

## 2. Advective Diffusion Equation

In nature, transport occurs in fluids through the combination of advection and diffusion. The previous chapter introduced diffusion and derived solutions to predict diffusive transport in stagnant ambient conditions. This chapter incorporates advection into our diffusion equation (deriving the advective diffusion equation) and presents various methods to solve the resulting partial differential equation for different geometries and contaminant conditions.

### 2.1 Derivation of the advective diffusion equation

Before we derive the advective diffusion equation, we look at a heuristic description of the effect of advection. To conceptualize advection, consider our pipe problem from the previous chapter. Without pipe flow, the injected tracer spreads equally in both directions, describing a Gaussian distribution over time. If we open a valve and allow water to flow in the pipe, we expect the center of mass of the tracer cloud to move with the mean flow velocity in the pipe. If we move our frame of reference with that mean velocity, then we expect the solution to look the same as before. This new reference frame is

$$\eta = x - (x_0 + ut) \tag{2.1}$$

where  $\eta$  is the moving reference frame spatial coordinate,  $x_0$  is the injection point of the tracer,  $u$  is the mean flow velocity, and  $ut$  is the distance traveled by the center of mass of the cloud in time  $t$ . If we substitute  $\eta$  for  $x$  in our solution for a point source in stagnant conditions we obtain

$$C(x, t) = \frac{M}{A\sqrt{4\pi Dt}} \exp\left(-\frac{(x - (x_0 + ut))^2}{4Dt}\right). \tag{2.2}$$

To test whether this solution is correct, we need to derive a general equation for advective diffusion and compare its solution to this one.

#### 2.1.1 The governing equation

The derivation of the advective diffusion equation relies on the principle of superposition: advection and diffusion can be added together if they are linearly independent. How do we know if advection and diffusion are independent processes? The only way that they can be dependent is if one process feeds back on the other. From the previous chapter,

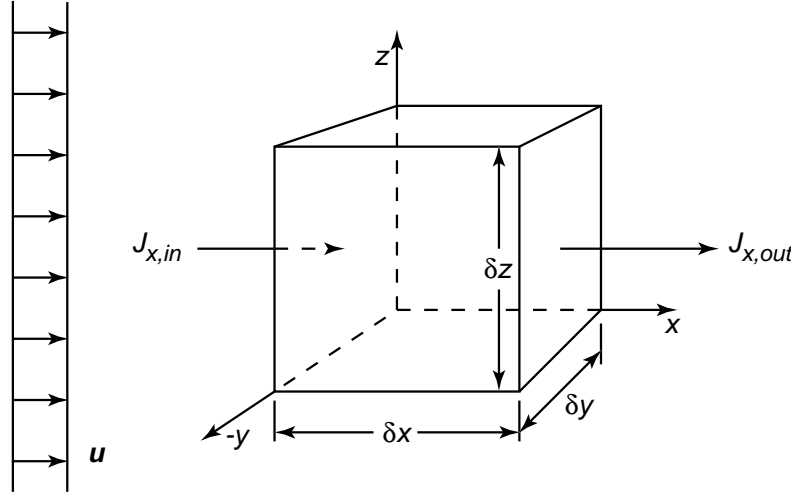


Fig. 2.1. Schematic of a control volume with crossflow.

diffusion was shown to be a random process due to molecular motion. Due to diffusion, each molecule in time  $\delta t$  will move either one step to the left or one step to the right (i.e.  $\pm \delta x$ ). Due to advection, each molecule will also move  $u \delta t$  in the cross-flow direction. These processes are clearly additive and independent; the presence of the crossflow does not bias the probability that the molecule will take a diffusive step to the right or the left, it just adds something to that step. The net movement of the molecule is  $u \delta t \pm \delta x$ , and thus, the total flux in the  $x$ -direction  $J_x$ , including the advective transport and a Fickian diffusion term, must be

$$\begin{aligned} J_x &= uC + q_x \\ &= uC - D \frac{\partial C}{\partial x}. \end{aligned} \quad (2.3)$$

We leave it as an exercise for the reader to prove that  $uC$  is the correct form of the advective term (hint: consider the dimensions of  $q_x$  and  $uC$ ).

As we did in the previous chapter, we now use this flux law and the conservation of mass to derive the advective diffusion equation. Consider our control volume from before, but now including a crossflow velocity,  $\mathbf{u} = (u, v, w)$ , as shown in Figure 2.1. Here, we follow the derivation in Fischer et al. (1979). From the conservation of mass, the net flux through the control volume is

$$\frac{\partial M}{\partial t} = \sum \dot{m}_{in} - \sum \dot{m}_{out}, \quad (2.4)$$

and for the  $x$ -direction, we have

$$\delta \dot{m}|_x = \left( uC - D \frac{\partial C}{\partial x} \right) \Big|_1 \delta y \delta z - \left( uC - D \frac{\partial C}{\partial x} \right) \Big|_2 \delta y \delta z. \quad (2.5)$$

As before, we use linear Taylor series expansion to combine the two flux terms, giving

$$uC|_1 - uC|_2 = uC|_1 - \left( uC|_1 + \frac{\partial(uC)}{\partial x} \Big|_1 \delta x \right)$$

$$= -\frac{\partial(uC)}{\partial x}\delta x \quad (2.6)$$

and

$$\begin{aligned} -D \frac{\partial C}{\partial x}\Big|_1 + D \frac{\partial C}{\partial x}\Big|_2 &= -D \frac{\partial C}{\partial x}\Big|_1 + \left( D \frac{\partial C}{\partial x}\Big|_1 + \frac{\partial}{\partial x} \left( D \frac{\partial C}{\partial x} \right)\Big|_1 \delta x \right) \\ &= D \frac{\partial^2 C}{\partial x^2} \delta x. \end{aligned} \quad (2.7)$$

Thus, for the  $x$ -direction

$$\delta \dot{m}|_x = -\frac{\partial(uC)}{\partial x} \delta x \delta y \delta z + D \frac{\partial^2 C}{\partial x^2} \delta x \delta y \delta z. \quad (2.8)$$

The  $y$ - and  $z$ -directions are similar, but with  $v$  and  $w$  for the velocity components, giving

$$\delta \dot{m}|_y = -\frac{\partial(vC)}{\partial y} \delta y \delta x \delta z + D \frac{\partial^2 C}{\partial y^2} \delta y \delta x \delta z \quad (2.9)$$

$$\delta \dot{m}|_z = -\frac{\partial(wC)}{\partial z} \delta z \delta x \delta y + D \frac{\partial^2 C}{\partial z^2} \delta z \delta x \delta y. \quad (2.10)$$

Substituting these results into (2.4) and recalling that  $M = C \delta x \delta y \delta z$ , we obtain

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{u}C) = D \nabla^2 C \quad (2.11)$$

or in Einsteinian notation

$$\frac{\partial C}{\partial t} + \frac{\partial u_i C}{\partial x_i} = D \frac{\partial^2 C}{\partial x_i^2}, \quad (2.12)$$

which is the desired advective diffusion (AD) equation. We will use this equation extensively in the remainder of this class.

Note that these equations implicitly assume that  $D$  is constant. When considering a variable  $D$ , the right-hand-side of (2.12) has the form

$$\frac{\partial}{\partial x_i} \left( D_{ij} \frac{\partial C}{\partial x_j} \right). \quad (2.13)$$

### 2.1.2 Point-source solution

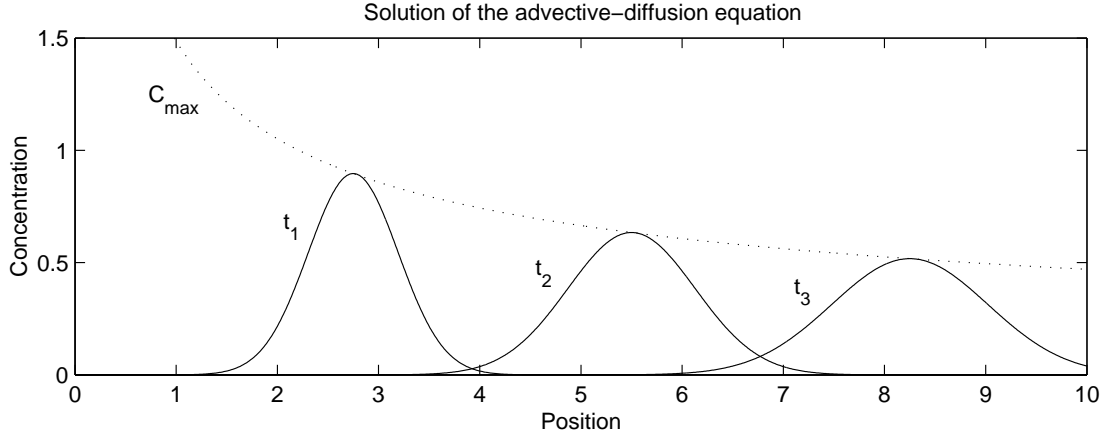
To check whether our initial suggestion (2.2) for a solution to (2.12) was correct, we substitute the coordinate transformation for the moving reference frame into the one-dimensional version of (2.12). In the one-dimensional case,  $\mathbf{u} = (u, 0, 0)$ , and there are no concentration gradients in the  $y$ - or  $z$ -directions, leaving us with

$$\frac{\partial C}{\partial t} + \frac{\partial(uC)}{\partial x} = D \frac{\partial^2 C}{\partial x^2}. \quad (2.14)$$

Our coordinate transformation for the moving system is

$$\eta = x - (x_0 + ut) \quad (2.15)$$

$$\tau = t, \quad (2.16)$$



**Fig. 2.2.** Schematic solution of the advective diffusion equation in one dimension. The dotted line plots the maximum concentration as the cloud moves downstream.

and this can be substituted into (2.14) using the chain rule as follows

$$\begin{aligned} \frac{\partial C}{\partial \tau} \frac{\partial \tau}{\partial t} + \frac{\partial C}{\partial \eta} \frac{\partial \eta}{\partial t} + u \left( \frac{\partial C}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial C}{\partial \tau} \frac{\partial \tau}{\partial x} \right) = \\ D \left( \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial}{\partial \tau} \frac{\partial \tau}{\partial x} \right) \left( \frac{\partial C}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial C}{\partial \tau} \frac{\partial \tau}{\partial x} \right) \end{aligned} \quad (2.17)$$

which reduces to

$$\frac{\partial C}{\partial \tau} = D \frac{\partial^2 C}{\partial \eta^2}. \quad (2.18)$$

This is just the one-dimensional diffusion equation (1.27) in the coordinates  $\eta$  and  $\tau$  with solution for an instantaneous point source of

$$C(\eta, \tau) = \frac{M}{A\sqrt{4\pi D\tau}} \exp\left(-\frac{\eta^2}{4D\tau}\right). \quad (2.19)$$

Converting the solution back to  $x$  and  $t$  coordinates (by substituting (2.15) and (2.16)), we obtain (2.2); thus, our intuitive guess for the superposition solution was correct. Figure 2.2 shows the schematic behavior of this solution for three different times,  $t_1$ ,  $t_2$ , and  $t_3$ .

### 2.1.3 Incompressible fluid

For an incompressible fluid, (2.12) can be simplified by using the conservation of mass equation for the ambient fluid. In an incompressible fluid, the density is a constant  $\rho_0$  everywhere, and the conservation of mass equation reduces to the continuity equation

$$\nabla \cdot \mathbf{u} = 0 \quad (2.20)$$

(see, for example Batchelor (1967)). If we expand the advective term in (2.12), we can write

$$\nabla \cdot (\mathbf{u}C) = (\nabla \cdot \mathbf{u})C + \mathbf{u} \cdot \nabla C. \quad (2.21)$$

by virtue of the continuity equation (2.20) we can take the term  $(\nabla \cdot \mathbf{u})C = 0$ ; thus, the advective diffusion equation for an incompressible fluid is

$$\frac{\partial C}{\partial t} + u_i \frac{\partial C}{\partial x_i} = D \frac{\partial^2 C}{\partial x_i^2}. \quad (2.22)$$

This is the form of the advective diffusion equation that we will use the most in this class.

### 2.1.4 Rules of thumb

We pause here to make some observations regarding the AD equation and its solutions.

First, the solution in Figure 2.2 shows an example where the diffusive and advective transport are about equally important. If the crossflow were stronger (larger  $u$ ), the cloud would have less time to spread out and would be narrower at each  $t_i$ . Conversely, if the diffusion were faster (larger  $D$ ), the cloud would spread out more between the different  $t_i$  and the profiles would overlap. Thus, we see that diffusion *versus* advection dominance is a function of  $t$ ,  $D$ , and  $u$ , and we express this property through the non-dimensional Peclet number

$$Pe = \frac{D}{u^2 t}, \quad (2.23)$$

or for a given downstream location  $L = ut$ ,

$$Pe = \frac{D}{uL}. \quad (2.24)$$

For  $Pe \gg 1$ , diffusion is dominant and the cloud spreads out faster than it moves downstream; for  $Pe \ll 1$ , advection is dominant and the cloud moves downstream faster than it spreads out. It is important to note that the Peclet number is dependent on our zone of interest: for large times or distances, the Peclet number is small and advection dominates.

Second, the maximum concentration decreases in the downstream direction due to diffusion. Figure 2.2 also plots the maximum concentration of the cloud as it moves downstream. This is obtained when the exponential term in (2.2) is 1. For the one-dimensional case, the maximum concentration decreases as

$$C_{max}(t) \propto \frac{1}{\sqrt{t}}. \quad (2.25)$$

In the two- and three-dimensional cases, the relationship is

$$C_{max}(t) \propto \frac{1}{t} \text{ and} \quad (2.26)$$

$$C_{max}(t) \propto \frac{1}{t\sqrt{t}}, \quad (2.27)$$

respectively.

Third, the diffusive and advective scales can be used to simplify the equations and make approximations. One of the most common questions in engineering is: when does a given equation or approximation apply? In contaminant transport, this question is usually answered by comparing characteristic advection and diffusion length and time scales to

the length and time scales in the problem. For advection (subscript  $a$ ) and for diffusion (subscript  $d$ ), the characteristic scales are

$$L_a = ut; \quad t_a = \frac{L}{u} \quad (2.28)$$

$$L_d = \sqrt{Dt}; \quad t_d = \frac{L^2}{D}. \quad (2.29)$$

From the Gaussian solution to a point-source, for instance, we can show that the time required before a cloud can be considered well-mixed over an area of length  $L$  is  $t_{m,d} = L^2/(8D)$ . These characteristic scales (easily derivable through dimensional analysis) should be memorized and used extensively to get a rough solution to transport problems.

## 2.2 Solutions to the advective diffusion equation

In the previous chapter we presented a detailed solution for an instantaneous point source in a stagnant ambient. In nature, initial and boundary conditions can be much different from that idealized case, and this section presents a few techniques to deal with other general cases. Just as advection and diffusion are additive, we will also show that superposition can be used to build up solutions to complex geometries or initial conditions from a base set of a few general solutions.

The solutions in this section parallel a similar section in Fischer et al. (1979). Appendix B presents analytical solutions for other initial and boundary conditions, primarily obtained by extending the techniques discussed in this section. Taken together, these solutions can be applied to a wide range of problems.

### 2.2.1 Initial spatial concentration distribution

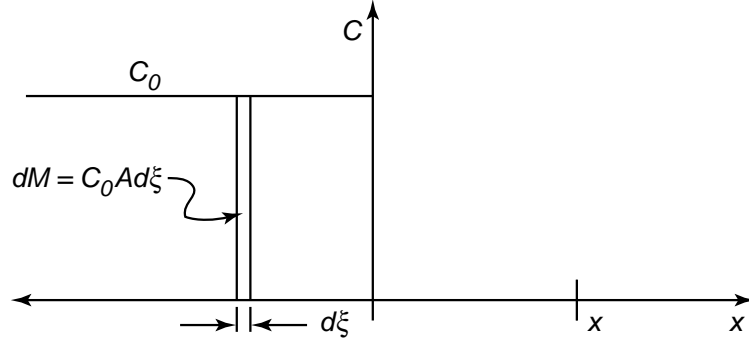
A good example of the power of superposition is the solution for an initial spatial concentration distribution. Since advection can always be included by changing the frame of reference, we will consider the one-dimensional stagnant case. Thus, the governing equation is

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}. \quad (2.30)$$

We will consider the homogeneous initial distribution, given by

$$C(x, t_0) = \begin{cases} C_0 & \text{if } x \leq 0 \\ 0 & \text{if } x > 0 \end{cases} \quad (2.31)$$

where  $t_0 = 0$  and  $C_0$  is the uniform initial concentration, as depicted in Figure 2.3. At a point  $x = \xi < 0$  there is an infinitesimal mass  $dM = C_0 A d\xi$ , where  $A$  is the cross-sectional area  $\delta y \delta z$ . For  $t > 0$ , the concentration at any point  $x$  is due to the diffusion of mass from all the differential elements  $dM$ . The contribution  $dC$  for a single element  $dM$  is just the solution of (2.30) for an instantaneous point source



**Fig. 2.3.** Schematic of an instantaneous initial concentration distribution showing the differential element  $dM$  at the point  $-\xi$ .

$$dC(x, t) = \frac{dM}{A\sqrt{4\pi Dt}} \exp\left(-\frac{(x - \xi)^2}{4Dt}\right), \quad (2.32)$$

and by virtue of superposition, we can sum up all the contributions  $dM$  to obtain

$$C(x, t) = \int_{-\infty}^0 \frac{C_0 d\xi}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x - \xi)^2}{4Dt}\right) \quad (2.33)$$

which is the superposition solution to our problem. To compute the integral, we must, as usual, make a change of variables. The new variable  $\zeta$  is defined as follows

$$\zeta = \frac{x - \xi}{\sqrt{4Dt}} \quad (2.34)$$

$$d\zeta = -\frac{d\xi}{\sqrt{4Dt}}. \quad (2.35)$$

Substituting  $\zeta$  into the integral solution gives

$$C(x, t) = \frac{C_0}{\sqrt{\pi}} \int_{-\infty}^{x/\sqrt{4Dt}} \exp(-\zeta^2) d\zeta. \quad (2.36)$$

Note that to obtain the upper bound on the integral we set  $\xi = 0$  in the definition for  $\zeta$  given in (2.34). Rearranging the integral gives

$$C(x, t) = \frac{C_0}{\sqrt{\pi}} \int_{x/\sqrt{4Dt}}^{\infty} \exp(-\zeta^2) d\zeta \quad (2.37)$$

$$= \frac{C_0}{\sqrt{\pi}} \left[ \int_0^{\infty} \exp(-\zeta^2) d\zeta - \int_0^{x/\sqrt{4Dt}} \exp(-\zeta^2) d\zeta \right]. \quad (2.38)$$

The first of the two integrals can be solved analytically—from a table of integrals, its solution is  $\sqrt{\pi}/2$ . The second integral is the so called error function, defined as

$$\text{erf}(\varphi) = \frac{2}{\sqrt{\pi}} \int_0^{\varphi} \exp(-\zeta^2) d\zeta. \quad (2.39)$$

Solutions to the error function are generally found in tables or as built-in functions in a spreadsheet or computer programming language. Hence, our solution can be written as

$$C(x, t) = \frac{C_0}{2} \left( 1 - \text{erf}\left(\frac{x}{\sqrt{4Dt}}\right) \right). \quad (2.40)$$

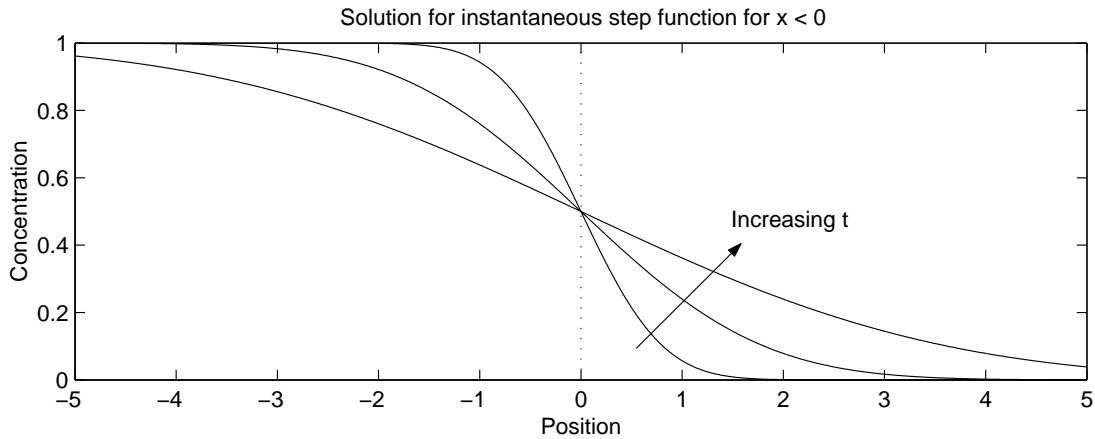


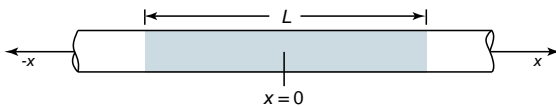
Fig. 2.4. Solution (2.40) for an instantaneous initial concentration distribution given by (2.31) with  $C_0 = 1$ .

Figure 2.4 plots this solution for  $C_0 = 1$  and for increasing times  $t$ .

**Example Box 2.1:**

**Diffusion of an intravenous injection.**

A doctor administers an intravenous injection of an allergy fighting medicine to a patient suffering from an allergic reaction. The injection takes a total time  $T$ . The blood in the vein flows with mean velocity  $u$ , such that blood over a region of length  $L = uT$  contains the injected chemical; the concentration of chemical in the blood is  $C_0$  (refer to the following sketch).



What is the distribution of chemical in the vein when it reaches the heart 75 s later?

This problem is an initial spatial concentration distribution, like the one in Section 2.2.1. Take the point  $x = 0$  at the middle of the distribution and let the coordinate system move with the mean blood flow velocity  $u$ . Thus, we have the initial concentration distribution

$$C(x, t_0) = \begin{cases} C_0 & \text{if } -L/2 < x < L/2 \\ 0 & \text{otherwise} \end{cases}$$

where  $t_0 = 0$  at the time  $T/2$ .

Following the solution method in Section 2.2.1, the superposition solution is

$$C(x, t) = \int_{-L/2}^{L/2} \frac{C_0 d\xi}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-\xi)^2}{4Dt}\right)$$

which can be expanded to give

$$C(x, t) = \frac{C_0}{\sqrt{4\pi Dt}} \cdot \left[ \int_{-\infty}^{L/2} \exp\left(-\frac{(x-\xi)^2}{4Dt}\right) d\xi - \int_{-\infty}^{-L/2} \exp\left(-\frac{(x-\xi)^2}{4Dt}\right) d\xi \right].$$

After substituting the coordinate transformation in (2.34) and simplifying, the solution is found to be

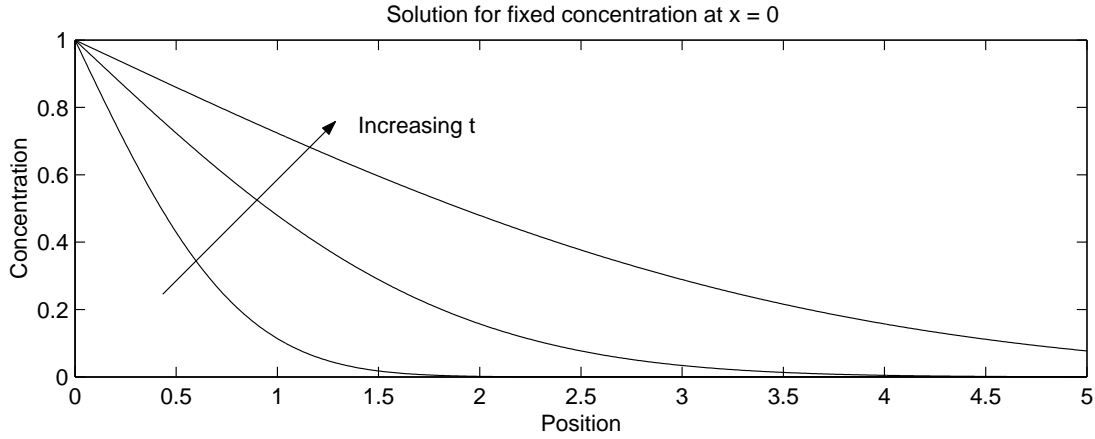
$$C(x, t) = \frac{C_0}{2} \left( \operatorname{erf}\left(\frac{x+L/2}{\sqrt{4Dt}}\right) - \operatorname{erf}\left(\frac{x-L/2}{\sqrt{4Dt}}\right) \right).$$

Substituting  $t = 75$  s gives the concentration distribution when the slug of medicine reaches the heart.

**2.2.2 Fixed concentration**

Another common situation is a fixed concentration at some point  $x_1$ . This could be, for example, the oxygen concentration at the air-water interface. The parameters governing





**Fig. 2.5.** Solution (2.43) for a fixed concentration at  $x = 0$  of  $C_0 = 1$ .

the solution are the fixed concentration  $C_0$ , the diffusion coefficient  $D$ , and the coordinates  $(x - x_0)$ , and  $t$ . Again, we will neglect advection since we can include it through a change of variables, and we will take  $x_0 = 0$  for simplicity. As we did for a point source, we form a similarity solution from the governing variables, which gives us the solution form

$$C(x, t) = C_0 f\left(\frac{x}{\sqrt{Dt}}\right). \quad (2.41)$$

If we define the similarity variable  $\eta = x/\sqrt{Dt}$  and substitute it into (2.30) we obtain, as expected, an ordinary differential equation in  $f$  and  $\eta$ , given by

$$\frac{d^2 f}{d\eta^2} + \frac{\eta}{2} \frac{df}{d\eta} = 0 \quad (2.42)$$

with boundary conditions  $f(0) = 1$  and  $f(\infty) = 0$ . Unfortunately, our ordinary differential equation is non-linear. A quick look at Figure 2.4, however, might help us guess a solution. The point at  $x = 0$  has a fixed concentration of  $C_0/2$ . If we substitute  $C_0$  as the leading coefficient in (2.40) (instead of  $C_0/2$ ), maybe that would be the solution. Substitution into the differential equation (2.42) and its boundary conditions proves, indeed, that the solution is correct, namely

$$C(x, t) = C_0 \left(1 - \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right) \quad (2.43)$$

is the solution we seek. Figure 2.5 plots this solution for  $C_0 = 1$ . Important note: this solution is *only* valid for  $x > x_0$ .

### 2.2.3 Fixed, no-flux boundaries

The final situation we examine in this section is how to incorporate no-flux boundaries. No-flux boundaries are any surface that is impermeable to the contaminant of interest. The discussion in this section assumes that no chemical reactions occur at the surface and that the surface is completely impermeable.

**Example Box 2.2:**

Dissolving sugar in coffee.

On a cold winter's day you pour a cup of coffee and add 2 g of sugar evenly distributed over the bottom of the coffee cup. The diameter of the cup is 5 cm; its height is 7 cm. If you do not stir the coffee, when does the concentration boundary layer first reach the top of the cup and when does all of the sugar dissolve? How would these answers change if you stir the coffee?

The concentration of sugar is fixed at the saturation concentration at the bottom of the cup and is initially zero everywhere else. These are the same conditions as for the fixed concentration solution; thus, the sugar distribution at height  $z$  above the bottom of the cup is

$$C(z, t) = C_0 \left( 1 - \operatorname{erf} \left( \frac{z}{\sqrt{4Dt}} \right) \right).$$

The characteristic height of the concentration boundary layer is proportional to  $\sigma = \sqrt{2Dt}$ . Assume the concentration boundary layer first reaches the top of the cup when  $2\sigma = h = 7$  cm. Solving for time gives

$$t_{mix,bl} = \frac{h^2}{8D}.$$

For an order-of-magnitude estimate, take  $D \sim 10^{-9}$  m<sup>2</sup>/s, giving

$$t_{mix,bl} \approx 6 \cdot 10^5 \text{ s.}$$

To determine how long it takes for the sugar to dissolve, we must compute the mass flux of sugar at  $z = 0$ . We already computed the derivative of the error function in Example Box 1.1. The mass flux of sugar at  $z = 0$  is then

$$\dot{m}(0, t) = \frac{ADC_{sat}}{\sqrt{\pi Dt}}$$

where  $A$  is the cross-sectional area of the cup. The total amount of dissolved sugar  $M_d$  is the time-integral of the mass flux

$$M_d = \int_0^t \frac{ADC_{sat}}{\sqrt{\pi D\tau}} d\tau$$

Integrating and solving for time gives

$$t_d = \frac{M_d^2 \pi}{4A^2 DC_{sat}^2}$$

where  $t_d$  is the time it takes for the mass  $M_d$  to dissolve. This expression is only valid for  $t < t_{mix,bl}$ ; for times beyond  $t_{mix,bl}$ , we must account for the boundary at the top of the cup. Assuming  $C_{sat} = 0.58$  g/cm<sup>3</sup>, the time needed to dissolve all the sugar is

$$t_d = 5 \cdot 10^4 \text{ s.}$$

By stirring, we effectively increase the value of  $D$ . Since  $D$  is in the denominator of each of these time estimates, we shorten the time for the sugar to dissolve and mix throughout the cup.

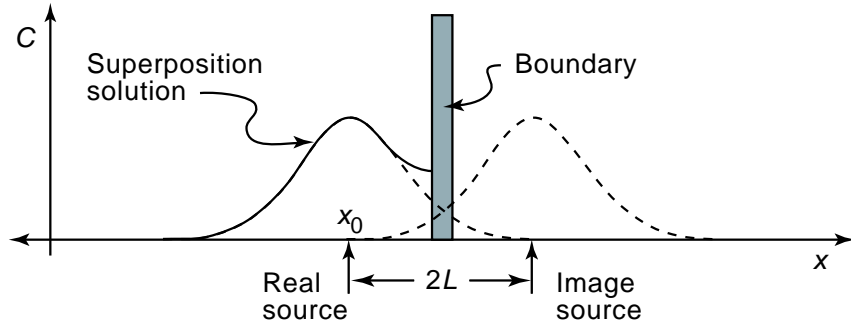
As you might expect, we first need to find a way to specify a no-flux boundary as a boundary condition to the governing differential equation. This is done easily using Fick's law. Since no-flux means that  $\mathbf{q} = 0$  (and taking  $D$  as constant), the boundary conditions can be expressed as

$$\begin{aligned} \mathbf{q}|_{S_b} \cdot \mathbf{n} &= 0 \\ \left( \frac{\partial C}{\partial x}, \frac{\partial C}{\partial y}, \frac{\partial C}{\partial z} \right) \Big|_{S_b} \cdot \mathbf{n} &= 0 \end{aligned} \quad (2.44)$$

where  $S_b$  is the function describing the boundary surface (i.e.  $S_b = f(x, y)$ ) and  $\mathbf{n}$  is the unit vector normal to the no-flux boundary. In the one-dimensional case, the no-flux boundary condition reduces to

$$\frac{\partial C}{\partial x} \Big|_{x_b} = 0, \quad (2.45)$$

where  $x_b$  is the boundary location. This property is very helpful in interpreting concentration measurements to determine whether a boundary, for instance, the lake bottom, is impermeable or not.



**Fig. 2.6.** Schematic of a no-flux boundary with real instantaneous point source to the left and an imaginary source to the right. The dotted lines indicate the individual contributions from the two sources; the solid line indicates the superposition solution.

To find a solution to a bounded problem, consider an instantaneous point source injected at  $x_0$  with a no-flux boundary a distance  $L$  to the right as shown in Figure 2.6. Our standard solution allows mass to diffuse beyond the no-flux boundary (as indicated by the dashed line in the figure). To replace this lost mass, an image source (imaginary source) is placed to the right of the boundary, such that it leaks the same amount of mass back to left of the boundary as our standard solution leaked to the right. Superposing (adding) these two solutions gives us the desired no-flux behavior at the wall. The image source is placed  $L$  to the right of the boundary, and the solution is

$$C(x, t) = \frac{M}{A\sqrt{4\pi Dt}} \left( \exp\left(-\frac{(x-x_0)^2}{4Dt}\right) + \exp\left(-\frac{(x-x_i)^2}{4Dt}\right) \right) \quad (2.46)$$

where  $x_i = x_0 + 2L$ . Naturally, the solution given here is only valid to the left of the boundary. To the right of the boundary, the concentration is everywhere zero. Compute the concentration gradient  $\partial C/\partial x$  at  $x = 0$  to prove to yourself that the no-flux boundary condition is satisfied.

The method of images becomes more complicated when multiple boundaries are concerned. This is because the mass diffusing from the image source on the right eventually will penetrate a boundary on the left and need its own image source. In general, when there are two boundaries, an infinite number of image sources is required. In practice, the solution usually converges after only a few image sources have been included (Fischer et al. 1979). For the case of an instantaneous point source at the origin with boundaries at  $\pm L$ , Fischer et al. (1979) give the image source solution

$$C(x, t) = \frac{M}{A\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} \exp\left(-\frac{(x+4nL)^2}{4Dt}\right) - \exp\left(-\frac{(x+(4n-2)L)^2}{4Dt}\right). \quad (2.47)$$

Obviously, the number of image sources required for the solution to converge depends on the time scale over which the solution is to be valid. These techniques will become more clear in the following examples and remaining chapters.

**Example Box 2.3:****Boundaries in a coffee cup.**

In the previous example box we said that we have to account for the free surface boundary when the concentration boundary layer reaches the top of the coffee cup. Describe the image source needed to account for the free surface and state the image-source solution for the concentration distribution.

We can ignore the boundaries at the sides of the cup because sugar is evenly distributed on the bottom of the cup. This even distribution results in  $\partial C/\partial x = \partial C/\partial y = 0$ , which results in no net diffusive flux toward the cup walls.

To account for the free surface, though, we must add an image source with a fixed concentration of  $C_{sat}$  somewhere above the cup. Taking  $z = 0$  at the bottom of the cup, the image source must be placed at  $z = 2h$ , where  $h$  is the depth of coffee in the cup.

Taking care that  $C(z, \infty) \rightarrow C_{sat}$ , the superposition solution for the sugar concentration distribution can be found to be

$$C(z, t) = C_{sat} \left( 1 + \operatorname{erf} \left( \frac{2h}{\sqrt{4Dt}} \right) - \operatorname{erf} \left( \frac{z}{\sqrt{4Dt}} \right) - \operatorname{erf} \left( \frac{2h - z}{\sqrt{4Dt}} \right) \right).$$

**2.3 Application: Diffusion in a Lake**

We return here to the application of arsenic contamination in a small lake presented in Chapter 1 (adapted from Nepf (1995)). After further investigation, it is determined that a freshwater spring flows into the bottom of the lake with a flow rate of 10 l/s.

*Advection.* Advection is due to the flow of spring water through the lake. Assuming the spring is not buoyant, it will spread out over the bottom of the lake and rise with a uniform vertical flux velocity (recall that  $z$  is positive downward, so the flow is in the minus  $z$ -direction)

$$\begin{aligned} v_a &= -Q/A \\ &= -5 \cdot 10^{-7} \text{ m/s.} \end{aligned} \tag{2.48}$$

The concentration of arsenic at the thermocline is 8  $\mu\text{g/l}$ , which results in an advective flux of arsenic

$$\begin{aligned} q_a &= C v_a \\ &= -4 \cdot 10^{-3} \text{ } \mu\text{g}/(\text{m}^2\text{s}). \end{aligned} \tag{2.49}$$

Thus, advection caused by the spring results in a vertical advective flux of arsenic through the thermocline.

*Discussion.* Taking the turbulent and advective fluxes of arsenic together, the net vertical flux of arsenic through the thermocline is

$$\begin{aligned} J_z &= -4.00 \cdot 10^{-3} + 2.93 \cdot 10^{-3} \\ &= -1.10 \cdot 10^{-3} \text{ } \mu\text{g}/(\text{m}^2\text{s}) \end{aligned} \tag{2.50}$$

where the minus sign indicates the net flux is upward. Thus, although the net diffusive flux is downward, the advection caused by the stream results in the net flux at the thermocline being upward. We can conclude that the arsenic source is likely at the bottom of the lake. The water above the thermocline will continue to increase in concentration until

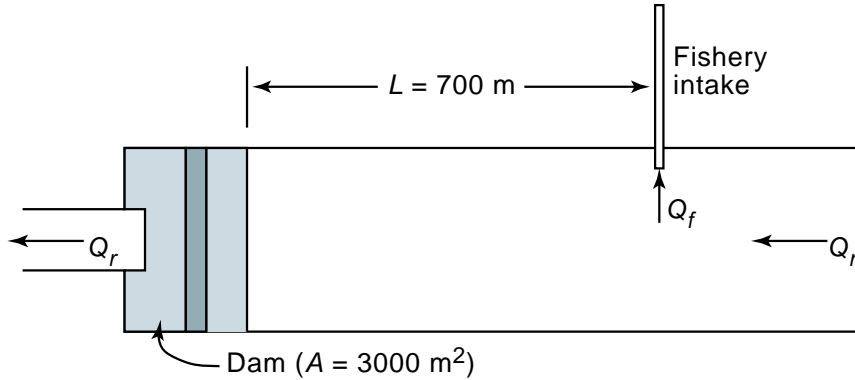


Fig. 2.7. Schematic diagram of the reservoir and fish farm intake for the copper contamination example.

the diffusive flux at the thermocline becomes large enough to balance the advective flux through the lake, at which time the system will reach a steady state.

## 2.4 Application: Fishery intake protection

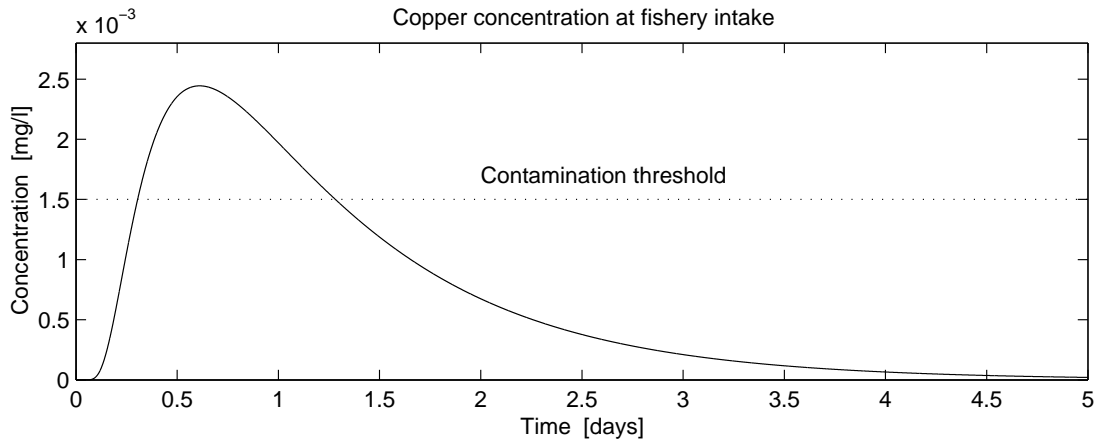
As part of a renovation project, the face of a dam is to be treated with copper sulfate to remove unsightly algae build-up. A fish nursery derives its water from the reservoir upstream of the dam and has contracted you to determine if the project will affect their operations. Based on experience, the fish nursery can accept a maximum copper concentration at their intake of  $1.5 \cdot 10^{-3} \text{ mg/l}$ . Refer to Figure 2.7 for a schematic of the situation.

The copper sulfate is applied uniformly across the dam over a period of about one hour. Thus, we might model the copper contamination as an instantaneous source distributed evenly along the dam face. After talking with the renovation contractor, you determine that 10 kg of copper will be dissolved at the dam face. Because the project is scheduled for the spring turnover in the lake, the contaminant might be assumed to spread evenly in the vertical (dam cross-sectional area  $A = 3000 \text{ m}^2$ ). Based on a previous dye study, the turbulent diffusion coefficient was determined to be  $2 \text{ m}^2/\text{s}$ . The average flow velocity past the fishery intake is  $0.01 \text{ m/s}$ .

*Advection or diffusion dominant.* To evaluate the potential risks, the first step is to see how important diffusion is to the transport of copper in the lake. This is done through the Peclet number, giving

$$\begin{aligned} Pe &= \frac{D}{uL} \\ &= 0.3 \end{aligned} \tag{2.51}$$

which indicates diffusion is mildly important, and the potential for copper to migrate upstream remains.



**Fig. 2.8.** Concentration of copper at the fishery intake as a function of time. The dotted line indicates the maximum allowable concentration of  $1.5 \cdot 10^{-3}$  mg/l.

*Maximum concentration at intake.* Because there is potential that copper will move upstream due to diffusion, the concentration of copper at the intake needs to be predicted. Taking the dam location at  $x = 0$  and taking  $x$  positive downstream, the concentration at the intake is

$$C(x_i, t) = \frac{M}{A\sqrt{4\pi Dt}} \exp\left(-\frac{(x_i - ut)^2}{4Dt}\right). \quad (2.52)$$

where  $x_i$  is the intake location (-700 m). Figure 2.8 shows the solution for the copper concentration at the intake from (2.52). From the figure, the maximum allowable concentration is expected to be exceeded for about 1 day between the times  $t = 0.3$  and  $t = 1.3$  days. The maximum copper concentration at the intake will be about  $2.4 \cdot 10^{-3}$  mg/l. Thus, the fish farm will have to take precautions to prevent contamination. What other factors do you think could increase or decrease the likelihood of copper poisoning at the fish farm?

## Summary

This chapter derived the advective diffusion equation using the method of superposition and demonstrated techniques to solve the resulting partial differential equation. Solutions for a stagnant ambient were shown to be easily modified to account for advection by solving in a moving reference frame. Solutions for distributed and fixed concentration distributions were presented, and the image-source method to account for no-flux boundaries was introduced. Engineering approximations should be made by evaluating the Peclet number and characteristic length and time scales of diffusion and advection.

## Exercises

**2.1** Integral evaluation. Define an appropriate coordinate transformation and show that

$$I = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{4Dt+x^2/\sqrt{Dt}} 2x\sqrt{Dt} \exp\left(-\left(\frac{x^2}{\sqrt{Dt}} + 4Dt\right)^2\right) dx \quad (2.53)$$

can also be written as

$$I = \frac{Dt}{2} \left( \operatorname{erf}\left(\frac{x^2}{\sqrt{Dt}} + 4Dt\right) - 1 \right) \quad (2.54)$$

**2.2** Peclet number. A river with cross section  $A = 20 \text{ m}^2$  has a flow rate of  $Q = 1 \text{ m}^3/\text{s}$ . The effective mixing coefficient is  $D = 1 \text{ m}^2/\text{s}$ . For what distance downstream is diffusion dominant? Where does advection become dominant? What is the length of stream where diffusion and advection have about equal influence?

**2.3** Advection in a stream. To estimate the mixing characteristics of a small stream, a scientist injects 5 g of dye instantaneously and uniformly over the river cross section ( $A = 5 \text{ m}^2$ ) at the point  $x = 0$ . A measurement station is located 1 km downstream and records a river flow rate of  $Q = 0.5 \text{ m}^3/\text{s}$ . In order to design the experiment, the scientist assumed that  $D = 0.1 \text{ m}^2/\text{s}$ . Use this value to answer the following equations.

- The fluorometer used to measure the dye downstream at the measuring station has a detection limit of  $0.1 \mu\text{g}/\text{l}$ . When does the measuring station first detect the dye cloud?
- When does the maximum dye concentration pass the measuring station, and what is this maximum concentration?
- After the maximum concentration passes the measuring station, the measured concentration decreases again. When is the measuring station no longer able to detect the dye?
- Why is the elapsed time between first detection and the maximum concentration different from the elapsed time between the last detection and the maximum concentration?

**2.4** Fixed concentration. A beaker in a laboratory contains a solution with dissolved methane gas ( $\text{CH}_4$ ). The concentration of methane in the atmosphere  $C_a$  is negligible; the concentration of methane in the uniformly-mixed portion of the beaker is  $C_w$ . The methane in the beaker dissolves out of the water and into the air, resulting in a fixed concentration at the water surface of  $C_{ws} = 0$ . Assume this process is limited by diffusion of methane through the water.

- Write an expression for the vertical concentration distribution of methane in the beaker. Assume the bottom boundary does not affect the profile (concentration at the bottom is  $C_w$ ) and that methane is uniformly distributed in the horizontal (use the one-dimensional solution).
- Use the expression found above to find an expression for the flux of methane into the atmosphere through the water surface.

**2.5** Concentration profiles. Figure 2.9 shows four concentration profiles measured very carefully at the bottom of four different lakes. For each profile, state whether the lake bottom is a no-flux or flux boundary and describe where you think the source is located and why.

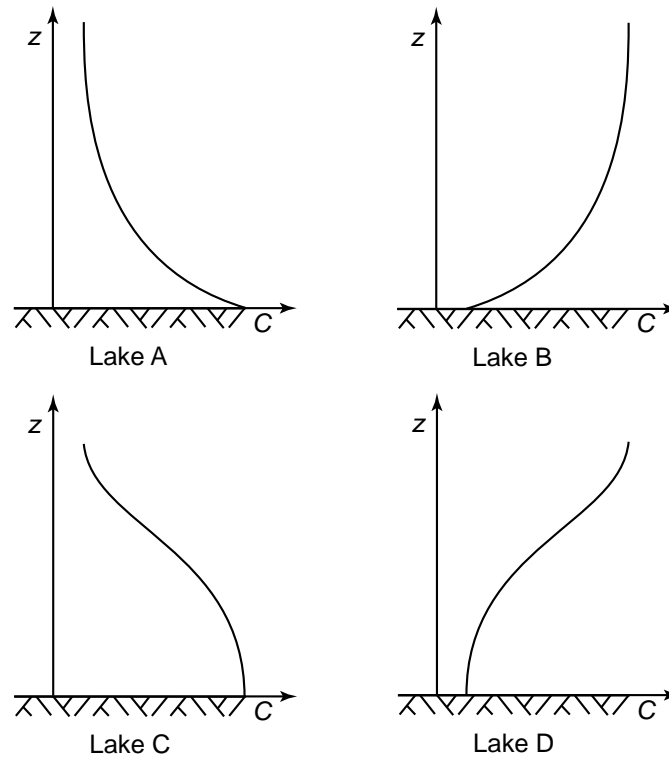


Fig. 2.9. Bottom concentration profiles for the four lakes in problem number 2.4.

**2.6 Double point sources.** To demonstrate the image-source method, a professor creates two instantaneous point sources of dye (three dimensional) a distance  $L$  apart and measures the concentration of dye at the point halfway between the two sources. Estimate the radius of the cloud for each point source by  $r = 2\sigma$ .

- Write an expression for the time  $t$  when the two sources first touch.
- Write an expression for the concentration distribution along the line connecting the two point sources.
- Differentiate this solution to show that the net flux through the measurement point along the axis of the two sources is zero.

**2.7 Smoke stack.** A chemical plant has a smoke stack 75 m tall that discharges a continuous flux of carbon monoxide (CO) of 0.01 kg/s . The wind blows with a velocity of 1 m/s due east (from the west to the east) and the transverse turbulent diffusion coefficient is 4.5 m<sup>2</sup>/s. Neglect longitudinal (downwind) diffusion.

- Write the unbounded solution for a continuous source in a cross wind.
- Add the appropriate image source(s) to account for the no-flux boundary at the ground and write the resulting image-source solution for concentration downstream of the release.
- Plot the two-dimensional concentration distribution downstream of the smoke stack for the plane 2 m above the ground.
- For radial distance  $r$  away from the smoke stack, where do the maximum concentrations occur?



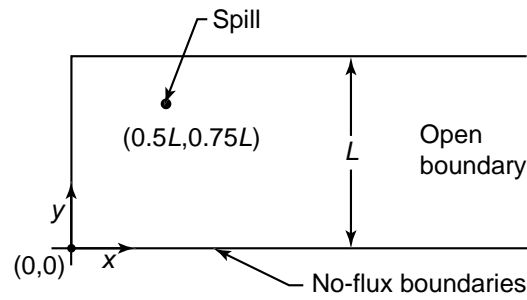


Fig. 2.10. Sketch of the boat arena and spill location for problem number 2.4.

**2.8 Damaged smoke stack.** After a massive flood, the smoke stack in the previous problem developed a leak at ground level so that all the exhaust exits at  $z = 0$ .

- How does this new release location change the location(s) of the image source(s)?
- Plot the maximum concentration at 2 m above the ground as a function of distance from the smoke stack for this damaged case.
- If a CO concentration of  $1.0 \mu\text{g}/\text{l}$  of CO is dangerous, should the factor be closed until repairs are completed?

**2.9 Boundaries in a boat arena.** A boat parked in an arena has a sudden gasoline spill. The arena is enclosed on three sides, and the spill is located as shown in Figure 2.10. Find the locations of the first 11 most important image sources needed to account for the boundaries and incorporate them into the two-dimensional instantaneous point-source solution.

**2.10 Image sources in a pipe.** A point source is released in the center of an infinitely long round pipe. Describe the image source needed to account for the pipe walls.

**2.11 Vertical mixing in a river.** Wastewater from a chemical plant is discharged by a line diffuser perpendicular to the river flow and located at the bottom of the river. The river flow velocity is  $15 \text{ cm/s}$  and the river depth is  $1 \text{ m}$ .

- Find the locations of the first four most important image sources needed to account for the river bottom and the free surface.
- Write a spreadsheet program that computes the ratio of  $C(x, z = h, t = x/u)$  to  $C_{max}(t = x/u)$ , where  $u$  is the flow velocity in the river and  $h$  is the water depth;  $x = z = 0$  at the release location.
- Use the spreadsheet program to find the locations where the concentration ratio is 0.90, 0.95, and 0.98.
- From dimensional analysis we can write that the time needed for the injection to mix in the vertical is given by

$$t_{mix} = \frac{x_{mix}}{u} = \frac{h^2}{\alpha D} \quad (2.55)$$

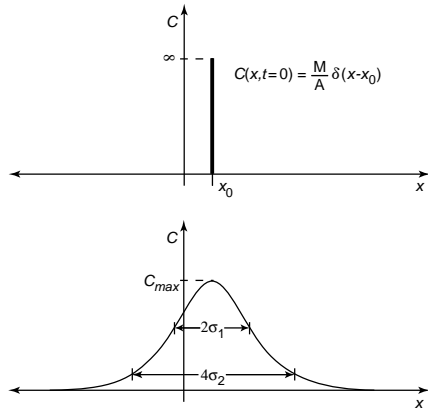
where  $D$  is the vertical diffusion coefficient. Compute the value of  $\alpha$  for the criteria  $C_{min}/C_{max} = 0.95$ .

- Why is the value of  $\alpha$  independent of  $D$ ?

Table 2.1: Table of solutions to the diffusion equation

Schematic and Solution

**Instantaneous point source, infinite domain**



$$C(x, t) = \frac{M}{A\sqrt{4\pi Dt}} \exp\left[-\frac{(x - x_0)^2}{4Dt}\right]$$

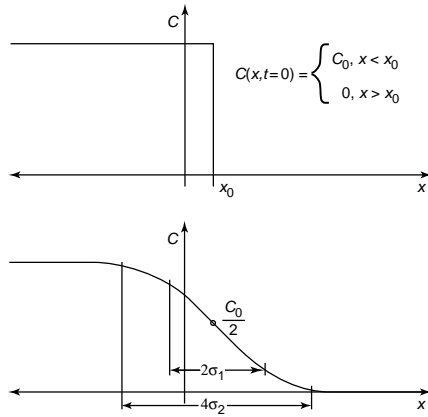
$$C_{max}(t) = \frac{M}{A\sqrt{4\pi Dt}}$$

$$q_x(x, t) = \frac{M(x - x_0)}{2At\sqrt{4\pi Dt}} \exp\left[-\frac{(x - x_0)^2}{4Dt}\right]$$

Let  $\sigma = \sqrt{2Dt}$  and  
 $(2\sigma)^2 = 8Dt$ .  
 For  $x_0 = 0$ :  
 $C(\pm\sigma, t) = 0.61C_{max}(t)$

Let  $\sigma = \sqrt{2Dt}$  and  
 $(4\sigma)^2 = 32Dt$ .  
 For  $x_0 = 0$ :  
 $C(\pm 2\sigma, t) = 0.14C_{max}(t)$

**Instantaneous distributed source, infinite domain**



$$C(x, t) = \frac{C_0}{2} \left[ 1 - \operatorname{erf} \left[ \frac{(x - x_0)}{\sqrt{4Dt}} \right] \right]$$

$$C_{max}(t) = C_0$$

$$q_x(x, t) = \frac{C_0\sqrt{D}}{\sqrt{4\pi t}} \exp\left[-\frac{(x - x_0)^2}{4Dt}\right]$$

Let  $\sigma = \sqrt{2Dt}$  and  
 $(2\sigma)^2 = 8Dt$ .  
 For  $x_0 = 0$ :  
 $C(+\sigma, t) = 0.16C_0$   
 $C(-\sigma, t) = 0.84C_0$

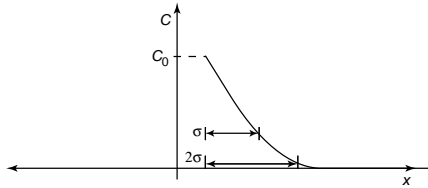
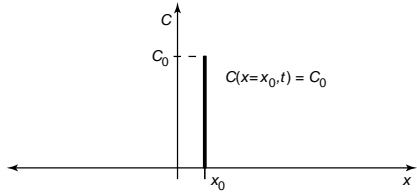
Let  $\sigma = \sqrt{2Dt}$  and  
 $(4\sigma)^2 = 32Dt$ .  
 For  $x_0 = 0$ :  
 $C(+2\sigma, t) = 0.02C_0$   
 $C(-2\sigma, t) = 0.98C_0$

Table 2.1: (continued)

Schematic

Solution

**Fixed concentration, semi-infinite domain**



$$C(x > x_0, t) = C_0 \left[ 1 - \operatorname{erf} \left[ \frac{(x - x_0)}{\sqrt{4Dt}} \right] \right]$$

$$C_{max}(t) = C_0$$

$$q_x(x > x_0, t) = \frac{2C_0\sqrt{D}}{\sqrt{4\pi t}} \exp \left[ -\frac{(x - x_0)^2}{4Dt} \right]$$

Let  $\sigma = \sqrt{2Dt}$  and  $\sigma^2 = 2Dt$ .

For  $x_0 = 0$ :

$$C(+\sigma, t) = 0.32C_0$$

$$C(-\sigma, t) = \text{Undefined}$$

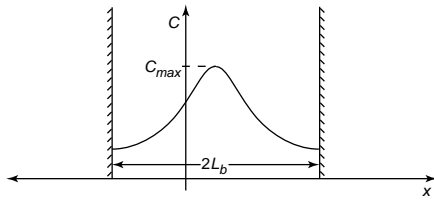
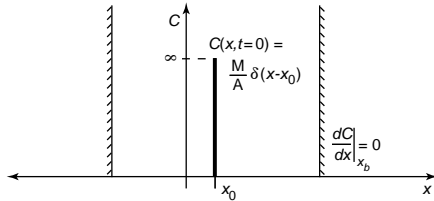
Let  $\sigma = \sqrt{2Dt}$  and  $(2\sigma)^2 = 8Dt$ .

For  $x_0 = 0$ :

$$C(+2\sigma, t) = 0.05C_0$$

$$C(-2\sigma, t) = \text{Undefined}$$

**Instantaneous point source, bounded domain**



$$C(x, t) = \frac{M}{A\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} \exp \left[ -\frac{(x - x_0 + 4nL_b)^2}{4Dt} \right] - \exp \left[ -\frac{(x - x_0 + (4n - 2)L_b)^2}{4Dt} \right]$$

$$C_{max}(t) = \frac{M}{A\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} \exp \left[ -\frac{(4nL_b)^2}{4Dt} \right] - \exp \left[ -\frac{(4n - 2)L_b)^2}{4Dt} \right]$$

$$q_x(x, t) = \frac{M}{2At\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} (x - x_0 + 4nL_b) \exp \left[ -\frac{(x - x_0 + 4nL_b)^2}{4Dt} \right] - (x - x_0 + (4n - 2)L_b) \exp \left[ -\frac{(x - x_0 + (4n - 2)L_b)^2}{4Dt} \right]$$

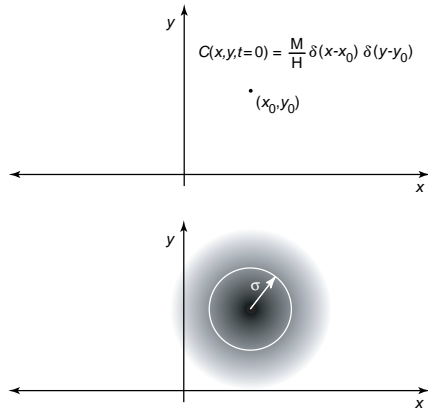
Using the image-source method, the first image on the opposite side of the boundary is at  $x_0 \pm 2L_b$ .

Table 2.1: (continued)

Schematic

Solution

**Instantaneous 2-D point source, infinite domain**



$$C(x, y, t) = \frac{M}{4\pi H t \sqrt{D_x D_y}} \exp \left[ -\frac{(x-x_0)^2}{4D_x t} - \frac{(y-y_0)^2}{4D_y t} \right]$$

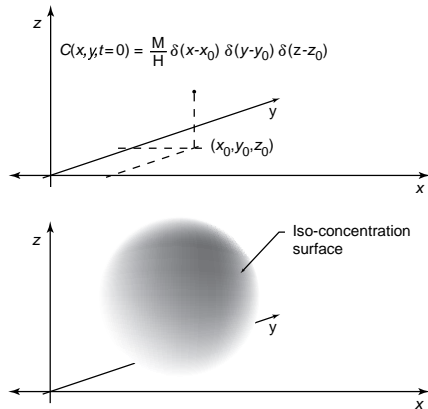
$$C_{max}(t) = \frac{M}{4\pi H t \sqrt{D_x D_y}}$$

$$\mathbf{q}(x, y, t) = \frac{M}{8\pi H t^2 \sqrt{D_x D_y}} \exp \left[ -\frac{(x-x_0)^2}{4D_x t} - \frac{(y-y_0)^2}{4D_y t} \right] ((x-x_0)\mathbf{i} + (y-y_0)\mathbf{j})$$

Let  $D_x = D_y, \sigma = \sqrt{2Dt}$ ,  
 $(2\sigma)^2 = 8Dt$ , and  
 $r^2 = (x-x_0)^2 + (y-y_0)^2$ .  
 For  $r = \sigma$ :  
 $C(\sigma, t) = 0.61C_{max}(t)$

Let  $D_x = D_y$ ,  
 $\sigma = \sqrt{2Dt}$ ,  
 $(4\sigma)^2 = 32Dt$ , and  
 $r^2 = (x-x_0)^2 + (y-y_0)^2$ .  
 For  $r = 2\sigma$ :  
 $C(2\sigma, t) = 0.14C_{max}(t)$

**Instantaneous 3-D point source, infinite domain**



$$C(x, y, z, t) = \frac{M}{4\pi t \sqrt{4\pi t D_x D_y D_z}} \exp \left[ -\frac{(x-x_0)^2}{4D_x t} - \frac{(y-y_0)^2}{4D_y t} - \frac{(z-z_0)^2}{4D_z t} \right]$$

$$C_{max}(t) = \frac{M}{4\pi t \sqrt{4\pi t D_x D_y D_z}}$$

$$\mathbf{q}(x, y, z, t) = \frac{M}{8\pi t^2 \sqrt{4\pi t D_x D_y D_z}} \exp \left[ -\frac{(x-x_0)^2}{4D_x t} - \frac{(y-y_0)^2}{4D_y t} - \frac{(z-z_0)^2}{4D_z t} \right] ((x-x_0)\mathbf{i} + (y-y_0)\mathbf{j} + (z-z_0)\mathbf{k})$$

Let  $D_x = D_y = D_z$ ,  
 $\sigma = \sqrt{2Dt}$ ,  $(2\sigma)^2 = 8Dt$ ,  
 and  
 $r^2 = (x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2$ .  
 For  $r = \sigma$ :  
 $C(\sigma, t) = 0.61C_{max}(t)$

Let  $D_x = D_y = D_z$ ,  
 $\sigma = \sqrt{2Dt}$ ,  
 $(4\sigma)^2 = 32Dt$ , and  
 $r^2 = (x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2$ .  
 For  $r = 2\sigma$ :  
 $C(2\sigma, t) = 0.14C_{max}(t)$