

## Chapter 4

### Parabolic Equations

Partial differential equations occur in abundance in a variety of areas from engineering, mathematical biology and physics. In this chapter we will concentrate upon the partial differential equations representing heat flow and diffusion which are parabolic equations.

#### Heat Equation

Heat can flow from regions of high temperature to regions of low temperature in essentially three different ways. These three ways are conduction, radiation and convection. Internal conduction occurs because of molecular motion within the body. That is, within solid bodies we have heat flowing from regions of high temperature, which have a large amount of molecular motion, (large velocities, large kinetic energy of the molecules) to regions of low temperature (smaller velocities, less kinetic energy of the molecules). Radiation heat transfer between two objects occurs when heat passes through space from the hotter object to the cooler object without heating the space between the objects. It is due to wave motion. A common example is the Sun heating the Earth. Heat transfer by convection occurs when some type of motion moves heat from one place to another. Forced convection occurs when a blower blows heat from one area to another. There are other types of heat transfer such as that which occurs during evaporation and condensation processes. All of these heat transfer methods are best studied in a course on the subject. For our purposes we will concentrate on heat transfer by conduction. Recall the Gauss<sup>†</sup> divergence theorem

For  $\vec{F} = \vec{F}(x, y, z, t)$  a continuous vector field defined everywhere within a simply connected volume  $V$  and surrounded by a closed surface  $S$  we have

$$\iiint_V \operatorname{div} \vec{F} \, d\tau = \iint_S \vec{F} \cdot \hat{n} \, d\sigma \quad (4.1)$$

where  $d\tau$  is a volume element,  $d\sigma$  is an element of surface area and  $\hat{n}$  is a unit exterior normal to the surface.

---

<sup>†</sup> See Appendix C

which can be used to convert surface integrals to volume integrals. We will use this theorem together with the Fourier law of heat conduction and a conservation law for energy transfer to derive the heat conduction equation. The Fourier law of heat conduction is given by

$$\vec{q} = -\kappa \text{grad } u = -\kappa \nabla u = -\kappa \left( \frac{\partial u}{\partial x} \hat{i} + \frac{\partial u}{\partial y} \hat{j} + \frac{\partial u}{\partial z} \hat{k} \right) \quad (4.2)$$

where  $\vec{q}$  (cal/cm<sup>2</sup>sec) is the rate of heat flow per unit area per unit of time,  $\kappa$  (cal/sec cm<sup>2</sup> °C/cm) is the thermal conductivity of the region where heat flows and depends upon the material properties in which heat is flowing. The quantity  $u = u(x, y, z)$  (°C) represents the temperature. The surfaces  $u(x, y, z) = c$ , where  $c$  is constant, are called isothermal surfaces or surfaces of constant temperature. Observe the gradient vector  $\nabla u$  is always normal to any point on an isothermal surface  $u(x, y, z) = \text{constant}$  and points in the direction of greatest increase of temperature. Because heat flows from hot to cold regions we need the above negative sign in Fourier's law. Thus, Fourier's law for heat conduction can be interpreted as representing heat flow in the direction which temperature decreases. The quantity  $\vec{q}$  is called the thermal current vector and represents the rate of heat flow per unit of area.

Introduce the following notation and units of measurements:

$c = c(x, y, z)$  is the specific heat of the solid, (cal/gm °C)

$\rho = \rho(x, y, z)$  is the volume density of the solid, (gm/cm<sup>3</sup>)

$\kappa = \kappa(x, y, z)$  is the thermal conductivity of the solid, (cal/sec cm<sup>2</sup> °C/cm)

$\vec{q} = \vec{q}(x, y, z, t)$  is the rate of heat flow per unit area, (cal/cm<sup>2</sup>sec)

$H = H(x, y, z, t)$  is the rate of heat generation per unit volume, (cal/sec cm<sup>3</sup>)

$u = u(x, y, z, t)$  denotes temperature, (°C)

We employ the above symbols and write out the law of conservation of energy for an arbitrary simply-connected region<sup>‡</sup>  $V$  with closed surface  $S$ . Let  $H_s$  denote the change in the amount of heat stored in the region  $V$  during a time interval  $\Delta t$ . We write  $H_s$  as the amount of heat  $H_c$  which crosses the surface  $S$  into or leaving the region during the time interval  $\Delta t$  plus any heat generated  $H_g$  within

---

<sup>‡</sup> A simply-connected region is such that any simple closed curve within the region can be continuously shrunk to a point without leaving the region. Regions which are not simply-connected are called multiply-connected.

the region  $V$  during this time interval. The conservation law is then written in either of the forms

$$H_s = H_c + H_g \quad \text{or} \quad H_c + H_g - H_s = 0. \quad (4.3)$$

The heat stored in a volume element  $d\tau$  of  $V$  is given by  $c \rho u d\tau$  in units of calories. The quantity  $H_s$  is the rate of change of heat stored within the volume element and is given by

$$H_s = \frac{\partial}{\partial t} \iiint_V c \rho u d\tau \quad \left( \frac{\text{cal}}{\text{sec}} \right). \quad (4.4)$$

The amount of heat which crosses into the region during a time interval  $\Delta t$ , or flux of heat into the region, is given by

$$H_c = \iint_S -\vec{q} \cdot \hat{n} d\sigma \quad \left( \frac{\text{cal}}{\text{sec}} \right). \quad (4.5)$$

where the negative sign is used to change the sign of the exterior unit normal vector  $\hat{n}$ . This surface integral is converted to a volume integral using the above Gauss divergence theorem to obtain

$$H_c = \iiint_V -\text{div } \vec{q} d\tau \quad \left( \frac{\text{cal}}{\text{sec}} \right). \quad (4.6)$$

The heat generated within the region is given by

$$H_g = \iiint_V H d\tau \quad \left( \frac{\text{cal}}{\text{sec}} \right). \quad (4.7)$$

The results from equations (4.4), (4.6), and (4.7) enable us to write the conservation law given by equation (4.3) in the form

$$\iiint_V \left\{ -\text{div } \vec{q} + H - \frac{\partial}{\partial t}(c \rho u) \right\} d\tau = 0 \quad (4.8)$$

which implies, for an arbitrary volume and arbitrary time  $\Delta t$ , the term inside the brackets must equal zero. Also note each term in equation (4.8) has the same units of (cal/cm<sup>3</sup>sec). Now substitute for  $\vec{q}$  from equation (4.2), representing Fourier's law of heat conduction, to obtain the heat conduction equation

$$\text{div}(\kappa \text{grad } u) + H = \frac{\partial}{\partial t}(c \rho u). \quad (4.9)$$

which has the expanded form

$$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial u}{\partial z} \right) + H = \frac{\partial}{\partial t} (c \rho u). \quad (4.10)$$

In the special case the thermal conductivity  $\kappa$  is constant, and does not vary with position, we can write

$$\text{div}(\kappa \text{grad } u) = \nabla(\kappa \nabla u) = \kappa \nabla^2 u. \quad (4.11)$$

where  $\nabla^2 u$  is called the Laplacian operator. In the case where all coefficients are constants we can write the heat equation in the form

$$\frac{\partial u}{\partial t} = K \nabla^2 u + Q, \quad K = \frac{\kappa}{c \rho}, \quad Q = \frac{H}{c \rho} \quad (4.12)$$

where  $K$  is called the diffusivity of the material. If  $\lim_{t \rightarrow \infty} \frac{\partial u}{\partial t} = 0$  the temperature is said to have reached steady state conditions. For steady state conditions we set  $\frac{\partial u}{\partial t} = 0$  in equation (4.12) and assume the temperature  $u$  depends only upon position. If there are no sources or sinks we set  $Q = 0$  and under these conditions the heat equation becomes homogeneous. The tables 4-1 and 4-2 show various representations of the heat equation in Cartesian coordinates. The construction of similar tables for cylindrical and spherical coordinates is left as an exercise.

Note in the table 4-1 that the exact differential forms are easily integrated. Also note the different forms of the Laplacian operator in one, two and three dimensions.

The Laplacian operator  $\nabla^2 u$  is sometimes written using the notation  $\Delta u$ . The Laplacian takes on different forms in different coordinate systems. Given a set of transformation equations  $x = x(\xi, \eta, \zeta)$      $y = y(\xi, \eta, \zeta)$      $z = z(\xi, \eta, \zeta)$  we form the position vector  $\vec{r} = \vec{r}(\xi, \eta, \zeta) = x(\xi, \eta, \zeta)\hat{i} + y(\xi, \eta, \zeta)\hat{j} + z(\xi, \eta, \zeta)\hat{k}$  and calculate the derivatives  $\frac{\partial \vec{r}}{\partial \xi}$ ,  $\frac{\partial \vec{r}}{\partial \eta}$ ,  $\frac{\partial \vec{r}}{\partial \zeta}$  which represent tangent vectors to the coordinate curves defining the  $(\xi, \eta, \zeta)$  coordinates.

From these tangent vectors one can calculate the magnitudes

$$h_\xi = \left| \frac{\partial \vec{r}}{\partial \xi} \right| \quad h_\eta = \left| \frac{\partial \vec{r}}{\partial \eta} \right| \quad h_\zeta = \left| \frac{\partial \vec{r}}{\partial \zeta} \right|$$

and the dot products  $\frac{\partial \vec{r}}{\partial \xi} \cdot \frac{\partial \vec{r}}{\partial \eta}$ ,  $\frac{\partial \vec{r}}{\partial \xi} \cdot \frac{\partial \vec{r}}{\partial \zeta}$ ,  $\frac{\partial \vec{r}}{\partial \eta} \cdot \frac{\partial \vec{r}}{\partial \zeta}$ . If these dot products are zero the coordinate curves have orthogonal intersections and under these conditions

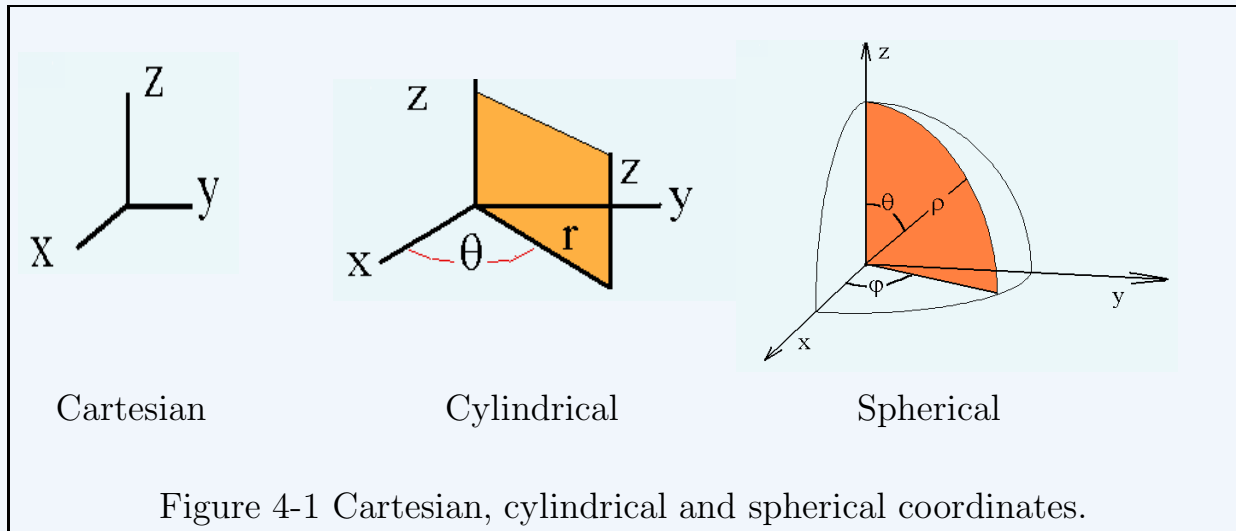
Special Cases	Operator Form	1-Dimensional Form
General	$\nabla (\kappa \nabla u) + H = \rho c \frac{\partial u}{\partial t}$	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + H = \rho c \frac{\partial u}{\partial t}$
Homogeneous Material	$\nabla^2 u + \frac{H}{\kappa} = \frac{\rho c}{\kappa} \frac{\partial u}{\partial t}$	$\frac{\partial^2 u}{\partial x^2} + \frac{H}{\kappa} = \frac{\rho c}{\kappa} \frac{\partial u}{\partial t}$
Steady State	$\nabla (\kappa \nabla u) + H = 0$	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + H = 0$
Source Free	$\nabla (\kappa \nabla u) = \rho c \frac{\partial u}{\partial t}$	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) = \rho c \frac{\partial u}{\partial t}$
Steady State Homogeneous Material	$\nabla^2 u + \frac{H}{\kappa} = 0$	$\frac{d^2 u}{dx^2} + \frac{H}{\kappa} = 0$
Steady State Source Free	$\nabla (\kappa \nabla u) = 0$	$\frac{d}{dx} \left( \kappa \frac{du}{dx} \right) = 0$
Homogeneous Material Source Free	$\nabla^2 u = \frac{\rho c}{\kappa} \frac{\partial u}{\partial t}$	$\frac{\partial^2 u}{\partial x^2} = \frac{\rho c}{\kappa} \frac{\partial u}{\partial t}$
Steady State Source Free Homogeneous Material	$\nabla^2 u = 0$	$\frac{d^2 u}{dx^2} = 0$

Special Cases	2-Dimensional Form	3-Dimensional Form
General	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right) + H = \rho c \frac{\partial u}{\partial t}$	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial u}{\partial z} \right) + H = \rho c \frac{\partial u}{\partial t}$
Homogeneous Material	$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + \frac{H}{\kappa} = \frac{\rho c}{\kappa} \frac{\partial u}{\partial t}$	$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + \frac{H}{\kappa} = \frac{\rho c}{\kappa} \frac{\partial u}{\partial t}$
Steady State	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right) + H = 0$	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial u}{\partial z} \right) + H = 0$
Source Free	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right) = \rho c \frac{\partial u}{\partial t}$	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial u}{\partial z} \right) = \rho c \frac{\partial u}{\partial t}$
Steady State Homogeneous Material	$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{H}{\kappa} = 0$	$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + \frac{H}{\kappa} = 0$
Steady State Source Free	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right) = 0$	$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial u}{\partial z} \right) = 0$
Homogeneous Material Source Free	$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{\rho c}{\kappa} \frac{\partial u}{\partial t}$	$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = \frac{\rho c}{\kappa} \frac{\partial u}{\partial t}$
Steady State Source Free Homogeneous Material	$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$	$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0$

we say the  $(\xi, \eta, \zeta)$  coordinate system is an orthogonal system. The Laplacian is calculated in an orthogonal system from the relation

$$\nabla^2 u = \frac{1}{h_\xi h_\eta h_\zeta} \left[ \frac{\partial}{\partial \xi} \left( \frac{h_\eta h_\zeta}{h_\xi} \frac{\partial u}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( \frac{h_\xi h_\zeta}{h_\eta} \frac{\partial u}{\partial \eta} \right) + \frac{\partial}{\partial \zeta} \left( \frac{h_\xi h_\eta}{h_\zeta} \frac{\partial u}{\partial \zeta} \right) \right]. \quad (4.13)$$

For a derivation of this relation see the reference by Spiegel in the bibliography section. The above representation is only valid in an orthogonal coordinate system. For future reference we list the representation of the Laplacian in Cartesian, cylindrical and spherical coordinate systems.



In rectangular coordinates  $(x, y, z)$  we have

$$\Delta u = \nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}. \quad (4.14)$$

In cylindrical coordinates  $(r, \theta, z)$  we have the transformation equations

$$x = r \cos \theta, \quad y = r \sin \theta, \quad z = z$$

which produces the Laplacian

$$\Delta u = \nabla^2 u = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{\partial^2 u}{\partial z^2} \quad (4.15)$$

or

$$\nabla^2 u = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{\partial^2 u}{\partial z^2}.$$

In spherical coordinates  $(\rho, \theta, \phi)$  we have the transformation equations

$$x = \rho \sin \theta \cos \phi, \quad y = \rho \sin \theta \sin \phi, \quad z = \rho \cos \theta$$

which produces the Laplacian

$$\begin{aligned} \Delta u = \nabla^2 u &= \frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left( \rho^2 \frac{\partial u}{\partial \rho} \right) + \frac{1}{\rho^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial u}{\partial \theta} \right) + \frac{1}{\rho^2 \sin^2 \theta} \frac{\partial^2 u}{\partial \phi^2} \\ \text{or} \quad \nabla^2 u &= \frac{\partial^2 u}{\partial \rho^2} + \frac{2}{\rho} \frac{\partial u}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{1}{\rho^2} \cot \theta \frac{\partial u}{\partial \theta} + \frac{1}{\rho^2 \sin^2 \theta} \frac{\partial^2 u}{\partial \phi^2} \end{aligned} \quad (4.16)$$

### Boundary and initial conditions for the heat equation

Let  $S$  denote a closed surface enclosing a volume  $V$  where we wish to solve the heat equation. The various boundary conditions that can be assigned are as follows:

**Dirichlet**<sup>†</sup> boundary conditions or boundary value problem of the first kind requires the temperature be specified on the boundary of the region where the heat equation is solved. This type of boundary condition can be written in the form

$$u(x, y, z, t) \Big|_{(x, y, z) \in S} = f_1(x, y, z, t) \quad (4.17)$$

where  $f_1$  is a specified temperature.

**Neumann**<sup>†</sup> boundary conditions or boundary value problem of the second kind requires the heat flux across the boundary be specified on the boundary of the region where the heat equation is solved. This type of boundary condition is expressed

$$\frac{\partial u}{\partial n} = \text{grad } u \cdot \hat{n} = f_2(x, y, z, t) \Big|_{(x, y, z) \in S} \quad (4.18)$$

where  $f_2$  is a specified heat flux.

Note for an insulated boundary we have  $\frac{\partial u}{\partial n} = \text{grad } u \cdot \hat{n} = 0$  and no heat flows across the boundary.

**Robin**<sup>†</sup> boundary condition or boundary value problem of the third kind requires that the heat loss from the boundary to the surrounding medium be specified. This type of condition can be expressed

$$\frac{\partial u}{\partial n} + hu = f_3(x, y, z, t) \Big|_{(x, y, z) \in S} \quad (4.19)$$

---

<sup>†</sup> See Appendix C

where  $h > 0$  is a constant and  $f_3$  is a specified function. Here the heat exchange depends upon the temperature difference with the surrounding medium. In this case we can think of  $u$  as representing  $T - T_0$  where  $T_0$  is the temperature of the surrounding medium.

**Mixed** boundary conditions or mixed boundary value problems require different types of boundary conditions be specified over different portions of the bounding surface of the region of interest. For example, temperature can be specified over one portion of the surface while the heat flux can be specified over the other part of the surface. This type of mixed boundary condition can be expressed

$$\begin{aligned} u(x, y, z, t) = f_1(x, y, z) \Big|_{(x, y, z) \in S_1} & \quad \text{where} \quad S_1 \cup S_2 = S \\ \frac{\partial u}{\partial n} = f_2(x, y, z) \Big|_{(x, y, z) \in S_2} & \quad S_1 \cap S_2 = \emptyset. \end{aligned} \quad (4.20)$$

Mixed boundary value problems are in general much harder to solve. In the Neumann and Robin conditions there occurs the normal derivative  $\frac{\partial u}{\partial n}$  which is calculated at a boundary point and given by  $\frac{\partial u}{\partial n} = \text{grad } u \cdot \hat{n}$  where  $\hat{n}$  is the exterior unit normal to the boundary surface.

The above boundary conditions can be represented in an alternative fashion by using a boundary operator

$$B(u) \Big|_{x, y, z \in S} = \left[ \alpha \frac{\partial u}{\partial n} + \beta u \right]_{x, y, z \in S} = \text{a specified condition.}$$

where a Dirichlet boundary condition results when  $\alpha = 0, \beta = 1$ , a Neumann condition results when  $\alpha = 1, \beta = 0$ , and a Robin condition results for the parameter values  $\alpha = 1, \beta = h$ .

**Initial conditions** are expressed

$$u(x, y, z, 0) = f_4(x, y, z) \quad \text{where } (x, y, z) \in V \quad (4.21)$$

Here  $f_4$  is a specified initial temperature distribution.

### Diffusion Equation

The equation (4.10) is sometimes referred to as the diffusion equation. For diffusion processes we replace the temperature  $u(x, y, z, t)$  ( $^{\circ}C$ ) by concentration  $C(x, y, z, t)$  ( $gm/cm^3$ ) which represents the concentration of diffusing material at

the point  $(x, y, z)$  at time  $t$ . The Fourier law of heat conduction is replaced by Fick's<sup>†</sup> law of diffusion which states that the rate of transfer of diffusing material across a unit area of cross section is proportional to the concentration gradient in the direction of diffusion. In terms of symbols one can write

$$\vec{J} = -D \text{grad } C = -D \nabla C \quad (4.22)$$

where  $\vec{J}$  (gm/cm<sup>2</sup>sec) is the mass flow rate per unit area,  $D$  (cm<sup>2</sup>/sec) is the diffusion coefficient or mass diffusivity, and  $C$  (gm/cm<sup>3</sup>) is the concentration. Fick's law is valid for isotropic media of gases, liquids and solids. The diffusion coefficient  $D$  depends upon the process being considered. Nonlinear diffusion equations result if  $D$  is a function of the concentration. For anisotropic material, Fick's law is written

$$\vec{J} = -J_x \hat{i} - J_y \hat{j} - J_z \hat{k} \quad (4.23)$$

where

$$\begin{aligned} -J_x &= D_{11} \frac{\partial C}{\partial x} + D_{12} \frac{\partial C}{\partial y} + D_{13} \frac{\partial C}{\partial z} \\ -J_y &= D_{21} \frac{\partial C}{\partial x} + D_{22} \frac{\partial C}{\partial y} + D_{23} \frac{\partial C}{\partial z} \\ -J_z &= D_{31} \frac{\partial C}{\partial x} + D_{32} \frac{\partial C}{\partial y} + D_{33} \frac{\partial C}{\partial z} \end{aligned} \quad (4.24)$$

and the  $D_{ij}$ ,  $i, j = 1, 2, 3$ , are the diffusion coefficients reflecting the different diffusion properties in different directions. If all the diffusion coefficients  $D_{ij}$  are constants, then the analog of the heat equation becomes

$$\begin{aligned} \frac{\partial C}{\partial t} &= D_{11} \frac{\partial^2 C}{\partial x^2} + D_{12} \frac{\partial^2 C}{\partial x \partial y} + D_{13} \frac{\partial^2 C}{\partial x \partial z} \\ &+ D_{21} \frac{\partial^2 C}{\partial x \partial y} + D_{22} \frac{\partial^2 C}{\partial y^2} + D_{23} \frac{\partial^2 C}{\partial z \partial y} \\ &+ D_{31} \frac{\partial^2 C}{\partial x \partial z} + D_{32} \frac{\partial^2 C}{\partial y \partial z} + D_{33} \frac{\partial^2 C}{\partial z^2}. \end{aligned} \quad (4.25)$$

In the special case  $D_{ij} = 0$  for  $i \neq j$  and  $D_{11} = D_{22} = D_{33} = D$  the equation (4.25) reduces to

$$\frac{\partial C}{\partial t} = D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) = D \nabla^2 C \quad (4.26)$$

which has the exact same form as the heat equation given by equation (4.9) when the coefficients are constant and the heat source term is zero.

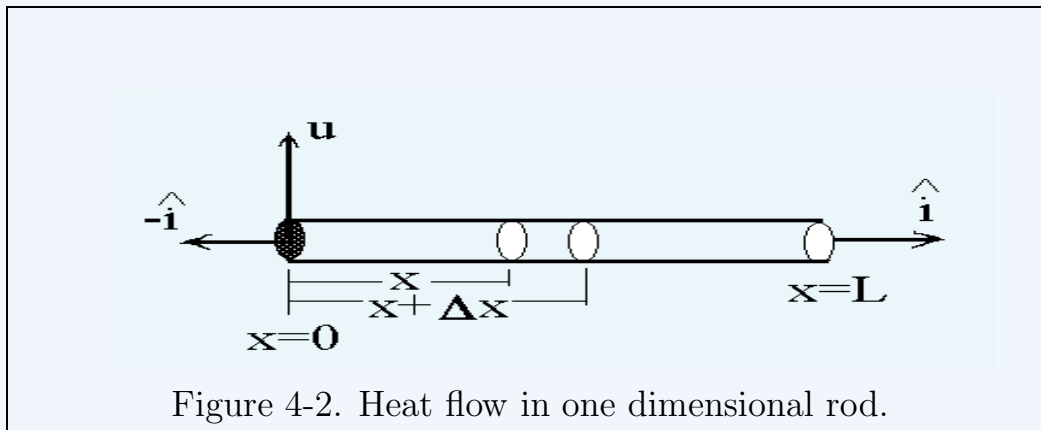
---

<sup>†</sup> See Appendix C

Boundary conditions associated with the diffusion equation are just like those of the heat equation. Dirichlet conditions require a specified concentration at the bounding surface. Neumann conditions require the flux of the diffusants be specified. A Robin condition requires a surface evaporation be proportional to the difference in concentration between the surface and surrounding medium.

**Example 4-1. (Heat flow one-dimension.)**

The previous derivation of the heat equation was for a general region of space. Sometimes the concepts are easier if one is not so general. Therefore, we will derive the one-dimensional heat equation for heat flow in a rod. With reference to figure 4-2 we formulate the equations describing the temperature distribution in a finite rod of length  $L$  which is insulated along its length and subject to end conditions. Imagine a thin rod made of a homogeneous material where the temperature remains constant at any cross section. Also assume the surface of the rod is insulated so heat flows only in the  $x$ -direction. We examine the law of conservation of energy for an arbitrary  $\Delta x$  section of the rod.



We use the notations

$c$ specific heat (cal/gm $^{\circ}$ C)	$t$ time (sec)
$\rho$ density (gm/cm $^3$ )	$\Delta x$ distance (cm)
$A$ cross sectional area (cm $^2$ )	$\kappa$ thermal conductivity (cal/cm $^2$ sec $^{\circ}$ C/cm)
$u = u(x, t)$ temperature ( $^{\circ}$ C)	$H$ heat generation source (cal/cm $^3$ )sec.

and assume  $c, \rho$  and  $\kappa$  are constants. The element of volume of the  $\Delta x$  section is given by  $A\Delta x$  and the conservation of energy requires the rate of change of