Chapter 2

Air Quality Modeling

2.1. Background

Air quality has become an important societal issue. Acid rain is a regional problem, affected by industrial by-products of toxic gas; it pollutes the ground and damages vegetation. In urban areas it is the ozone concentration that is considered to be the biggest health hazard. Air quality models are mathematical descriptions of atmospheric transport, diffusion, and chemical reaction of pollutants. The unknown variables are concentrations of chemical species in the air. The aim in developing and studying such models is to be able to predict how peak concentrations will change in response to prescribed changes in meteorology and in the source of pollution. Ozone air quality modeling has been one of the main areas of emphasis in the United States in the last twenty years; it is of particular interest to the automobile industry. In this chapter we consider the modeling of transport and diffusion of a single chemical, say ozone, ignoring the various underlying processes.

Putting the problem in a more personal context, suppose there is an industrial plant emitting noxious fumes. Also suppose that once an hour, as part of the manufacturing process, the plant emits a very concentrated batch of these offensive fumes for a few minutes and then stops. Exactly one mile away there is a beautiful house you would like to buy. If the wind is blowing in the direction of the house (the "worst possible" direction), how objectionable will the fumes be by the time they reach "your" house? In other words, what will be the maximum concentration of the fumes as they pass your house?

Assuming there are no chemical changes taking place as the fumes travel, there are basically two processes at work here: *advection* and *diffusion*.

Advection is essentially the effect of the wind "blowing" the fumes in a given direction without significantly dispersing them. A good example is a distant cloud moving with a fixed velocity in a given direction without apparently altering its size or shape.

Let us first consider the one-dimensional situation where there is advection but no diffusion (see Fig. 2.1).

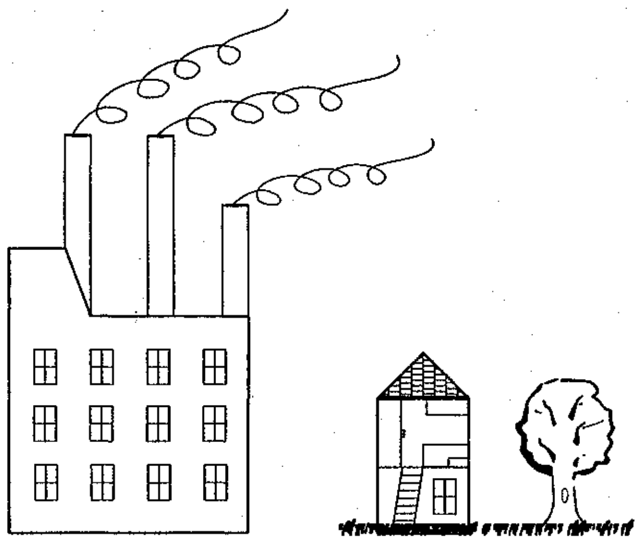


FIG. 2.1.

Suppose at time $t = 0$ the density of the fumes has a distribution given by profile $c_0(x)$ shown in Fig. 2.2.

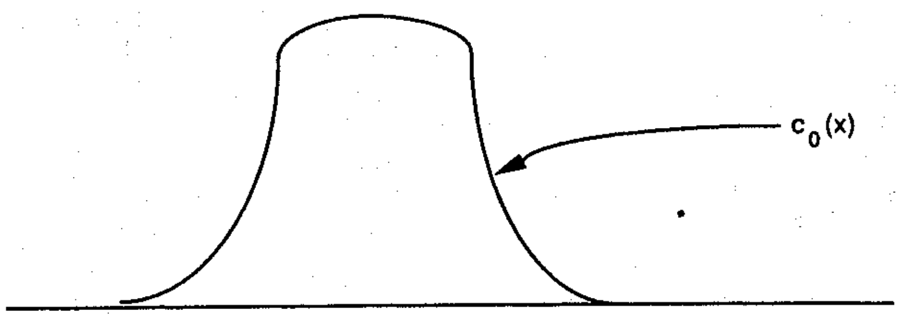


FIG. 2.2.

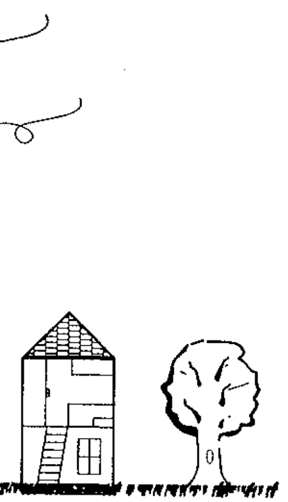
This profile moves to the right with the constant wind velocity U, giving rise to the moving profile for the concentration

$$c(x,t) = c_0(x - Ut). \tag{2.1}$$

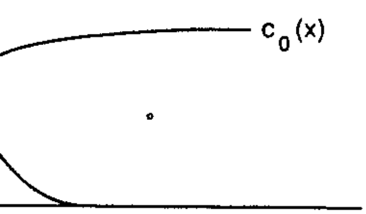
Differentiating partially, using the chain rule, we get

$$\frac{\partial c}{\partial x}\,(x,t) = c_0'(x - Ut), \qquad \frac{\partial c}{\partial t}\,(x,t) = c_0'(x - Ut) \cdot (-U),$$

l situation where there is advection



e fumes has a distribution given by



nstant wind velocity U, giving the

$- Ut)$.

e, we get

$,t) = c_0'(x - Ut) \cdot (-U),$

thus giving us the "advection equation"

$$\frac{\partial c}{\partial t}(x,t) + \frac{\partial (Uc)}{\partial x}(x,t) = 0 \tag{2.2}$$

with "initial" condition $c(x,0) = c_0(x)$. In the particular situation described here, we knew the solution of the partial differential equation in advance. In a more complicated situation, such as when the "wind velocity" U is not a constant, this will not be the case.

Looking at the form with the concentration profile (2.1) we see that the noxious fumes will arrive at "your" house in the same concentration as they left the factory: very high! This is bad news indeed.

Luckily all is not lost! As we have hinted earlier, there is another process at work: *diffusion*. This is the reason that even without the presence of wind, foul-smelling odors usually disappear after a time. For example, a newly painted house stops smelling of paint after a day or two, if not earlier. Taking into account advection and diffusion, there is at least the possibility that by the time the fumes have reached your house, diffusion has had a big enough effect, so that the fumes are barely noticeable.

In the remainder of this chapter we will give a more detailed mathematical description of the processes of advection and diffusion, how these can be investigated numerically, and finally how the two processes combined can be described by a simple "advection diffusion equation" that can be studied numerically.

2.2. The model

We denote by c the concentration of one species; it is a function of position (x_1, x_2, x_3) and of time t. The species is being transported by the wind, whose velocity $\vec{u} = \vec{u}\,(x_1, x_2, x_3, t)$ is assumed to be known. Particles of the species are also diffusing locally; they tend to move from areas of high concentration to areas of low concentration. If diffusion is ignored then the transport equation is

$$\frac{\partial c}{\partial t} + \nabla \cdot (\vec{u}\, c) = 0. \tag{2.3}$$

This is in some contexts also called the *continuity equation*. If we integrate (2.3) over any bounded domain D in $\mathbb{R}^3$ we get

$$\frac{d}{dt} \iiint_D c(x_1, x_2, x_3, t)\,dx_1 dx_2 dx_3 = -\iint_{\partial D} c\, \vec{u} \cdot \vec{n}\; dS, \tag{2.4}$$

where ∂D is the boundary of D and $\vec{n}$ is the outward unit normal to ∂D. This equation says that the rate of increase of the chemical in any domain D is equal to the flow of chemicals across the boundary. Conversely, if (2.4) holds for any domain D then, upon taking a sequence of domains D_j shrinking to a point, we can recover the relation (2.3) at that point.

If diffusion is not ignored then (2.3) is replaced by a more complicated partial differential equation:

$$\frac{\partial c}{\partial t} + \nabla \cdot (\vec{u}\ c) = \sum_{i,j=1}^{3} \frac{\partial}{\partial x_i}\left(k_{ij}\frac{\partial c}{\partial x_j}\right), \tag{2.5}$$

where (k_{ij}) is a positive definite matrix, called the *diffusion matrix*.

In either case, (2.3) or (2.5), we are given the concentration c at an initial time, say at $t = 0$,

$$c(x_1, x_2, x_3, 0) = c_0(x_1, x_2, x_3) \tag{2.6}$$

and our task is to compute the concentration $c(x_1, x_2, x_3, t)$ at subsequent times. In particular we wish to find out the maximum values of the concentration at a prescribed time; government regulations for pollution control often take the maximum concentration of pollution as a critical factor.

2.3. The advection equation

In this section we ignore diffusion and assume that the wind velocity is only in the horizontal direction. For simplicity we also assume that the direction of the wind is fixed, say, in the x-direction. Then $\vec{u} = (U, 0, 0)$ and the transport equation reduces to

$$\frac{\partial c}{\partial t} + \frac{\partial (Uc)}{\partial x} = 0; \tag{2.7}$$

this is called the *advection equation*. We also assume that initially c depends only on x, i.e.,

$$c(x, 0) = c_0(x), \qquad -\infty < x < \infty. \tag{2.8}$$

The velocity $U = U(x)$ is a function of x.

To solve (2.7), (2.8), we rewrite (2.7) in the form

$$\frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} = f \qquad (f = -U_x c) \tag{2.9}$$

and assume that $U(x)$ is continuously differentiable ($U_x = dU/dx$).

Consider the differential equation

$$\begin{cases} \dfrac{dx}{dt} = U(x), & t > 0, \\ x(0) = x_0 \end{cases} \tag{2.10}$$

oundary. Conversely, if (2.4) holds
ience of domains D_j shrinking to a
that point.
s replaced by a more complicated

$$\frac{\partial}{\partial x_i}\left(k_{ij}\frac{\partial c}{\partial x_j}\right),$$

lled the *diffusion matrix*.
en the concentration c at an initial

(x_1, x_2, x_3)

ation $c(x_1, x_2, x_3, t)$ at subsequent
out the maximum values of the
ernment regulations for pollution
ion of pollution as a critical factor.

ume that the wind velocity is only
ve also assume that the direction of
hen $\vec{u} = (U, 0, 0)$ and the transport

$= 0;$

lso assume that initially c depends

$-\infty < x < \infty.$

$x.$
the form

$(f = -U_x c)$

rentiable ($U_x = dU/dx$).

$t > 0,$

and denote its solution $x(t)$ by $x(t; x_0)$. Geometrically, $x(t; x_0)$ determines a unique curve γ_{x_0} passing through the point $(x_0, 0)$. We can show that $x(t; x_0)$ is actually differentiable in the parameter x_0 and the derivative

$$z(t) \equiv \frac{\partial x(t; x_0)}{\partial x_0}$$

satisfies

$$\frac{dz}{dt} = U_x(x(t; x_0))z, \qquad z(0) = 1.$$

PROBLEM 2.3.1. Prove the last statement.

We now examine the function

$$c(x(t; x_0), t)$$

as a function of the variable t. We find that

$$\frac{dc}{dt} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x}\frac{dx}{dt} = \frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} = f = -U_x(x(t; x_0))c,$$

or

$$\frac{d}{dt}\log c = -U_x(x(t; x_0)).$$

It follows that

$$c(x(t; x_0), t) = c_0(x_0)\exp\left\{-\int_0^t U_x(x(s; x_0))ds\right\}. \tag{2.11}$$

Note that d/dt is simply differentiation along the curve γ_{x_0}, parametrized by t.

We have shown that the solution of (2.7), (2.8) must be given by the formula (2.11). Conversely we can show that if the curves $(x(t; x_0), t)$ cover the upper half ($t \geq 0$) of the (x, t) plane, then the right-hand side of (2.11) is a solution to (2.7), (2.8).

PROBLEM 2.3.2. Prove the last statement.

DEFINITION 2.3.1. The curves (2.10) are called *characteristics* of (2.9) (for any f). The method described above for computing the solution c is called the *method of characteristics*.

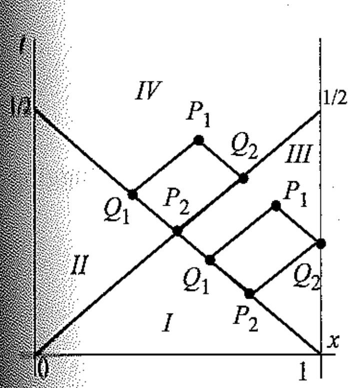


Figure 8

(c) Using (2), show that $u_t(0, t) = u_t(L, t) = 0$ for all $t > 0$.
(d) Prove the principle of conservation of energy, which states that the energy during the free vibrations of a string is constant for all time. [Hint: Prove that $dE/dt = 0$, using (b) and (c).]

19. Refer to Example 3.
(a) What are the characteristic lines?
(b) Find the intervals of dependence of the points (.5, .2) and (.3, 2).
(c) Describe the region I in this case. Which one of the points in (b) belongs to the region I?
(d) Find $u(x, t)$ for all points in the region I.

20. Refer to Example 3. Find $u(x, t)$ for all points in the region II.

21. Refer to Example 4. Find $u(x, t)$ for all points in the region III (see Figure 8).

22. Refer to Example 4. Find $u(x, t)$ for all points in the region IV (see Figure 8).

3.5 The One Dimensional Heat Equation

In this and the following section we study the temperature distribution in a uniform bar of length L with insulated lateral surface and no internal sources of heat, subject to certain boundary and initial conditions. To describe the problem, let $u(x, t)$ $(0 < x < L, t > 0)$ represent the temperature of the point x of the bar at time t (Figure 1). Given that the initial temperature distribution of the bar is $u(x, 0) = f(x)$, and given that the ends of the bar are held at constant temperature 0, we ask, What is $u(x, t)$ for $0 < x < L, t > 0$? As you would expect, to answer this question, we must solve a boundary value problem. We will show in the appendix at the end of this section that u satisfies the **one dimensional heat equation**

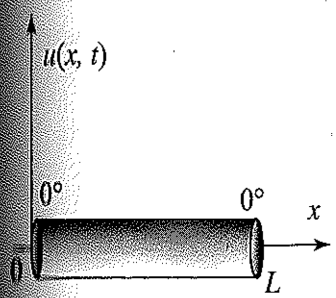


Figure 1 Insulated bar with ends kept at 0°.

$$\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < L, \quad t > 0.$$

In addition, u satisfies the **boundary conditions**

$$u(0, t) = 0 \quad \text{and} \quad u(L, t) = 0 \quad \text{for all } t > 0$$

and the **initial condition**

$$u(x, 0) = f(x) \quad \text{for } 0 < x < L.$$

Since the problem is first order in t, we only need one initial condition, unlike the wave problem where two conditions were needed.

We solve this problem using the method of separation of variables. After doing so, we will introduce the notion of steady-state temperature and use it to solve a related heat problem with nonzero boundary data. Interesting and important variations on these problems are presented in the following section.

Separation of Variables

We start by looking for product solutions of the form

$$u(x,t) = X(x)T(t),$$

where $X(x)$ is a function of x alone and $T(t)$ is a function of t alone. Plugging into the heat equation and separating variables, we obtain

$$\frac{T'}{c^2T} = \frac{X''}{X}.$$

For the equality to hold we must have

$$\frac{T'}{c^2T} = k \quad \text{and} \quad \frac{X''}{X} = k,$$

where k is the **separation constant**. From these equations, we get two *ordinary differential equations*

$$X'' - kX = 0 \quad \text{and} \quad T' - kc^2T = 0.$$

Separating variables in the boundary conditions, we get

$$X(0)T(t) = 0 \quad \text{and} \quad X(L)T(t) = 0 \text{ for all } t > 0.$$

To avoid trivial solutions we require

$$X(0) = 0 \quad \text{and} \quad X(L) = 0.$$

We thus obtain the boundary value problem in X:

$$X'' - kX = 0, \quad X(0) = 0 \quad \text{and} \quad X(L) = 0.$$

This problem is exactly the one that we solved in Section 3.3 for the vibrating string. We found that

$$k = -\mu^2, \quad \text{where } \mu = \mu_n = \frac{n\pi}{L}, \quad n = 1, 2, \ldots,$$

and

$$\boxed{X = X_n = \sin\frac{n\pi}{L}x, \quad n = 1, 2, \ldots.}$$

Substituting the values of k in the differential equation for T, we get the first order ordinary differential equation

$$T' + \left(c\frac{n\pi}{L}\right)^2 T = 0$$

whose general solution is

$$\boxed{T_n(t) = b_n e^{-\lambda_n^2 t}, \quad n = 1, 2, \ldots .}$$

where we set

$$\boxed{\lambda_n = c\,\frac{n\pi}{L}, \quad n = 1, 2, \ldots}$$

(see Theorem 1, Appendix A.1). We thus arrive at the product solution, or **normal mode**,

$$u_n(x,t) = b_n e^{-\lambda_n^2 t} \sin \frac{n\pi}{L} x, \quad n = 1, 2, \ldots .$$

By construction, each u_n is a solution of the heat equation and the given (homogeneous) boundary conditions. Motivated by the superposition principle (Theorem 1, Section 3.1) we let

$$\boxed{u(x,t) = \sum_{n=1}^{\infty} b_n e^{-\lambda_n^2 t} \sin \frac{n\pi}{L} x.}$$

Our next step is to determine the coefficients b_n so as to satisfy the initial condition $u(x,0) = f(x)$.

Fourier Series Solution of the Entire Problem

We set $t = 0$, use the initial condition, and get

$$f(x) = u(x,0) = \sum_{n=1}^{\infty} b_n \sin \frac{n\pi}{L} x.$$

Recognizing this sum as the half-range sine series expansion of f, we get from (4), Section 2.4,

$$b_n = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi}{L} x \, dx \quad n = 1, 2, \ldots,$$

which completely determines the solution. We summarize our findings as follows.

SOLUTION OF THE ONE DIMENSIONAL HEAT EQUATION

The solution of the one dimensional heat boundary value problem

(1) $$\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2} \qquad 0 < x < L, \quad t > 0,$$

(2) $$u(0,t) = 0 \quad \text{and} \quad u(L,t) = 0 \qquad \text{for all } t > 0,$$

(3) $$u(x,0) = f(x) \qquad \text{for } 0 < x < L,$$

is

(4) $$u(x,t) = \sum_{n=1}^{\infty} b_n e^{-\lambda_n^2 t} \sin \frac{n\pi}{L} x,$$

where

(5) $$b_n = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi}{L} x \, dx \quad \text{and} \quad \lambda_n = c\frac{n\pi}{L}, \qquad n = 1, 2, \ldots .$$

EXAMPLE 1 Temperature in a bar with ends held at 0°C
A thin bar of length π units is placed in boiling water (temperature 100°C). After reaching 100°C throughout, the bar is removed from the boiling water. With the lateral sides kept insulated, suddenly, at time $t = 0$, the ends are immersed in a medium with constant freezing temperature 0°C. Taking $c = 1$, find the temperature $u(x,t)$ for $t > 0$.

Solution The boundary value problem that we need to solve is

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < \pi, \quad t > 0,$$
$$u(0,t) = 0 \quad \text{and} \quad u(\pi,t) = 0, \quad t > 0,$$
$$u(x,0) = 100, \quad 0 < x < \pi.$$

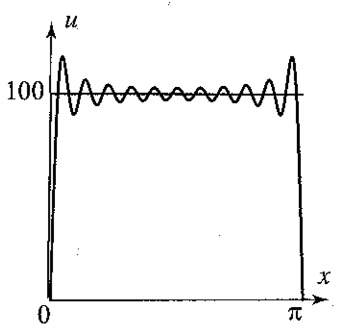


Figure 2 Partial sum of the sine Fourier series expansion of the initial temperature distribution (with k up to 10) $100 = \frac{400}{\pi} \sum_{k=0}^{\infty} \frac{\sin(2k+1)x}{2k+1}$ $0 < x < \pi$. (See Exercise 1, Section 2.3.)

From (4), we have

$$u(x,t) = \sum_{n=1}^{\infty} b_n e^{-n^2 t} \sin nx$$

where

$$b_n = \frac{2}{\pi} \int_0^{\pi} 100 \sin nx \, dx = \frac{200}{n\pi}(1 - \cos n\pi).$$

Substituting the values of b_n and using the fact that $(1 - \cos n\pi) = 0$ if n is even and 2 if n is odd, we get

$$u(x,t) = \frac{400}{\pi} \sum_{\substack{n=0 \\ n \text{ odd}}}^{\infty} \frac{e^{-n^2 t}}{n} \sin nx = \frac{400}{\pi} \sum_{k=0}^{\infty} \frac{e^{-(2k+1)^2 t}}{2k+1} \sin(2k+1)x.$$

If we plug a given value of t into the series solution, we obtain a function of x alone. This function gives the temperature distribution of the bar at the given time t. In particular, when $t = 0$, $u(x, 0)$ yields the half-range sine series expansion of the initial temperature distribution $f(x)$, illustrated in Figure 2 and the first picture in Figure 4. In Figures 3 and 4, we have approximated the series solution by summing it through the terms with $k = 0$ and $k = 10$, respectively, and have shown the temperature distribution at various values of t. Notice the rapid exponential decay of the higher order terms of the series solution. The exponent of the second nonzero term is 9 times bigger and the third is 25 times bigger than the exponent of the first term. This shows that the higher order terms die exceedingly fast. Because of this fast fall off of the higher order terms, the Gibbs phenomenon, which is apparent in the first frame in Figure 4, disappears very quickly from the partial sums. ■

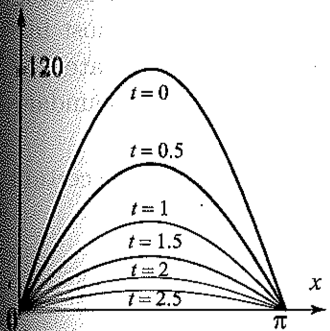


Figure 3 Approximation of the temperature by the first normal mode $u_1(x,t) = \frac{400}{\pi} e^{-t} \sin x$.

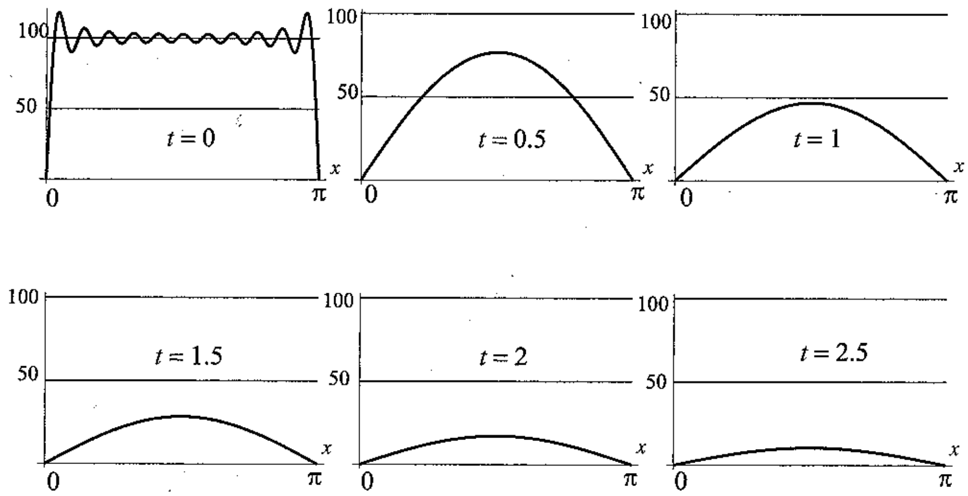


Figure 4 Temperature distribution in a bar with ends held at 0°. The temperature decays to 0 as t increases. Note that for large t, the shape of the graph is dominated by the first normal mode. Indeed, comparison with Figure 3 shows that the two curves are virtually indistinguishable for $t \geq 0.5$.

Steady-State Temperature Distribution

The graphs in Figure 4 show that the temperature in the bar tends to zero as t increases. This is intuitively clear, since the ends of the bar are kept at 0° and there is no internal source of heat. In general, the temperature distribution that we get as $t \to \infty$ is a function of x alone called the **steady-state solution** (or **time-independent solution**). So, in Example 1, the steady-state solution is the function that is identically 0.

For general boundary conditions, since the steady-state solution is independent of t, we must have $\partial u/\partial t = 0$. Substituting this in (1), we see that the steady-state distribution satisfies the differential equation $\frac{\partial^2 u}{\partial x^2} = 0$, or simply $\frac{d^2 u}{dx^2} = 0$, because u, the steady-state solution, is a function of x only. The general solution of this simple differential equation is $u(x) = Ax + B$, where A and B are constants that are determined using the boundary conditions. We illustrate with an example.