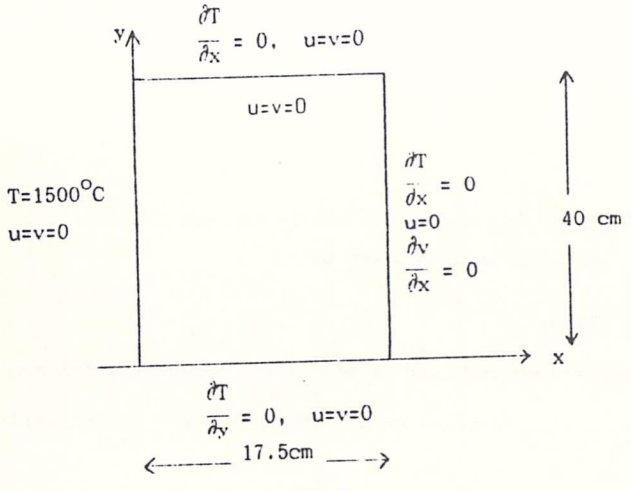


Figure 10.2

We consider the steady state problem. In nondimensionalised variables this is:

$$(\underline{u}.\nabla)\underline{u} = -\nabla p + \nabla\left[\left[\frac{1}{Re(T)}\right]\nabla\underline{u}\right] + \theta T\underline{e}_1 \tag{10.1}$$

$$\nabla.\underline{u} = \underline{0} \tag{10.2}$$

$$(\underline{u}.\nabla)T = \frac{1}{Pe(T)}\nabla^2 T - q \quad \text{if} \quad T < T_m \tag{10.3}$$

$$= \frac{1}{Pe(T)}\nabla^2 T \qquad \text{if} \quad T \geq T_m.$$

The viscosity of glass is strongly dependent on temperature:

$$\nu(T) = \nu_o \exp\left[\frac{b}{T-c}\right]$$

where

$$\nu_o = 8.65 \times 10^{-4}$$

$$b = 88.7$$

$$c = -7.8.$$

Thus the Reynolds number $Re = \frac{UL}{\nu(T)} = Re(T)$. Here L = 1 cm and U = 1 cm/s.

The constant $\beta = \frac{Gr}{(Re)^2} = -0.0176$ where the Grashof number Gr equals

$$Gr = L^3 bg(T_1 - T_o)/\nu^2 \quad (T_1 - T_o \text{ typical temperature range}).$$

The Peclet number Pe is a function of temperature

$$Pe(T) = \frac{\nu(T) L \rho_o c_p}{K(T)}$$

where ρ_o, the density of glass, is 2.30 gm cm^{-3}. The thermal conductivity cannot be assumed to be a constant and is given by

$$K(T) = 2.02 \times 10^7 + (1.83 \times 10^6)T$$

q denotes a heat sink/unit volume required to melt the glass: the total heat sink is 6Kw. The nondimensional temperature $T = \frac{\theta - 1000}{100}$ where θ is the original dimensional temperature in ^oC.

In the bulk of the fluid T ~ constant (approx. 1.0) and we have

Re ~ 1.0

Pe ~ 3500

Pr ~ 3000

Gr ~ 20.

The objective is to calculate the heat required to melt a given weight of glass in a given time. Since we know how much heat melts a given weight of glass it is only necessary to calculate

$$\int_0^a \frac{\partial T}{\partial x}\, dy \qquad \text{where a = 40 cm.}$$

It is highly unlikely that a clever analytic treatment of this problem is possible. The industrial concern in question used a finite element approach. Finite differences could equally well have been used employing staggered grids in the usual way (see eg. Chorin). However, problems arose (and will arise) with these techniques due to the rapid change in the viscosity of glass as one crosses from the molten region to the solid region.

A more satisfactory approach would be an integral formulation for $\frac{\partial T}{\partial x}$ on the boundary, but this is as yet an open problem.

Bibliography

These notes were compiled for the most part from the following literature:

Beckett, P.M., Mousavi, A., Poots, G. and Gent, R.W. (1987). Mathematical model of an electrothermal deicing system for a helicopter rotor. Part I: one dimensional transient solutions. Math. Enging. in Indust. 1, No.2, 97-168.

Crank, J. (1983). The Mathematics of Diffusion, 2nd ed. Oxford University Press.

Crank, J. (1987). Free and Moving Boundary Problems, Oxford University Press.

Elliott, C.M. and Ockendon, J.R. (1982). Weak and Variational Methods for Moving Boundary Problems. Pitman.

Gradshteyn, I.S. and Ryzhik, I.M. (1980). Tables of Integrals, Series and Products. Academic Press.

Klamkin, M.S. (Ed.) (1987). Mathematical Modelling: classroom notes in applied mathematics. SIAM publications.

Mans, R., de Vries, S. and Zwartkruis, T. (1989). Furnace Reaction Analysis, Eindhoven technical report, No. 89-05.

Phillips, J. (1986). The NAG Library: a beginner's guide. Oxford University Press.

Scott, J.A., Thoma, M., Burgess, N. and Jones, S. (1986). A reaction-diffusion study. McKee, S. (Ed.), UCINA Report No. 8612.

Spiegel, M. (1965). Theory and problems of Laplace Transforms. McGraw-Hill.

Tayler, A.B. (1986). Mathematical Models in Applied Mechanics, Oxford University Press.

Another useful text is

Abramowitz, M. and Stegun, I. (1964). Handbook of Mathematical Functions. Dover Publications.

APPEND A

Table of Laplace Transforms

	$F(s) = \mathcal{L}\{f(t)\}$	$f(t)$
1	$1/s$	1
2	$1/s^2$	t
3	$1/s^n, \quad (n = 1, 2, \cdots)$	$t^{n-1}/(n-1)!$
4	$1/\sqrt{s}$	$1/\sqrt{\pi t}$
5	$1/s^{3/2}$	$2\sqrt{t/\pi}$
6	$1/s^a \quad (a > 0)$	$t^{a-1}/\Gamma(a)$
7	$\dfrac{1}{s-a}$	e^{at}
8	$\dfrac{1}{(s-a)^2}$	te^{at}
9	$\dfrac{1}{(s-a)^n} \quad (n = 1, 2, \cdots)$	$\dfrac{1}{(n-1)!}t^{n-1}e^{at}$
10	$\dfrac{1}{(s-a)^k} \quad (k > 0)$	$\dfrac{1}{\Gamma(k)}t^{k-1}e^{at}$
11	$\dfrac{1}{(s-a)(s-b)} \quad (a \neq b)$	$\dfrac{1}{(a-b)}(e^{at} - e^{bt})$
12	$\dfrac{s}{(s-a)(s-b)} \quad (a \neq b)$	$\dfrac{1}{(a-b)}(ae^{at} - be^{bt})$
13	$\dfrac{1}{s^2+\omega^2}$	$\dfrac{1}{\omega}\sin \omega t$
14	$\dfrac{s}{s^2+\omega^2}$	$\cos \omega t$
15	$\dfrac{1}{s^2-a^2}$	$\dfrac{1}{a}\sinh at$
16	$\dfrac{s}{s^2-a^2}$	$\cosh at$
17	$\dfrac{1}{(s-a)^2+\omega^2}$	$\dfrac{1}{\omega}e^{at}\sin \omega t$
18	$\dfrac{s-a}{(s-a)^2+\omega^2}$	$e^{at}\cos \omega t$
19	$\dfrac{1}{s(s^2+\omega^2)}$	$\dfrac{1}{\omega^2}(1 - \cos \omega t)$
20	$\dfrac{1}{s^2(s^2+\omega^2)}$	$\dfrac{1}{\omega^3}(\omega t - \sin \omega t)$
21	$\dfrac{1}{(s^2+\omega^2)^2}$	$\dfrac{1}{2\omega^3}(\sin \omega t - \omega t \cos \omega t)$
22	$\dfrac{s}{(s^2+\omega^2)^2}$	$\dfrac{t}{2\omega}\sin \omega t$
23	$\dfrac{s^2}{(s^2+\omega^2)^2}$	$\dfrac{1}{2\omega}(\sin \omega t + \omega t \cos \omega t)$
24	$\dfrac{s}{(s^2+a^2)(s^2+b^2)} \quad (a^2 \neq b^2)$	$\dfrac{1}{b^2-a^2}(\cos at - \cos bt)$

Systems of Units. Some Important Conversion Factors

The most important systems of units are shown in the table below. The Mks System is also known as the *International System of Units* (abbreviated *SI System*), and the abbreviations s (instead of sec) and N (instead of nt) are also used.

System of units	Length	Mass	Time	Force
Cgs system	centimeter (cm)	gram (gm)	second (sec)	dyne
Mks system	meter (m)	kilogram (kg)	second (sec)	newton (nt)
Engineering system	foot (ft)	slug	second (sec)	pound (lb)

1 inch (in.) = 2.54000 51 cm

1 foot (ft) = 12 in. = 30.48006 12 cm

1 yard (yd) = 3 ft = 91.44018 36 cm

1 statute mile (mi) = 5280 ft = 1.60935 km

1 nautical mile = 6080.2 ft = 1.8532 km

1 acre = 4840 yd^2 = 4046.773 m^2

1 mi^2 = 640 acres = 2.58999 87 km^2

1 fluid ounce = 29.5737 cm^3

1 U.S. gallon = 4 quarts (liq) = 8 pints (liq) = 128 fl oz = 3785.432 cm^3

1 British Imperial and Canadian gallon = 1.20094 U.S. gallons = 4546.1 cm^3

1 slug = 14.59390 kg

1 pound (lb) = 4.448444 nt

1 newton (nt) = 10^5 dynes

1 British thermal unit (Btu) = 1054.8 joules

1 joule = 10^7 ergs

1 calorie (cal) = 4.1840 joules

1 kilowatt-hour (kWh) = 3413 Btu = $3.6 \cdot 10^6$ joules

1 horsepower (hp) = 2545 Btu/h = 178.2 cal/sec = 0.74570 kW

1 kilowatt (kW) = 1000 watts = 3413 Btu/h = 238.9 cal/sec

°F = °C · 1.8 + 32

1° = 60′ = 3600′ = 0.01745 radian

For further details see, e.g., D. Halliday and R. Resnick, *Physics*, 3rd ed., New York: Wiley, 1978. See also AN American National Standard, ASTM/IEEE Standard Metric Practice, Institute of Electrical and Electronics Engineers, Inc., 345 East 47th Street, New York, N.Y. 10017.

Some Constants

$e = 2.71828\ 18284\ 59045\ 23536$
$\sqrt{e} = 1.64872\ 12707\ 00128\ 14685$
$e^2 = 7.38905\ 60989\ 30650\ 22723$

$\pi = 3.14159\ 26535\ 89793\ 23846$
$\pi^2 = 9.86960\ 44010\ 89358\ 61883$
$\sqrt{\pi} = 1.77245\ 38509\ 05516\ 02730$

$\log_{10} \pi = 0.49714\ 98726\ 94133\ 85435$
$\ln \pi = 1.14472\ 98858\ 49400\ 17414$
$\log_{10} e = 0.43429\ 44819\ 03251\ 82765$
$\ln 10 = 2.30258\ 50929\ 94045\ 68402$

$\sqrt{2} = 1.41421\ 35623\ 73095\ 04880$
$\sqrt[3]{2} = 1.25992\ 10498\ 94873\ 16477$
$\sqrt{3} = 1.73205\ 08075\ 68877\ 29353$
$\sqrt[3]{3} = 1.44224\ 95703\ 07408\ 38232$
$\ln 2 = 0.69314\ 71805\ 59945\ 30942$
$\ln 3 = 1.09861\ 22886\ 68109\ 69140$

$\gamma = 0.57721\ 56649\ 01532\ 86061$
$\ln \gamma = -0.54953\ 93129\ 81644\ 82234$
(cf. p. 214)
$1^\circ = 0.01745\ 32925\ 19943\ 29577$ rad
1 rad $= 57.29577\ 95130\ 82320\ 87680^\circ$
$= 57°17'44.806''$

Polar Coordinates

$x = r \cos\theta \qquad r = \sqrt{x^2 + y^2}$

$y = r \sin\theta \qquad \theta = \arctan \frac{y}{x}$

$dx\,dy = r\,dr\,d\theta$

Series

$$\frac{1}{1-x} = \sum_{m=0}^{\infty} x^m \quad (|x| < 1)$$

$$e^x = \sum_{m=0}^{\infty} \frac{x^m}{m!}$$

$$\sin x = \sum_{m=0}^{\infty} \frac{(-1)^m x^{2m+1}}{(2m+1)!}$$

$$\cos x = \sum_{m=0}^{\infty} \frac{(-1)^m x^{2m}}{(2m)!}$$

$$\ln(1-x) = -\sum_{m=0}^{\infty} \frac{x^m}{m} \quad (|x| < 1)$$

$$\arctan x = \sum_{m=0}^{\infty} \frac{(-1)^m x^{2m+1}}{2m+1} \quad (|x| < 1)$$

Greek Alphabet

α	Alpha	ν	Nu
β	Beta	ξ	Xi
γ, Γ	Gamma	o	Omicron
δ, Δ	Delta	π	Pi
ϵ	Epsilon	ρ	Rho
ζ	Zeta	σ, Σ	Sigma
η	Eta	τ	Tau
$\theta, \vartheta, \Theta$	Theta	υ, Υ	Upsilon
ι	Iota	ϕ, φ, Φ	Phi
κ	Kappa	χ	Chi
λ, Λ	Lambda	ψ, Ψ	Psi
μ	Mu	ω, Ω	Omega

Vectors

$$\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + a_3 b_3$$

$$\mathbf{a} \times \mathbf{b} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix}$$

$$\text{grad } f = \nabla f = \frac{\partial f}{\partial x}\mathbf{i} + \frac{\partial f}{\partial y}\mathbf{j} + \frac{\partial f}{\partial z}\mathbf{k}$$

$$\text{div } \mathbf{v} = \nabla \cdot \mathbf{f} = \frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y} + \frac{\partial v_3}{\partial z}$$

$$\text{curl } \mathbf{v} = \nabla \times \mathbf{v} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ v_1 & v_2 & v_3 \end{vmatrix}$$

ANNEX B

A simple example of matched asymptotic expansions

Consider the mass-spring-damper system:

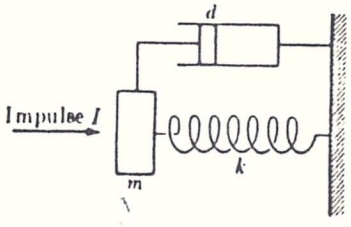


Figure B.1

The governing differential equation and associated boundary conditions are:

$$m\frac{d^2x}{dt^2} + d\frac{dx}{dt} + kx = 0 \qquad \text{(B-1)}$$

$$u(0) = \left[\frac{dx}{dt}\right]_{t=0} = I/m \qquad \text{(B-2)}$$

$$x(0) = 0. \qquad \text{(B-3)}$$

This admits the solution

$$x(t) = (I/d)(e^{-\lambda_2 t} - e^{-\lambda_1 t})/\sqrt{1-4mk/d^2} \qquad \text{(B-4)}$$

where

$$\lambda_{1,2} = \frac{d}{2m}(1 \pm \sqrt{1-4mk/d^2}) \qquad \text{(B-5)}$$

This will be the reference solution used in assessing the approximate solutions that follow.

First introduce dimensionless variables

$$t' = \frac{kt}{d}\ ;\quad x' = (d/I)x \qquad \text{(B-6)}$$

which transforms the original problem to

$$\epsilon \frac{d^2x'}{dt'^2} + \frac{dx'}{dt'} + x' = 0 \tag{B-7}$$

$$\left[\frac{dx'}{dt'}\right]_{t'=0} = \frac{1}{\epsilon} \tag{B-8}$$

$$x'(0) = 0 \tag{B-9}$$

where $\epsilon = mk/d^2$.

We assume we are given that $m \ll 1$. Thus $\epsilon \ll 1$. We therefore seek a series solution in this small parameter.

First consider an outer expansion of the form

$$x' = x^o = \Sigma\, x_n^o\, \epsilon^n. \tag{B-10}$$

Upon substituting into (B-7) and equating like powers of ϵ, we obtain

$$\frac{dx_o^o}{dt'} + x_o^o = 0 \tag{B-11}$$

$$\frac{dx_n^o}{dt'} + x_n^o = -\frac{d^2x_{n-1}^o}{dt'^2}, \quad n > 0. \tag{B-12}$$

The solution is

$$x_o^o = A_o^o\, e^{-t'}. \tag{B-13}$$

This corresponds to the solution for long times (hence 'outer' expansion).

The inner solution happens in a very short time. Therefore, in order to be able to study the solution with some resolution, we need to "magnify" the region of interest. This is achieved by stretching the independent variable. For the inner solution $x' = x^i$ this is achieved by

$$\bar{t} = t'/\epsilon$$

which transforms the differential equation (B-7) and the boundary conditions (B-8) and (B-9) into

$$\frac{d^2x^i}{d\bar{t}^2} + \frac{dx^i}{d\bar{t}} + \epsilon x^i = 0 \tag{B-14}$$

$$\left[\frac{dx^i}{d\bar{t}}\right]_{\bar{t}=0} = 1 \tag{B-15}$$

$$x^i(0) = 0. \tag{B-16}$$

With $\bar{t}$ fixed the inner expansion is

$$x^i = \Sigma\, x^i_n(\bar{t})\epsilon^n \tag{B-17}$$

and, on equating powers of ϵ^n,

$$\frac{d^2x^i_o}{d\bar{t}^2} + \frac{dx^i_o}{d\bar{t}} = 0 \tag{B-18}$$

$$\frac{d^2x^i_n}{d\bar{t}^2} + \frac{dx^i_n}{d\bar{t}} = -x^i_{n-1}, \qquad n > 0. \tag{B-19}$$

The solution of (B-18) together with (B-15) and (B-16) is

$$x^i_o = 1 - e^{-\bar{t}}. \tag{B-20}$$

Note it is important to provide the right amount of stretching. If, for instance, we had defined

$$\bar{t} = t'/\epsilon^2$$

then we would have obtained, as the equation for the lowest order term,

$$\frac{d^2x^i_o}{d\bar{t}^2} = 0$$

with the solution

$$x^i_o \sim \epsilon\bar{t}.$$

The features of the inner solution which allow us to match the outer solution have been lost: there has been too much 'stretching' and we are only viewing the initial linear portion of the solution (see Figure B.2).

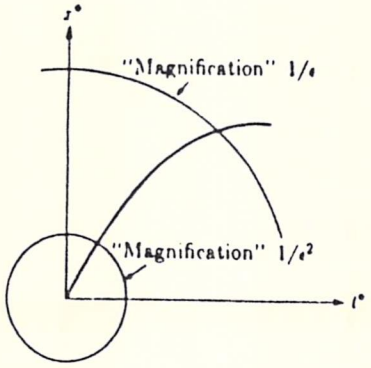


Figure B.2

Whether the expansion works is the best guide to what stretching should be used, although physical intuition can often be helpful.

(NB: (B-20) for small $\bar{t}$ gives $x_o^i \sim 0(\bar{t}) = \epsilon\bar{t}$ (in notation above) i.e. the solution obtained above with much greater stretching.)

To complete the zeroth-order solution it remains to determine the constant A_o^o in (B-13). Let us assume that the validity of the inner and outer solutions overlaps in some region of t and that in this region we can find a $t = \delta(t)$ such that we have

$$\lim_{\epsilon \to 0} \delta = 0$$

and

$$\lim_{\epsilon \to 0} (\delta/\epsilon) = \infty.$$

Such a choice would be, for example, $\delta = \sqrt{\epsilon}$. Requiring the two expansions to overlap in the limit gives (since the inner solution is expressed as a function of $\bar{t} = t/\epsilon$)

$$\lim_{\epsilon \to 0} x_o^i (\delta/\epsilon) = \lim_{\epsilon \to 0} x_o^o(\delta)$$

or

$$x_o^i (\infty) = x_o^o(0). \qquad \text{(B-21)}$$

This is termed the <u>limit matching principle</u> which may be stated as follows:

<u>The outer limit of the inner expansion</u> = <u>the inner limit of the outer expansion</u>.

From (B-20) it follows that

$$x_o^{i}(\infty) \equiv x_o^{io} = 1 \tag{B-21a}$$

and from (B-13)

$$x_o^{o}(0) \equiv x_o^{oi} = A_o^{o}.$$

Applying the limit matching principle

$$x_o^{io} = x_o^{oi} \tag{B-22}$$

gives

$$A_o^{o} = 1. \tag{B-23}$$

We may now construct a <u>composite solution</u> that is uniformly valid to order ϵ over the whole region by setting

$$x_o^{c} \sim x_o^{o} + x_o^{i} - x_o^{oi}. \tag{B-24}$$

It is seen that this solution, in view of the matching, approaches the inner and outer solutions in the inner and outer regions, and carries over smoothly between them. In the problem considered, the zeroth-order composite solution becomes

$$x_o^{c} \sim e^{-t} - e^{-\bar{t}} = e^{-t} - e^{-t/\epsilon} \tag{B-25}$$

from (B-13), (B-20) and (B-21a).

We now seek the next higher approximation.

From (B-12) and (B-13) (with $A_o^{o} = 1$) we have

$$\frac{dx_1^{o}}{dt} + x_1^{o} = -e^{-t}$$

which has the general solution

$$x_1^{o} = -t'e^{-t'} + A_1^{o}e^{-t'}. \tag{B-26}$$

From (B-19) and (B-20) the first-order inner solution must satisfy

$$\frac{d^2x_1^{i}}{d\bar{t}^2} + \frac{dx_1^{i}}{d\bar{t}} = e^{-\bar{t}} - 1. \tag{B-27}$$

The general solution of this equation is

$$x_1^i = A_1^i + B_1^i e^{-\bar{t}} - \bar{t} - \bar{t}e^{-\bar{t}}. \tag{B-28}$$

The constants A_1^i and B_1^i are to be determined such that the inner boundary conditions (B-15) and (B-16) are fulfilled. Since the lowest-order term has already taken care of these, x_1^i and its first derivative must both be zero, i.e.

$$x_1^i(0) = \frac{dx^i(0)}{dt} = 0;$$

this gives

$$A_1^i = -B_1^i = 2$$

and hence

$$x_1^i = 2(1-e^{-\bar{t}}) - \bar{t}(1+e^{-\bar{t}}) \tag{B-29}$$

The two-term inner expansion is thus

$$x^i \sim x_o^i + \epsilon x_1^i = 1-e^{-\bar{t}} + \epsilon[2(1-e^{-\bar{t}}) - \bar{t}(1+e^{-\bar{t}})] \tag{B-30}$$

or, expressed in the outer (physical) variable

$$x^i \sim 1-t' - (1-t')e^{-t'/\epsilon} + 2\epsilon(1-e^{-t'/\epsilon}). \tag{B-31}$$

The two term outer solution, obtained from (B-13) and (B-26), is

$$x^o \sim x_o^o + \epsilon x_1^o = e^{-t'} - \epsilon t'e^{-t'} + \epsilon A_1^o e^{-t'}. \tag{B-32}$$

The behaviour of this near the inner limit may be obtained by a series expansion in small t', i.e.

$$x^{oi} \sim 1-t'-\epsilon(t'-A_1^o). \tag{B-33}$$

In the inner expansion, on the other hand, for large t' the exponential term will be negligible in the outer limit and thus

$$x^{io} \sim 1-t'+2\epsilon. \tag{B-34}$$

It is evident from a comparison of (B-33) and (B-34) that the two expressions match if

$$A_1^o = 2.$$

(Bear in mind that for small t' when $\epsilon \ll 1$

$$x^{oi} \sim 1-t' + \epsilon(A_1^o.)$$

Finally, it is possible to obtain the two-term composite expansion (valid to first order) by setting

$$x^c \sim x^i + x^o - x^{io}$$

$$\therefore \quad x^c \sim 1-t'-(1-t')e^{-t'/\epsilon} + 2\epsilon(1-e^{-t'/\epsilon})$$

$$+ e^{-t'} - \epsilon t'e^{-t'} + 2\epsilon e^{-t'}$$

$$-(1-t') - 2\epsilon$$

or

$$x^c \sim (1+2\epsilon)e^{-t'} + (1-2\epsilon)e^{-t'/\epsilon}$$

$$+ t'(e^{-t'/\epsilon} - \epsilon e^{-t'}).$$

A comparison of the various approximations is given graphically in Fig. B3.

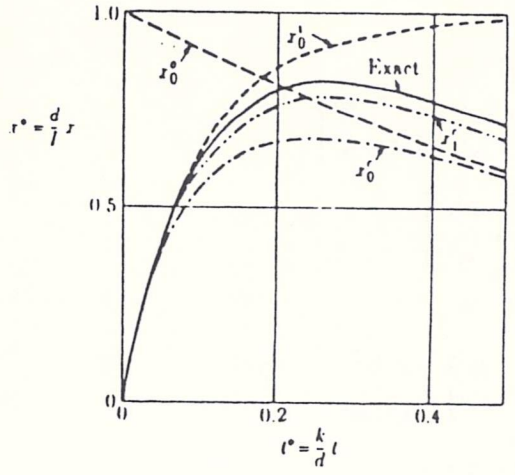


Figure B.3

Ex.

Consider the conservation of energy equation (4.3)

$$\rho c\left[\frac{\partial T}{\partial t} + (\underline{q}.\nabla)T\right] = K\nabla^2 T. \qquad (1)$$

Use the following scalings to reduce the equation to non-dimensional form:

$$\underline{x}' = \underline{x}/L, \quad \underline{q}' = \underline{q}/V, \quad t' = tU/L,$$

$$T' = T/(T_1 - T_o). \quad \text{(Here } \underline{x} = (x,y)^T; \quad \underline{q} = (u,v)^T\text{).}$$

In two dimensions equation (1) may be written as

$$\rho c\left[\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y}\right] = K\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right].$$

We note

$$\frac{\partial}{\partial t} \equiv \frac{\partial t'}{\partial t}\frac{\partial}{\partial t'} \equiv \frac{U}{L}\frac{\partial}{\partial t'}$$

$$\frac{\partial}{\partial x} \equiv \frac{\partial x'}{\partial x}\frac{\partial}{\partial x'} \equiv \frac{1}{L}\frac{\partial}{\partial x'}.$$

Thus we obtain

$$\rho c(T_1 - T_o)\left[\frac{U}{L}\frac{\partial T'}{\partial t'} + \frac{U}{L}u'\frac{\partial T'}{\partial x'} + \frac{U}{L}v'\frac{\partial T'}{\partial y'}\right]$$

$$= K \cdot \frac{(T_1 - T_o)}{L^2}\left[\frac{\partial^2 T'}{\partial x'^2} + \frac{\partial^2 T'}{\partial y'^2}\right]$$

or

$$\frac{\rho cU}{L}\left[\frac{\partial T'}{\partial t'} + u'\frac{\partial T'}{\partial x'} + v'\frac{\partial T'}{\partial y'}\right] = \frac{K}{L^2}\left[\frac{\partial^2 T'}{\partial x^2} + \frac{\partial^2 T'}{\partial y^2}\right].$$

Now $Re = \rho UL/\mu$ and $1/Pr = K/\mu c$.

Thus

$$Re\left[\frac{\partial T'}{\partial t'} + (\underline{q}'.\nabla')T'\right] = \frac{1}{Pr}\nabla'^2 T'.$$

TROCADORES DE CALOR

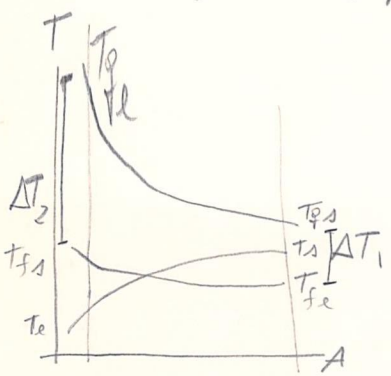
CORRENTES: PARALELAS, OPOSTAS, CRUZADAS

$q = U.A.\overline{\Delta T}$

$q = F.UA.\Delta T$, F - fator de correção p/ Trocadores de multiplos passos

$q = \dot{m}_q . C_{p_q} (T_{q_e} - T_{q_s})$

$q = \dot{m}_f . C_{p_f} (T_{f_s} - T_{f_e})$



$$\overline{\Delta T} = \frac{\Delta T_2 - \Delta T_1}{\ln\left(\frac{\Delta T_2}{\Delta T_1}\right)}$$

$$\overline{\Delta T} = \frac{(T_{q_e} - T_{f_s}) - (T_{q_s} - T_{f_e})}{\ln\left(\frac{T_{q_e} - T_{f_s}}{T_{q_s} - T_{f_e}}\right)}$$

$$U_2 = \frac{1}{\frac{1}{h_{12}} + \frac{r_2 \ln r_3/r_2}{k_{23}} + \frac{r_2}{r_3 h_{34}}}$$

$$U_3 = \frac{1}{\frac{r_3}{r_2 h_{12}} + \frac{r_3 \ln r_3/r_2}{k_{23}} + \frac{1}{h_{34}}}$$

$$U = \frac{h_{12} . h_{34}}{h_{12} + h_{34}} \quad \text{(quase ideal)}$$

$$E = \frac{\text{transf. calor real}}{\text{máx. transf. calor}} = \frac{q_{real}}{q_{max}}$$

$$q_{real} = (\dot{m} C_p)_q (T_{q_e} - t_{q_1}) = (\dot{m} C_p)_f (T_{f_s} - T_{f_e})$$

$$q_{max} = (\dot{m} C_p)_{min} \cdot (T_{q_e} - T_{f_e})$$

$C_{min} = (\dot{m} C_p)_{min}$, $C_{max} (\dot{m} C_p)_{max}$

$$q_{real} = E . C_{min} (T_{q_e} - T_{f_e})$$

$$E = \frac{(\dot{m} C_p)_q (T_{q_e} - T_{q_1})}{C_{min} (T_{q_e} - T_{f_e})} = \frac{(\dot{m} C_p)_f (T_{f_1} - T_{f_e})}{C_{min} (T_{q_e} - T_{f_e})}$$

Se $C_{min} = (\dot{m} C_p)_q \rightarrow E = \frac{(T_{q_e} - T_{q_s})}{(T_{q_e} - T_{f_e})}$

Se $C_{min} = (\dot{m} C_p)_f \rightarrow E = \frac{(T_{f_s} - T_{f_e})}{(T_{q_e} - T_{f_e})}$

E pode ser obtido (em função de 2 parâmetros) através de diagramas:

$$\frac{C_{min}}{C_{max}} = \frac{(\dot{m} C_p)_{min}}{(\dot{m} C_p)_{max}} \quad \text{e} \quad NTU = \frac{UA}{C_{min}}$$

NTU - nº unidade de transferência de calor