

Chapter 2

DIFFUSION

2.1 The Diffusion Equation

Formulation

As we saw in the previous chapter, the flux of a substance consists of an advective component, due to the mean motion of the carrying fluid, and of a so-called diffusive component, caused by the unresolved random motions of the fluid (molecular agitation and/or turbulence). In this chapter, we explore some consequences of the existence of a diffusive flux by concentrating on cases in which there is no mean flow in the system and thus investigating the effects caused by concentration variations across the system.

The mass balance on an infinitesimal stretch of a one-dimensional system (Figure 2-1 – a river, for example) yields:

$$V \frac{dc}{dt} = \text{Import} - \text{Export} = q(x,t) A - q(x + \Delta x, t) A,$$

where the volume of the element is $V = A\Delta x$, and the Import and Export are simply the flux times the cross-sectional area. The preceding equation can be rewritten as:

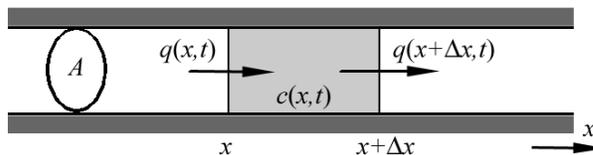


Figure 2-1. Infinitesimal control volume in one dimension.

$$\frac{dc}{dt} = - \frac{q(x + \Delta x, t) - q(x, t)}{\Delta x},$$

and in the limit of an infinitesimally small stretch Δx ,

$$\frac{\partial c}{\partial t} = - \frac{\partial q}{\partial x}. \quad (2.1)$$

(A switch from total to partial derivatives was necessary since at this stage there is more than one independent variables.)

It is important to note that the above equation, being a simple mass balance, is valid regardless of whether the flux q is purely diffusive or contains an advective component. In the absence of a transporting flow ($u = 0$), the substance flux given by (1.4), with j given by (1.5), reduces to:

$$q = - D \frac{\partial c}{\partial x}, \quad (2.2)$$

which is the diffusive flux caused by the unresolved fluctuating motions such as those caused by turbulence. We suppose that the diffusion coefficient D is known. After elimination of q , Equation (2.1) contains the single unknown c :

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right). \quad (2.3)$$

This equation is called the one-dimensional diffusion equation or Fick's second law. It can be solved for the spatially and temporally varying concentration $c(x, t)$ with sufficient initial and boundary conditions.

In general, the diffusion coefficient D may vary with the local condition of turbulence, but an interesting case is, of course, that of a constant D :

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}. \quad (2.4)$$

Initial and boundary conditions

The above diffusion equation is hardly solved in any general way. Each solution depends critically on boundary and initial conditions specific to the problem at hand.

First and foremost, we need to know how many initial and boundary conditions are necessary so that the problem is neither underspecified or overspecified. For this, we determine the order of the problem's governing equation. The time derivative ($\partial c / \partial t$) is of first order and thus calls for a single initial condition (at all x values); typically, the initial concentration distribution is given

$$c = c_0(x) \quad \text{at} \quad t = 0. \quad (2.5)$$

The spatial derivative ($\partial^2 c / \partial x^2$) is of second order and thus calls for two boundary conditions; typically, any problem will include one boundary condition at each end of the domain (say $x = x_1$ and $x = x_2$). While it would be easier from a mathematical perspective to have the end concentrations imposed, for example,

$$c = c_1(t) \quad \text{at} \quad x = x_1 \quad (2.6)$$

$$c = c_2(t) \quad \text{at} \quad x = x_2, \quad (2.7)$$

it is much more typical to encounter flux boundary conditions

$$-D \frac{\partial c}{\partial x} = q_1 \quad \text{at} \quad x = x_1 \quad (2.8)$$

$$-D \frac{\partial c}{\partial x} = q_2 \quad \text{at} \quad x = x_2. \quad (2.9)$$

An impermeable boundary implies no flux and thus no concentration gradient at that boundary. Of course, mixed conditions (e.g., concentration given at one end of the domain and flux specified at the other) are possible.

As a first example showing how a diffusion problem may be solved analytically, we shall now derive the solution to an ideal but most important problem.

Prototypical solution

The diffusion equation is a linear one, and a solution can, therefore, be obtained by adding several other solutions. An elementary solution ('building block') that is particularly useful is the solution to an instantaneous, localized release in an infinite domain initially free of the substance.

Mathematically, the problem is stated as follows:

- Infinite domain: $-\infty < x < +\infty$,
- $D = \text{constant}$,
- No initial concentration, except for the localized release: $c_0(x) = M\delta(x)$ at $t = 0$.
- Since the substance will take an infinite time to reach the infinitely far ends of the domain, we impose:

$$\lim_{x \rightarrow +\infty} c = \lim_{x \rightarrow -\infty} c = 0$$

at finite times ($t < \infty$).

In the above, M is the total mass of the substance released per unit cross-sectional area, and $\delta(x)$ is the Dirac function [$\delta(x) = 0$ for $x \neq 0$, $\delta(x) = +\infty$ at $x = 0$, and area under the infinitely tall and infinitely narrow peak is unity].

Physically, we anticipate a behavior as displayed in Figure 2-2. The pollutant patch gradually spreads on both sides of the release location, with a commensurate decrease in the maximum center value. Curves at later times

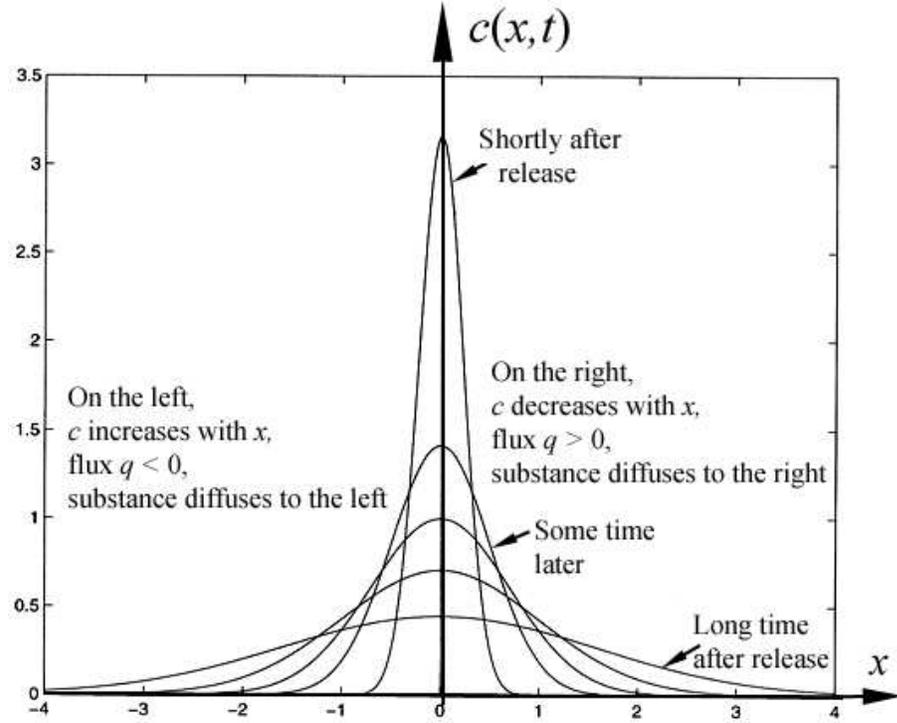


Figure 2-2. Diffusion in time of an initially localized pollutant distribution. While the pollution patch spreads, the maximum concentration decreases, preserving the area under the curve.

appear similar to those at earlier times, only being flatter and wider. Anticipating such similarity in the solution, we write:

$$c(x,t) = t^{-\alpha} F(\eta) \quad \text{with} \quad \eta = \frac{x^2}{4Dt}, \quad (2.10)$$

where $t^{-\alpha}$ (with the dimensionless exponent α expected to be positive) is a ‘size factor’ to represent the temporal decay of the maximum concentration value (at $x = 0$), and where the function $F(\eta)$ is the ‘shape factor’ giving the similar curve profile. This function has a ‘stretched coordinate’ so that the same value $F(\eta)$ is obtained for increasing values of x as time goes on (constant x^2/t). This is to take into account the spreading of the pollutant patch. The exponent 2 of x is an educated guess, to render the functional dependency compatible with the equation at hand. [The choice is rooted in the fact that t appears in the equation as a first-order derivative, while x enters the equation as a second-order derivative.] The factor D in the denominator of η is there to make the ratio dimensionless; η therefore has no units, and its function $F(\eta)$ takes on a universal character. Finally, the factor 4 is introduced for pure mathematical

convenience.

From (2.10), we calculate the derivatives of c needed to solve Equation (2.4):

$$\begin{aligned}\frac{\partial c}{\partial t} &= -\alpha t^{-\alpha-1} F(\eta) + t^{-\alpha} \frac{dF}{d\eta} \frac{\partial \eta}{\partial t} = -\alpha t^{-\alpha-1} F(\eta) - \eta t^{-\alpha-1} \frac{dF}{d\eta} \\ \frac{\partial c}{\partial x} &= t^{-\alpha} \frac{dF}{d\eta} \frac{\partial \eta}{\partial x} = \frac{x t^{-\alpha-1}}{2D} \frac{dF}{d\eta} \\ \frac{\partial^2 c}{\partial x^2} &= \frac{t^{-\alpha-1}}{2D} \frac{dF}{d\eta} + \frac{x t^{-\alpha-1}}{2D} \frac{d^2 F}{d\eta^2} \frac{\partial \eta}{\partial x} = \frac{t^{-\alpha-1}}{2D} \frac{dF}{d\eta} + \frac{t^{-\alpha-1}}{D} \eta \frac{d^2 F}{d\eta^2}.\end{aligned}$$

Then, substitution of $\partial c/\partial t$ and $\partial^2 c/\partial x^2$ in the diffusion equation yields:

$$-\alpha t^{-\alpha-1} F(\eta) - \eta t^{-\alpha-1} \frac{dF}{d\eta} = \frac{1}{2} t^{-\alpha-1} \frac{dF}{d\eta} + \eta t^{-\alpha-1} \frac{d^2 F}{d\eta^2}.$$

The time factors cancel out (thanks to the careful definition of η), and the partial-differential equation is reduced to an ordinary differential equation, with variable η :

$$\eta \frac{d}{d\eta} \left(\frac{dF}{d\eta} + F \right) + \frac{1}{2} \left(\frac{dF}{d\eta} + 2\alpha F \right) = 0. \quad (2.11)$$

Since the exponent α is still free, we will now choose it so that the two groups in the parentheses are identical, *i.e.* $\alpha = 1/2$. A solution is one that obeys

$$\frac{dF}{d\eta} + F(\eta) = 0,$$

which is:

$$F(\eta) = A e^{-\eta},$$

where A is an arbitrary constant of integration.

Putting all the pieces together, we arrive at the following solution:

$$c(x, t) = A t^{-1/2} \exp\left(-\frac{x^2}{4Dt}\right).$$

We note that this solution already meets the boundary conditions (vanishing concentrations far away on both sides). The remaining, initial condition determines the constant of integration. Conservation of the total amount of the substance requires that

$$\int_{-\infty}^{+\infty} c(x, t) dx = \int_{-\infty}^{+\infty} c_0(x) dx = M$$

at all times. Calculations yield $A = M/\sqrt{4\pi D}$, and the final solution is therefore:

$$c(x, t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right). \quad (2.12)$$

Let us now verify not only that the amount of substance is right but also that the initial profile is the peak distribution with $c = 0$ for $x \neq 0$ and $c = \infty$ for $x = 0$. For $x \neq 0$ and fixed, the ratio $x^2/4Dt$ increases toward infinity as t goes to zero, and the exponential goes to zero. Since the exponential function goes to zero faster than $t^{-1/2}$ goes to infinity, the limit is $c \rightarrow 0$ for $t \rightarrow 0$. At $x = 0$, however, $x^2/4Dt = 0$, and the exponential is unity; $c(0, t)$ behaves as $t^{-1/2}$ and goes to infinity as t goes to zero. Thus, expression (2.12) satisfies the original equation, (2.4), meets the boundary and initial conditions, and is therefore the correct solution to the stated problem. A graphical representation is shown in Figure 2-2.

We shall now demystify this solution by deriving it from a totally different angle, the random-walk process.

2.2 Random-Walk Model

Random-walk process

In one of his celebrated papers of 1905, Albert Einstein showed that a random-walk process representing Brownian motion in a gas was mathematically equivalent to Fickian diffusion¹. Here, we present a very simplified form of this analogy between diffusion and random walk.

Take a one-dimensional domain (1D axis), divide it in a series of boxes of identical lengths ('bins'), and place one particle in one of the bins (Figure 2-3). Imagine now that this particle is endowed with a mechanism that makes it jump randomly every time interval, Δt , according to the following rules:

- there is a 25% chance that the particle will hop one bin to the left,
- there is a 25% chance that it will hop one bin to the right, and
- there is a 50% chance that it will remain in the same bin.

[This is the 1D version of the more general 2D random walk, commonly referred to as the drunkard's path: Late into the night, an inebriated fellow leaves a bar and has no recollection of where he is and where he is going; every second or so, he makes a step forward, backward (he turns completely around), leftward or rightward, making a random path that may look like that displayed on Figure 2-4. The question is: Where is this drunkard expected to be after m steps?]

Because of the random nature of the problem, the answer can only be in terms of probabilities. We thus define

$$p(n\Delta x, m\Delta t)$$

¹The 1905 paper in German was later translated into English in book form: Einstein, A., *Investigations on the Theory of Brownian Movement*, Dover Publications, 1956, 122 pages.

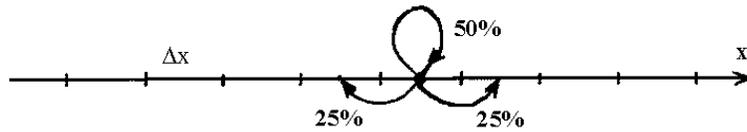


Figure 2-3. One-dimensional random walk. Percentages refer to the probabilities that the particle will move as depicted by the corresponding arrows. The repetition of this process obeys the same law as one-dimensional diffusion but in a discretized way.

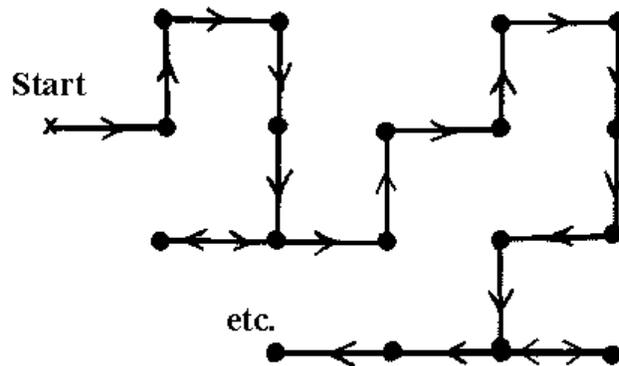


Figure 2-4. Two-dimensional random walk, also called the drunkard's path.

as the probability that the particle is in bin number n at time $t = m\Delta t$. We can calculate the probability at one time step based on the previous time step: At time $(m + 1)\Delta t$, the probability that the particle is in bin n is equal to the probability that it was already there times the probability that it stayed there, plus the probability that it was one bin to the left times the probability that it jumped to the right, plus the probability that it was one bin to the right times the probability that it jumped to the left. Mathematically, we have:

$$\begin{aligned} p[n\Delta x, (m + 1)\Delta t] &= \frac{1}{2} p(n\Delta x, m\Delta t) \\ &+ \frac{1}{4} p[(n - 1)\Delta x, m\Delta t] \\ &+ \frac{1}{4} p[(n + 1)\Delta x, m\Delta t]. \end{aligned} \quad (2.13)$$

Given the location of the particle at the initial time, say $n = 0$, the solution can be found by iterations from

$$p(0, 0) = 1 \quad , \quad p(n\Delta x, 0) = 0 \quad \text{for } n \neq 0.$$

Relation of random walk to diffusion equation

The connection with the diffusion equation is made when we take the limit of the random-walk process to infinitesimally small bin sizes and time steps (Δx and Δt both vanishingly small). For small incremental values of its argument, the probability function can be approximated using a Taylor expansion:

$$\begin{aligned} p[(n \pm 1)\Delta x, m\Delta t] &= p(n\Delta x, m\Delta t) \pm \Delta x \frac{\partial p}{\partial x} + \frac{1}{2} \Delta x^2 \frac{\partial^2 p}{\partial x^2} \\ &\pm \frac{1}{6} \Delta x^3 \frac{\partial^3 p}{\partial x^3} + O(\Delta x^4) \\ p[n\Delta x, (m + 1)\Delta t] &= p(n\Delta x, m\Delta t) + \Delta t \frac{\partial p}{\partial t} + O(\Delta t^2), \end{aligned}$$

where all the derivatives are taken at $(x = n\Delta x, t = m\Delta t)$, and equation (2.13) becomes

$$\begin{aligned} p(x, t) + \Delta t \frac{\partial p}{\partial t} + O(\Delta t^2) &= \frac{1}{2} p(x, t) \\ &+ \frac{1}{4} \left[p(x, t) - \Delta x \frac{\partial p}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 p}{\partial x^2} - \frac{\Delta x^3}{6} \frac{\partial^3 p}{\partial x^3} + O(\Delta x^4) \right] \\ &+ \frac{1}{4} \left[p(x, t) + \Delta x \frac{\partial p}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 p}{\partial x^2} + \frac{\Delta x^3}{6} \frac{\partial^3 p}{\partial x^3} + O(\Delta x^4) \right]. \end{aligned}$$

Mathematical simplifications then yield

$$\Delta t \frac{\partial p}{\partial t} = \frac{\Delta x^2}{4} \frac{\partial^2 p}{\partial x^2} + O(\Delta t^2, \Delta x^4).$$

Finally, a division by Δt makes the equation similar to a diffusion equation:

$$\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2} + O\left(\Delta t, \frac{\Delta x^4}{\Delta t}\right),$$

where the ‘diffusivity’, D , is defined by

$$D = \frac{\Delta x^2}{4\Delta t}. \quad (2.14)$$

In order that this coefficient be finite in the limit of vanishing Δx and Δt it is necessary that Δt goes to zero at the same pace as Δx^2 (i.e. halving the bin size requires dividing the time step by four). Now, if $\Delta x^2/\Delta t$ remains finite, the error on the order of $\Delta x^4/\Delta t$ goes to zero in the limit, and the equation for the continuous probability-distribution function $p(x, t)$ obeys exactly the diffusion equation, (2.4).

The conclusion is that diffusion and random walk (in the continuous limit) are two processes that share the same mathematical representation. Therefore, the solution or intuition obtained from one problem can be helpful in understanding or predicting the behavior of the other.

Numerical verification of random walk

We now present a numerical example to have an idea of how well the discrete random-walk process mimics continuous diffusion. Instead of performing a larger number of realizations with random numbers, let us go directly for the expected values by using (2.10) recursively. The result is shown in the table below (where an empty space indicates a zero probability there).

$n =$	-5	-4	-3	-2	-1	0	+1	+2	+3	+4	+5
$m=0$						1.000					
$m=1$					0.250	0.500	0.250				
$m=2$				0.063	0.250	0.375	0.250	0.063			
$m=3$			0.016	0.094	0.234	0.313	0.234	0.094	0.016		
$m=4$		0.004	0.031	0.109	0.219	0.273	0.219	0.109	0.031	0.004	
$m=5$	0.0010	0.010	0.044	0.117	0.205	0.246	0.205	0.117	0.044	0.010	0.0010
$m=6$	0.0029	0.016	0.054	0.121	0.193	0.226	0.193	0.121	0.054	0.016	0.0029

To compare with the continuous solution (2.12), we map p onto c and write

$$\begin{aligned} p(n\Delta x, m\Delta t) &= p(x, t) = \frac{P}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \\ &= \frac{P}{\Delta x \sqrt{\pi m}} \exp\left(-\frac{n^2}{m}\right), \end{aligned}$$

where x , t and D have been replaced respectively by $n\Delta x$, $m\Delta t$ and $\Delta x^2/4\Delta t$.

To set a value to the factor $P/\Delta x$, we choose to match the number of particles in the central bin ($n = 0$) at the last time level ($m = 5$) and obtain

$$p(n, m) = 0.246 \sqrt{\frac{5}{m}} \exp\left(-\frac{n^2}{m}\right).$$

The table constructed with these estimates from the continuous solution is:

$n =$	-5	-4	-3	-2	-1	0	+1	+2	+3	+4	+5
$m=0$						∞					
$m=1$				0.010	0.202	0.550	0.202	0.010			
$m=2$			0.004	0.053	0.236	0.389	0.236	0.053	0.004		
$m=3$		0.002	0.016	0.084	0.228	0.318	0.228	0.084	0.016	0.002	
$m=4$	0.0005	0.005	0.029	0.101	0.214	0.275	0.214	0.101	0.029	0.005	0.0005
$m=5$	0.0017	0.010	0.041	0.111	0.201	0.246	0.201	0.111	0.041	0.010	0.0017
$m=6$	0.0035	0.016	0.050	0.115	0.190	0.225	0.190	0.115	0.050	0.016	0.0035

The poor fit at the early time levels is naturally a consequence of the gross mismatch between values in a few discrete places, on one hand, and a continuous distribution, on the other. The quality of the fit improves as the distribution spreads in time. Thus, the discrete, random-walk process provides an adequate representation of the diffusive process if the spread is sufficiently wide (say, over 10 or more bins).

Suggested exercises:

1. Verify the temporal decay of the maximum value at $n = 0$ as m increases beyond 5.
2. Using a personal computer, generate a random number between 0 and 1 for each particle at every time level; if that number falls below 0.25 move the particle to the left, above 0.75 move the particle to the right and, otherwise, leave the particle where it is. Make a large number of runs and average the results over all runs. Compare with the values presented in the first of the two tables above.

2.3 A Graphical Iteration

Curve smoothing

The graphical method described below was actually used to solve the diffusion equation before computers existed.

A curve $c(x)$ is given graphically as a succession of points, Δx apart, in the (x, c) plane (heavy dots in Figure 2-5), and line segments connecting adjacent points approximate the curve (solid line). The following graphical constructions are then made:

1. Join the midpoints of adjacent line segments (dashed lines),

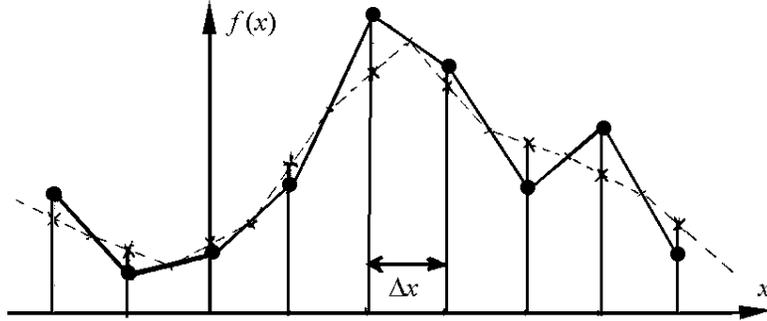


Figure 2-5. A graphical smoothing operation. By joining centers of curve segments, a new and smoother curve is obtained. The repetition of this operation mimics diffusion and forms a method to solve iteratively the one-dimensional diffusion equation.

2. At each location, move the function value to the level of the dashed line (crosses),

3. Repeat these steps again and again.

The obvious result of this manipulation is the cutting of spikes, filling of valleys, and overall smoothing of the curve (Figure 2-5).

Mathematically, we have replaced the local value $c(x)$ by a new value that is halfway between the values at the segment midpoints, the values at the segment midpoints being themselves halfway between adjacent values of c . Thus,

$$\begin{aligned} \text{new } c(x) &= \frac{1}{2} \left[\frac{c(x - \Delta x) + c(x)}{2} + \frac{c(x) + c(x + \Delta x)}{2} \right] \\ &= \frac{1}{4} [c(x - \Delta x) + 2c(x) + c(x + \Delta x)]. \end{aligned} \quad (2.15)$$

In other words, we have performed a running $(\frac{1}{4}, \frac{1}{2}, \frac{1}{4})$ average.

Comparison with diffusion and random walk

Since the values $(\frac{1}{4}, \frac{1}{2}, \frac{1}{4})$ are none other than (25%, 50%, 25%), we note the immediate analogy between the preceding graphical iteration and the random-walk process. Mathematically, Equations (2.13) and (2.15) are isomorphic, and the graphical iteration accomplishes the same process as the one-dimensional random walk. And, since the random walk is analogous to diffusion, so is the graphical iteration.

What we gain by introducing the above graphical procedure is the intuition that diffusion is essentially a smoothing process: No matter what the initial concentration distribution might be, diffusion will always act to smooth it and to make it ultimately uniform.

To complete the analogy, it is noteworthy to discretize the continuous diffusion equation, as it is done in preparation to being solved on the computer. This is to do in reverse what we did to turn the discrete random walk into a continuous process. Using Taylor expansions, we write

$$\begin{aligned}\frac{\partial c}{\partial t} &\simeq \frac{c(x, t + \Delta t) - c(x, t)}{\Delta t} \\ \frac{\partial^2 c}{\partial x^2} &\simeq \frac{1}{\Delta x} \left[\frac{c(x + \Delta x, t) - c(x, t)}{\Delta x} - \frac{c(x, t) - c(x - \Delta x, t)}{\Delta x} \right] \\ &\simeq \frac{c(x + \Delta x, t) - 2c(x, t) + c(x - \Delta x, t)}{\Delta x^2}\end{aligned}$$

and the diffusion equation $\partial c / \partial t = D \partial^2 c / \partial x^2$ is turned into

$$\frac{1}{\Delta t} [c(x, t + \Delta t) - c(x, t)] = \frac{D}{\Delta x^2} [c(x + \Delta x, t) - 2c(x, t) + c(x - \Delta x, t)].$$

Solving for the new value of c at position x , we have

$$c(x, t + \Delta t) = \left(1 - \frac{2D\Delta t}{\Delta x^2}\right) c(x, t) + \frac{D\Delta t}{\Delta x^2} [c(x + \Delta x, t) + c(x - \Delta x, t)]. \quad (2.16)$$

Comparing this update with (2.15) resulting from the graphical iteration, we note that both schemes are one and the same for $D\Delta t / \Delta x^2 = 1/4$. In other words, the graphical procedure accomplishes the numerical integration with time step set to

$$\Delta t = \frac{\Delta x^2}{4D}. \quad (2.17)$$

Note that the time step provided by (2.17) is in the same relation to the grid size and diffusivity as in (2.14).

To recapitulate, we conclude that the processes of diffusion, random walk and graphical smoothing are analogous. All three represent a process that is characterized by down-gradient propagation, spreading and smoothing over time. Further, they share identical mathematical representations, either continuous or discrete.

2.4 Spreading

Spreading induced by diffusion implies that the spatial extent of contamination grows with time. For practical purposes, we wish therefore to quantify this spreading, namely to have an answer to the question: How large is the zone affected by the contaminant?

Patch width

We easily conceive that the quantity that tells us how wide is a diffusing patch of contamination should be a function of time. However, what should be its precise definition is not trivial. Indeed, the prototypical solution

$$c(x, t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

does exhibit spreading over time but does not yield a specific width: c is nonzero all the way to infinity, starting immediately after the moment of release². Therefore, looking for the edges of the concentration distribution does not provide a value for the patch width.

To obtain a practical value for the width of a pollutant patch, we then resort to integral quantities. Let us explore a few of them. A first integral is

$$\int_{-\infty}^{+\infty} c \, dx = M = \text{constant},$$

giving the total amount of substance. This, obviously, tells nothing about the width of the patch. A second integral is formed by inserting the coordinate x , to inject the notion of distance,

$$\int_{-\infty}^{+\infty} xc \, dx = 0,$$

which vanishes by symmetry. This tells us where the mean position, \bar{x} , of the patch is ($\bar{x} = 0$ for this solution) but still nothing about the width. A third integral is

$$\int_{-\infty}^{+\infty} (x - \bar{x})^2 c \, dx,$$

which is a function of time, positive and nonzero. Because $(x - \bar{x})^2$ represents the squared distance to the mean position, the above integral says something about the average distance to the center of the patch and therefore holds information about the patch width. The time evolution of this width should then provide information about the rate of spreading.

For convenience, we define the normalized quantity

$$\sigma^2 = \frac{1}{M} \int_{-\infty}^{+\infty} (x - \bar{x})^2 c \, dx, \quad (2.18)$$

in which, in general, M and \bar{x} are defined as:

$$M = \int_{-\infty}^{+\infty} c \, dx, \quad \bar{x} = \frac{1}{M} \int_{-\infty}^{+\infty} xc \, dx.$$

By definition, σ has the dimension of a length, and this length can then be interpreted as proportional to the patch width.

²This instantaneous infinitely wide effect is obviously unrealistic and is attributed to the mathematical simplification of a continuum medium.

For the prototypical solution recalled above, calculations yield

$$\begin{aligned}\sigma^2 &= \frac{1}{M} \int_{-\infty}^{+\infty} x^2 \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) dx \\ &= \frac{4Dt}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \left(\frac{x}{\sqrt{4Dt}}\right)^2 \exp\left[-\left(\frac{x}{\sqrt{4Dt}}\right)^2\right] d\left(\frac{x}{\sqrt{4Dt}}\right) \\ &= \frac{4Dt}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \zeta^2 \exp(-\zeta^2) d\zeta,\end{aligned}$$

noting $\zeta = x/\sqrt{4Dt}$. The last integral contains no parameter and thus assumes a universal value, found to be $\sqrt{\pi}/2$. The result is

$$\sigma^2 = 2Dt$$

or

$$\sigma = \sqrt{2Dt}. \quad (2.19)$$

We immediately note that the distance σ grows in time, but as the square root of time rather than time itself. Thus, the spreading goes on with time, never stopping but gradually slowing down. The curve σ -versus- t is displayed in Figure 2-6.

The next question is by which numerical factor (such as 4, 1/2, or whatever) should σ be multiplied to yield a practical definition of the patch width. The $c(x, t)$ distribution at any given time obeys the so-called Gaussian (or ‘bell’) curve (Figure 2-7). Normalizing distance x by σ and concentration c by its maximum, central value $c_{\max} = M/\sqrt{4\pi Dt}$, the function becomes

$$\frac{c}{c_{\max}} = \exp\left[-\frac{1}{2}\left(\frac{x}{\sigma}\right)^2\right],$$

which contains no parameter. Graphically, the curve is universal (Figure 2-7).

A property of this function³ is that 95% of the area under the curve lies in the interval $-1.96 < (x/\sigma) < +1.96$, leaving 2.5% of the area under each tail. Rounding the value 1.96 to 2.00, we conclude that the interval $-2\sigma < x < +2\sigma$ contains 95% of the pollutant. This appears to be a practical criterion, and we adopt the length of this interval, 4σ , as the width of the patch:

$$\text{Width} = 4\sigma = 4\sqrt{2Dt} = 5.66\sqrt{Dt}. \quad (2.20)$$

Important remark

In some rare instances, when the pollutant is very toxic and small doses can be fatal, it is not as important to track the bulk of the pollutant as to

³See books on probability and statistics.

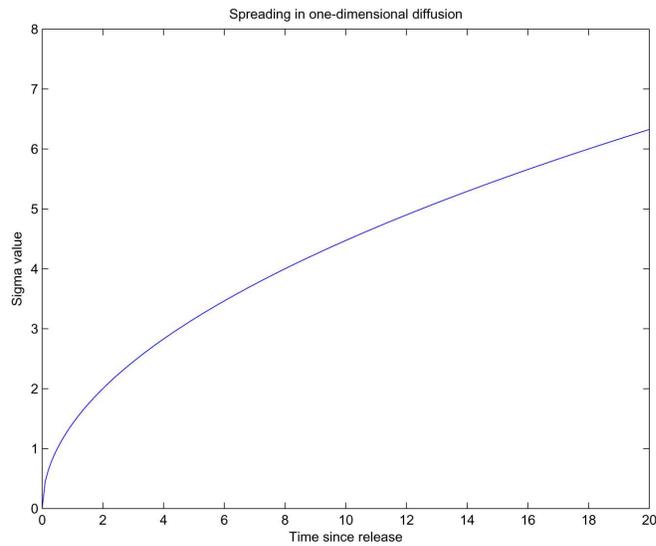


Figure 2-6. Curve σ versus time, showing continuous growth but at a decreasing rate. The width of a diffusing patch of pollutant is proportional to σ .

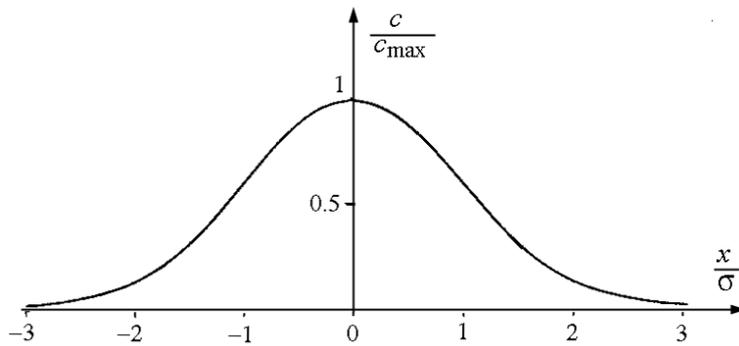


Figure 2-7. The universal ‘bell’ curve, also called Gaussian function. It provides the 1D concentration distribution following an instantaneous and localized release, after proper scaling of both concentration and distance.

pay attention to the edges of the patch. Discarding the 2.5% on each side may not be acceptable. Precaution would dictate taking a more conservative approach, such as choosing a width of 6σ (leaving 0.13% on each side). Better, one should use a random-walk model and follow in time the precise edge of the distribution.

Comparison with edge of random walk

In the random-walk process, nonzero probabilities invade new cells at the rate of one new cell on each side at every time step. This implies a linear growth in time: 1 cell at $t = 0$, 3 cells at $t = \Delta t$, 5 cells at $t = 2\Delta t$, and so on, with the result at time $t = m\Delta t$

$$\begin{aligned} \text{width} &= \text{width of } (2m + 1) \text{ cells} \\ &= (2m + 1)\Delta x \\ &\simeq 2m\Delta x = 2 \frac{\Delta x}{\Delta t} t, \end{aligned}$$

for large values of m . This implies a widening of the patch as the first power of time rather than the slower $t^{1/2}$ rate derived above. How do we reconcile both results?

The resolution lies in considering the values at the edges. Recalling the first table in Section 2-2, we note that, yes, the width increases linearly with time, but that the end values become gradually smaller. The bulk of the particles remain around the center, spreading outward at a weaker rate, essentially because the random aspect of the motion returns some particles toward the center as much as it sends others outward. There are thus two rates of spreading:

1. spreading of the bulk of the pollutant: width = $4\sigma = 4\sqrt{2Dt}$,
2. propagation of the edge particles: width = $(2\Delta x/\Delta t)t$.

The former is slower, while the latter is faster.

When dealing with very toxic substances, the tracking of the edge particles is what is important. One should then determine the appropriate value of the coefficient $2\Delta x/\Delta t$ to place in front of t to determine the width. [Here, be precise by noting that the distance from the release location is only half of that, $(\Delta x/\Delta t)t$.] In reality, one does not have Δx and Δt values with which to work, but a simple consideration shows that the ratio $\Delta x/\Delta t$ is a velocity, which is none other than the exchange velocity u' introduced in Section 1-2. In a turbulent fluid, this velocity is the average eddy orbital velocity u_* , which can generally be estimated from a knowledge of the intensity of the turbulence in the fluid. More on this point will be found in later chapters.

Example

A tank aboard a barge traveling along the Chicago Ship Canal suddenly collapses, releasing its benzene content (C_6H_6 , density = 0.879 g/cm^3), of which

100 liters find their way quickly to the water. The rest of the benzene remains contained on the barge. Assuming rapid mixing across the canal section (8.07 m deep and 48.8 m wide) and estimating the turbulent diffusion coefficient at $3.0 \text{ m}^2/\text{s}$, what are the concentrations of benzene 2, 6, 12 and 24 hours after the accident, at the site of the spill and 300 m away?

To solve this problem, we first determine the mass of benzene that was spilled. Since the density of benzene is $0.879 \text{ g/cm}^3 = 0.879 \text{ kg/L}$, this mass m is:

$$m = \text{density} \times \text{volume} = 0.879 \text{ kg/L} \times 100 \text{ L} = 87.9 \text{ kg}.$$

Over the cross-section of the canal, we have

$$M = \frac{m}{\text{cross-sectional area}} = \frac{87.9 \text{ kg}}{393.8 \text{ m}^2} = 0.2232 \text{ kg/m}^2.$$

The concentration over time is given by (2.12), which yields at the site of the spill ($x = 0$):

$$c = \frac{M}{\sqrt{4\pi Dt}} = \frac{0.0364 \text{ kg/m}^3}{\sqrt{t(\text{in sec})}} = \frac{0.606 \text{ mg/L}}{\sqrt{t(\text{in hrs})}}.$$

After 2, 6, 12 and 24 hours, the concentration values are, respectively, 0.428, 0.247, 0.175 and 0.124 mg/L. At the distance of 300 m ($x = 300 \text{ m}$), we have:

$$\frac{x^2}{4Dt} = \frac{7,500}{t(\text{in sec})} = \frac{2.083}{t(\text{in hrs})},$$

and the concentrations are:

$$c(2 \text{ hours}) = (0.428 \text{ mg/L}) \exp\left(\frac{-2.083}{2}\right) = 0.151 \text{ mg/L},$$

$$c(6 \text{ hours}) = (0.247 \text{ mg/L}) \exp\left(\frac{-2.083}{6}\right) = 0.175 \text{ mg/L},$$

$$c(12 \text{ hours}) = (0.175 \text{ mg/L}) \exp\left(\frac{-2.083}{12}\right) = 0.147 \text{ mg/L},$$

$$c(24 \text{ hours}) = (0.124 \text{ mg/L}) \exp\left(\frac{-2.083}{24}\right) = 0.113 \text{ mg/L}.$$

Note how the concentration at 300 m first increases (because it takes time for the benzene to diffuse over that distance) and then decreases (because further diffusion leads to dilution). We can actually calculate the exact time at which the concentration reaches its maximum and what that maximum is. Setting to zero the time derivative of solution (2.12), we obtain the time t_{\max} of the maximum concentration for any distance x from the release location:

$$t_{\max} = \frac{x^2}{2D}. \quad (2.21)$$

Substitution in the solution then yields the maximum concentration:

$$c_{\max} = \frac{M}{\sqrt{2\pi x}} \exp\left(-\frac{1}{2}\right) = 0.2420 \frac{M}{x}. \quad (2.22)$$

For $M=0.2232$ kg/m² and $x=300$ m, the values are:

$$c_{\max} = 0.180 \text{ mg/L} \quad \text{at} \quad t_{\max} = 4 \text{ hrs } 10 \text{ min.}$$

2.5 Problems with Other Conditions

Initial release over a finite area

This problem can be solved by superposition of many prototypical solutions. If a localized release occurs not at $x = 0$ but at $x = \xi$, then the solution is simply shifted by the distance ξ :

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

The difference $(x - \xi)$ represents the distance to the point of release. The quantity M is also made a function of ξ because we shall now consider a series of releases at various ξ locations and of various amounts.

If there are two releases, one of magnitude $M(\xi_1)$ at ξ_1 and one of magnitude $M(\xi_2)$ at ξ_2 , both at time $t = 0$, then the concentration distribution is:

$$c(x, t) = \frac{M(\xi_1)}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x - \xi_1)^2}{4Dt}\right] + \frac{M(\xi_2)}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x - \xi_2)^2}{4Dt}\right].$$

The generalization to three and more punctual releases is straightforward. For a continuous release, we add an infinite number of tiny releases collectively covering a finite interval. If the release in the $[\xi, \xi + d\xi]$ interval is $dM(\xi) = c_0(\xi)d\xi$, then

$$c(x, t) = \int_{-\infty}^{+\infty} \frac{c_0(\xi)}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x - \xi)^2}{4Dt}\right] d\xi. \quad (2.23)$$

The function $c_0(\xi)$ is none other than the initial concentration⁴. It is taken as zero wherever there is no release.

The preceding form of superposition is called *convolution*. In short, convolution accomplishes a transformation on a function using another intermediary

⁴The reader can verify this assertion by considering its dimensions or by returning to the definition of the quantity M .

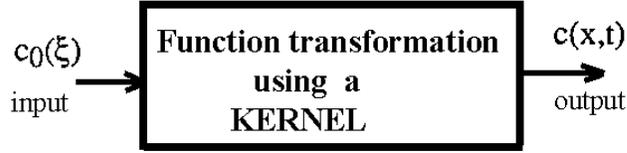


Figure 2-8. Diagram illustrating the convolution process: A tool function, called kernel, is used to transform an original function into another one. In the case of diffusion, the input function is the initial concentration distribution, and the output is the concentration distribution at any later time.

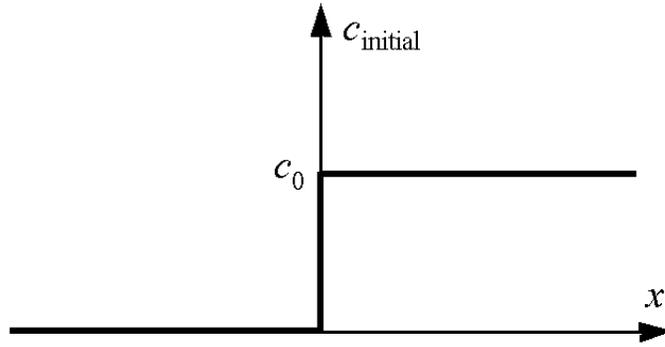


Figure 2-9. Initial condition corresponding to a uniform release over one side of an infinite domain.

function, called a kernel or Green's function (Figure 2-8). In our present case, the kernel is:

$$\frac{1}{\sqrt{4\pi Dt}} \exp \left[-\frac{(x - \xi)^2}{4Dt} \right],$$

representing the unit prototypical solution in a shifted form.

Consider now the problem corresponding to the initial condition shown on Figure 2-9. The release is nil for negative values of the coordinate and uniform of concentration c_0 , for positive values of the coordinate. From (2.23), the solution follows:

$$c(x, t) = \int_0^{\infty} \frac{c_0}{\sqrt{4\pi Dt}} \exp \left[-\frac{(x - \xi)^2}{4Dt} \right] d\xi.$$

Using the variable $\zeta = (x - \xi)/\sqrt{4Dt}$ with $d\zeta = -d\xi/\sqrt{4Dt}$, the preceding integral takes a more universal form:

$$c(x, t) = \frac{c_0}{\sqrt{\pi}} \int_{-\infty}^{x/\sqrt{4Dt}} \exp(-\zeta^2) d\zeta.$$

The remaining integral cannot be expressed in terms of elementary functions and must be tabulated. Because a number of problems in statistics involve a similar integral, it has become traditional to define the function

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\zeta^2) d\zeta, \quad (2.24)$$

which represents twice the area under the bell curve, starting at the middle. It is called the *error function*. Some properties of this function are:

$$\operatorname{erf}(0) = 0, \quad \operatorname{erf}(+\infty) = +1.$$

$$\operatorname{erf}(-z) = -\operatorname{erf}(z).$$

Other numerical values are tabulated below (Table 2-1).

$\frac{x}{\sigma}$	$\operatorname{erf} \frac{x}{\sigma}$
0.0	0.0
0.1	0.1129
0.2	0.2227
0.3	0.3286
0.4	0.4284
0.5	0.5205
0.6	0.6309
0.7	0.6778
0.8	0.7421
0.9	0.7969
1.0	0.8427
1.2	0.9103
1.4	0.9523
1.6	0.9763
1.8	0.9891
2.0	0.9953
2.5	0.9996
3.0	$1-2.32 \cdot 10^{-5}$
3.5	$1-7.71 \cdot 10^{-7}$
4.0	$1-1.59 \cdot 10^{-8}$
5.0	$1-1.57 \cdot 10^{-12}$
6.0	$1-2.18 \cdot 10^{-17}$
7.0	$1-2.10 \cdot 10^{-45}$
∞	1.0000

Table 2-1. Values of the error function.

Using (2.24), our solution finally takes the form

$$c(x, t) = \frac{c_0}{2} \left[1 + \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right], \quad (2.25)$$

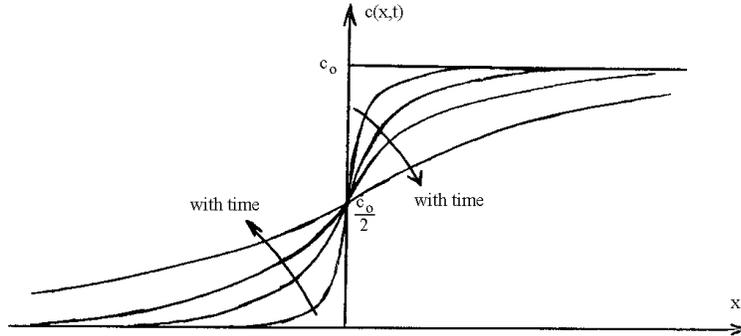


Figure 2-10. Gradual spreading of an initially one-sided release (depicted in Figure 2-9). The curves are obtained from solution (2.25).

in the case of a semi-infinite, uniform release. Graphically, concentration profiles take the aspect of a step that is gradually eroded (Figure 2-10). Physically, the pollutant spreads over the initially clean area, while on the dirty side its concentration falls gradually. After an infinitely long time, a uniform concentration equal to the average $c_0/2$ is reached.

Constant concentration specified at a fixed location

As a second application, consider the case where the concentration at a fixed location is maintained constant over time, starting at some initial time $t = 0$. Our initial and boundary conditions are then:

$$c = 0 \quad \text{at} \quad t = 0$$

$$c = c_0 \quad \text{at} \quad x = 0,$$

and we need to consider only half of the space ($x > 0$), the other half being symmetric.

Recalling our similar solution in section 2-1, we write

$$c(x, t) = t^{-\alpha} F(\eta) \quad \text{with} \quad \eta = \frac{x^2}{4Dt}.$$

At $x = 0$, η vanishes, and the function F takes the value $F(0)$, a constant. Since c must be a constant there, we must now choose $\alpha = 0$. The F equation (2.8) then becomes

$$\eta \frac{d^2 F}{d\eta^2} + \left(\eta + \frac{1}{2} \right) \frac{dF}{d\eta} = 0.$$

This can be integrated once to yield

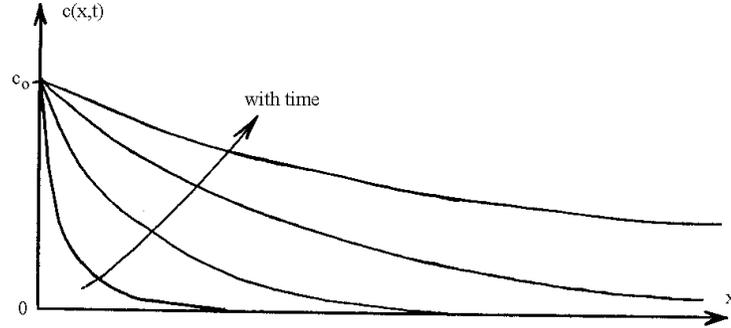


Figure 2-11. Gradual spreading away from a point where the concentration is maintained constant over time, according to solution (2.26).

$$\frac{dF}{d\eta} = \frac{A}{\sqrt{\eta}} e^{-\eta},$$

where A is a constant of integration. A second integration involves the error function:

$$F(\eta) = A \sqrt{\pi} \operatorname{erf}(\sqrt{\eta}) + B,$$

where B is another constant of integration. Imposing the initial and boundary conditions stated above yields the values of the constants, and the solution becomes:

$$c(x,t) = c_0 \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right]. \quad (2.26)$$

[Exercise: Check the limits $x \rightarrow 0$, $x \rightarrow \infty$, $t \rightarrow 0$, $t \rightarrow \infty$.]

Physically, the concentration rises in the vicinity of the dirty spot, gradually contaminating the entire domain (Figure 2-11). The concentration, however, never exceeds the value specified at the boundary.

Example

As an example, consider again the Chicago Ship Canal in the following situation. A side pipeline has suddenly developed a leak of benzene, which locally maintains the concentration of benzene in water at 0.020 mg/L. What is the extent of the patch over which the benzene concentration exceeds the drinking-water standard of 0.005 mg/L? Assume again thorough mixing across the canal cross-section and neglect benzene decay under bacterial action.

The solution to this problem proceeds by application of (2.26) in reverse: Given the concentration value $c=0.020$ mg/L, we determine the distance x at which it is reached by writing:

$$\operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right) = 1 - \frac{c}{c_0} = 0.75,$$

and we find by interpolating tabulated values of the error function:

$$\frac{x}{\sqrt{4Dt}} = 0.8144.$$

With $D=3.0 \text{ m}^2/\text{s}$, we have:

$$x(\text{in m}) = 2.821 \sqrt{t(\text{in sec})} = 169.3 \sqrt{t(\text{in hrs})}.$$

Some values of the patch width $2x$ are: 339 m after 1 hour, 479 m after 2 hours, 829 m after 6 hours, 1.17 km after 12 hours, and 1.66 km after 24 hours.

Initial punctual release at some distance from a boundary

Because physical boundaries are generally impermeable (such as the bank of a river), problems with domain boundaries require the implementation of a no-flux condition. If $x = 0$ designates the location of a boundary, we impose

$$-D \frac{\partial c}{\partial x} = 0 \quad \text{at} \quad x = 0. \quad (2.27)$$

The prototypical solution (2.9) spreads to infinity on both sides and exhibits a gradient everywhere. It thus cannot meet the above boundary condition, and using it would be tantamount to accepting an unphysical leak of the substance through the boundary. This flux across the boundary, however, can be cancelled by an equal and opposite flux from a hypothetical and symmetric release on the other side of the boundary. In other words, the situation with one release and a boundary is equivalent to another with two releases and no boundary. The solution is thus

$$c(x,t) = \frac{M}{\sqrt{4\pi Dt}} \left[\exp\left(-\frac{(x-L)^2}{4Dt}\right) + \exp\left(-\frac{(x+L)^2}{4Dt}\right) \right]. \quad (2.28)$$

Because of the addition of another solution, the concentration c is everywhere higher in the presence of the boundary than in its absence. Physically, the boundary prevents leakage to one side, and the substance is confined to less space. In other words, what would have gone beyond the boundary is “folded back” onto the real domain, increasing the concentration there. There is a resulting “piling-up” along the boundary (Figure 2-12).

As time goes on, the piling up along the boundary ($x = 0$) starts to overtake the decreasing peak at the release location ($x = L$), and thereafter the concentration is maximal at the boundary and decreasing inward. [**Exercise:** Can you determine the time at which this reversal occurs? How does it depend on the distance of the release to the boundary?]

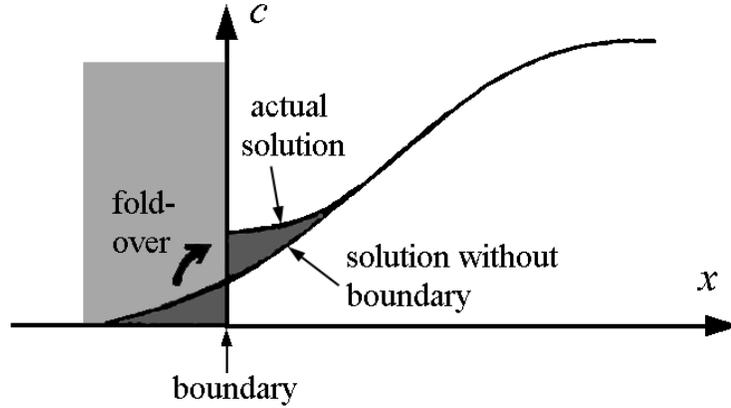


Figure 2-12. Diffusion in the vicinity of an impermeable boundary. The “piling up” along the boundary can be interpreted as a folding of the tail of the curve onto itself.

Initial punctual release between two boundaries

For a 1D interval of finite length L and the origin of the x -axis placed at the left end, the boundary conditions become:

$$-D \frac{\partial c}{\partial x} = 0 \quad \text{at both } x = 0 \text{ and } x = L.$$

If the release takes place at the arbitrary position $x = a$ ($0 \leq a \leq L$), we take into account each wall by introducing virtual releases at $x = -a$ and $x = +2L - a$. But, this is not enough because the virtual release on the right (at $x = +2L - a$) will leak through the left wall ($x = 0$) unless another virtual release is placed at $x = -2L + a$, which in turn needs to have its own image across the right wall, at $x = +4L - a$, et cetera ad infinitum. Likewise, the left image (at $x = -a$) must be compensated by an image on the right at $x = +2L + a$, which needs its own image on the left at $x = -2L - a$, etc. All in all, we must add the solutions due to a doubly infinite set of source and images at $x = \pm a, x = \pm 2L \pm a, \pm 4L \pm a, \pm 6L \pm a$, and so on (Figure 2-13). The solution can be succinctly written as:

$$c(x, t) = \frac{M}{\sqrt{4\pi Dt}} \sum_{m=-\infty}^{m=+\infty} \left[\exp\left(\frac{-(x - 2mL - a)^2}{4Dt}\right) + \exp\left(\frac{-(x - 2mL + a)^2}{4Dt}\right) \right]. \quad (2.29)$$

Note: Because of the steep exponential decay of each function, only the first few (typically five or seven) terms of the infinite sum need to be retained in practice.

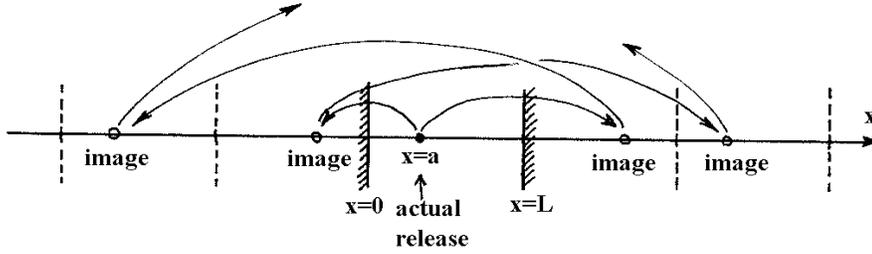


Figure 2-13. Diffusion from a localized release between two impermeable boundaries.

Exercises:

- 1) For a release at the center of the domain ($a = L/2$), study the temporal variation of the concentration at one of the boundaries. Does it first increase and then decrease as in the one-boundary situation?
- 2) What is the ultimate steady state? Derive its value from physical principles and verify it numerically for a particular value of a .

Example

We illustrate the solution in this case by returning to our example with the Chicago Ship Canal. This time, however, we shall be concerned with the earlier-time evolution of the benzene spill, namely when diffusion proceeds vertically in the canal, from the actual time of the accident to the time of nearly completed vertical homogenization of the benzene concentration. This problem requires information beyond that provided earlier: The horizontal extent of the spill is 2 m^2 , and the vertical diffusion coefficient is $0.010 \text{ m}^2/\text{s}$.

In this problem, there are two domain boundaries, the bottom (say $x = 0$) and the surface (say $x = H = 8.07 \text{ m}$, the canal depth). Since the benzene spill occurred at the surface ($x = H$), the following virtual releases must be considered: One at $x = H$ (the image with respect to the surface, that is on top of the spill itself, as if there were a double spill but no surface boundary), two at $x = -H$ (their images with respect to the bottom), two at $x = +3H$ (the images of these images with respect to the surface), two at $x = -3H$ (the images of these last images with respect to the bottom), etc. Thus, the solution is:

$$c(x, t) = \frac{2M}{\sqrt{4\pi Dt}} \left[\exp\left(-\frac{(x-H)^2}{4Dt}\right) + \exp\left(-\frac{(x+H)^2}{4Dt}\right) \right] \\ + \frac{2M}{\sqrt{4\pi Dt}} \left[\exp\left(-\frac{(x-3H)^2}{4Dt}\right) + \exp\left(-\frac{(x+3H)^2}{4Dt}\right) + \dots \right]$$

where M is the amount of benzene released per horizontal area of spill, the 2

Time	c at surface	c at bottom
1 min	32.01 g/L	0.000 g/L
10 min	10.12 g/L	1.342 g/L
20 min	7.221 g/L	3.686 g/L
30 min	6.158 g/L	4.734 g/L
1 hr	5.493 g/L	5.400 g/L
1.5 hrs	5.449 g/L	5.443 g/L
2 hrs	5.446 g/L	5.446 g/L

Table 2-2. Evolution of benzene concentration values. See example in text.

m^2 area. So, $M = 87.9 \text{ kg} / 2 \text{ m}^2 = 43.95 \text{ kg/m}^2$. The concentrations at the surface ($x = H$) and at the bottom ($x = 0$) are, respectively:

$$c_{\text{surface}}(t) = \frac{M}{\sqrt{\pi Dt}} \left[1 + 2 \exp\left(-\frac{H^2}{Dt}\right) + 2 \exp\left(-\frac{4H^2}{Dt}\right) + \dots \right]$$

$$c_{\text{bottom}}(t) = \frac{M}{\sqrt{\pi Dt}} \left[2 \exp\left(-\frac{H^2}{4Dt}\right) + 2 \exp\left(-\frac{9H^2}{4Dt}\right) + \dots \right].$$

With $H = 8.07 \text{ m}$ and $D = 0.010 \text{ m}^2/\text{s}$, we obtain the values listed in Table 2-2. Thus, homogenization over the vertical takes place in about one hour. (This justifies our assumption of complete vertical mixing in the earlier problems dealing with diffusion along the canal over time spans of several hours.)

Time for nearly complete mixing

When a release occurs in a domain of finite length, the ultimate state is one of complete homogenization, with uniform concentration equal to the amount released divided by the extent of the domain, i.e.

$$c_{\text{ultimate}} = c_{\text{average}} = \frac{M}{L}. \quad (2.30)$$

A pertinent question is: What is the time necessary to reach such state? Mathematically, the final state is only reached asymptotically and therefore this time is theoretically equal to infinity, but using a subjective criterion we may derive a practical criterion.

Let us consider the case of a release at the center of the domain ($a = L/2$) and follow the concentration at that same location ($x = L/2$) as a function of time, which is obviously the highest concentration in the domain and which monotonically decreases over time:

$$c_{\text{max}} = c(x = L/2, t) = \frac{M}{\sqrt{4\pi Dt}} \left[1 + 2 \sum_{n=1}^{+\infty} \exp\left(-\frac{n^2 L^2}{4Dt}\right) \right].$$

Let us then ask how long it takes for this maximum value to become only 1% more than the ultimate average value M/L . Defining the dimensionless variable τ by $t = (L^2/D)\tau$, the preceding expression can be written as

$$c_{\max}(\tau) = \frac{M}{L} \left[\frac{1}{\sqrt{4\pi\tau}} \left(1 + 2 \sum_{n=1}^{+\infty} e^{-n^2/4\tau} \right) \right],$$

where the part within brackets is a parameter-free (universal) function of τ that monotonically decreases toward unity. This function reaches the value 1.01 at $\tau = 0.134$. Thus, a practical criterion for the estimation of the time necessary for nearly complete homogenization of the concentration in a one-dimensional finite domain of length L following a punctual release at the center and in the presence of a diffusivity D is:

$$T = 0.134 \frac{L^2}{D}. \quad (2.31)$$

In the case of vertical mixing in the Chicago Ship Canal, the length L is to be taken as $H = 8.07$ m, whereas the vertical diffusivity is $D = 0.010$ m²/s. The result is a mixing time of 873 s, which is about 15 minutes. Considering the previously tabulated values, we note that 20 minutes after the spill the surface and bottom benzene concentrations still differ significantly. This is because the preceding theory assumed an initial release at the center of the domain, while in the example of the Chicago Ship Canal, the release was at one of the boundaries. Naturally, it takes longer to spread something when it first comes from one extremity than when it originates at the center. In the case of an instantaneous punctual release at one of the extremities, a reasonable approach is to replace L by $2L$ in the preceding formula, which increases the front factor by a factor 4

$$T = 0.536 \frac{L^2}{D}. \quad (2.32)$$

For the Chicago Ship Canal, the revised value is 3491 s, or about 58 minutes. This compares favorably with the concentrations at the surface and bottom, which are within 1% of their ultimate values 1 hour after the spill.

The rule to determine the time to complete mixing is then as follows: If the release occurred in the middle, use (2.31); if the release occurred at one boundary, use (2.32); and, if the release occurred at some off-center location, construct an intermediate criterion or, at the risk of overestimating the time taken, use (2.32).

2.6 Diffusion with Source and Decay

We now extend our analysis to include cases when the contaminant is not only diffusing but also replenished and decaying over time.

Governing equation

Recalling the mass budget (1.6) and applying it to an infinitesimal control volume of length Δx and cross-section A , we determine the import and export fluxes:

$$\begin{aligned} q_{\text{in}} A_{\text{in}} &= q(x, t) A \\ q_{\text{out}} A_{\text{out}} &= q(x + \Delta x, t) A, \end{aligned}$$

and state:

$$V \frac{dc}{dt} = - q(x + \Delta x, t) A - K V c + q(x, t) A + S,$$

where $V = A\Delta x$ is the volume of the interval under consideration, K is the decay rate, and S is the source. Division by V yields:

$$\frac{dc}{dt} = - \frac{q(x + \Delta x, t) - q(x, t)}{\Delta x} - K c + s,$$

where $s = S/V$ is the source per volume (of dimensions M/L³T). In the limit of an infinitesimal control volume ($\Delta x \rightarrow 0$), this budget becomes a partial-differential equation:

$$\frac{\partial c}{\partial t} = - \frac{\partial q}{\partial x} - K c + s.$$

Finally, in the absence of advection, the flux is purely diffusive ($q = -D\partial c/\partial x$), we obtain an equation governing the spatial and temporal variability of the concentration distribution:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right) - K c + s. \quad (2.33)$$

Whereas the diffusion coefficient D may vary with the local turbulence intensity, an important case for which we can derive analytical solutions is that of a constant D :

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - K c + s. \quad (2.34)$$

The solution to this equation corresponding to an instantaneous and localized release in the absence of subsequent source is the prototypical solution adjusted for temporal decay:

$$c(x, t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt} - Kt\right). \quad (2.35)$$

Continuous input at a fixed location

As an application, consider the case of a continuous release at a fixed location, as is the case of a point source. Because the time-dependent problem is

rather difficult to solve and also because the practical question in such situation may be limited to finding the ultimate state, we shall consider here only the steady-state solution to the problem (by putting $\partial c/\partial t$ to zero). Since the source is punctual (say, at $x = 0$), there is no source anywhere else, and Equation (2.31) reduces to:

$$0 = D \frac{\partial^2 c}{\partial x^2} - Kc.$$

The solution is made of two exponential functions,

$$c = A e^{\lambda x} + B e^{-\lambda x},$$

where A and B are two constants of integration to be determined by application of boundary conditions, and the exponent λ is given by

$$\lambda = \sqrt{\frac{K}{D}}.$$

By virtue of left-right symmetry, we need only consider the half axis $x > 0$. As we expect the decay process to limit the presence of the pollutant to the vicinity of the source, we impose the condition $c \rightarrow 0$ as $x \rightarrow \infty$ and put the coefficient A of the growing exponential to zero. The determination of the remaining constant B requires specification of the source rate at $x = 0$. Since this source is punctual, it must be expressed in mass per unit cross-area per time (M/L²T). Let us denote it by \dot{M} . Because half of the pollutant being released goes to the left and half to the right, we impose at $x \rightarrow 0+$:

$$-D \frac{\partial c}{\partial x} = q(0+, t) = \frac{\dot{M}}{2},$$

which leads to:

$$B = \frac{\dot{M}}{2D\lambda} = \frac{\dot{M}}{2\sqrt{DK}}.$$

The final solution is (Figure 2-14):

$$c = \frac{\dot{M}}{2\sqrt{DK}} \exp\left(-\sqrt{\frac{K}{D}} x\right) \quad \text{for } x > 0 \quad (2.36)$$

$$c = \frac{\dot{M}}{2\sqrt{DK}} \exp\left(+\sqrt{\frac{K}{D}} x\right) \quad \text{for } x < 0. \quad (2.37)$$

Of interest is the maximum concentration at the site of the source:

$$c_{\max} = \frac{\dot{M}}{2\sqrt{DK}}. \quad (2.38)$$

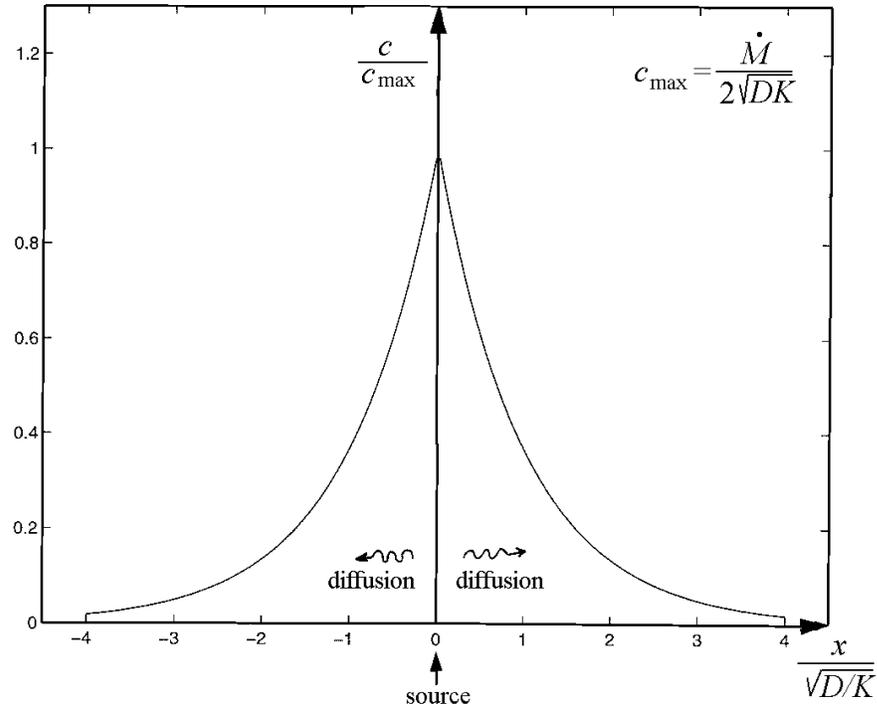


Figure 2-14. Steady-state concentration distribution around a punctual and continuous source and under decay, according to (2.36)–(2.37).

This value is naturally proportional to the rate of release, \dot{M} . Increasing diffusion implies greater spreading and thus a lower maximum concentration, while increasing decay obviously leads also to a lower maximum concentration.

Finally, we seek a formula that provides a practical expression for the patch width. As for the earlier case of a spreading concentration (Section 2-4), we are faced with an exponential solution that yields non-zero values all the way to infinity, and we need to apply a somewhat arbitrary cut-off criterion. If we define the width of the patch as the interval containing 95% of the total amount present, the width is defined as:

$$\text{Width} = \frac{6.0}{\lambda} = 6.0 \sqrt{\frac{D}{K}}, \quad (2.39)$$

and 95% of the substance is contained in the interval $[-\text{Width}/2, +\text{Width}/2]$. Naturally, the patch is wider if diffusion is more vigorous, and is narrower if decay is faster.

Example

We again return to our example with the Chicago Ship Canal and now take into account that benzene in water is subject to bacterial decay (aerobic degradation) at the known rate of 0.11/day. If a stationary barge containing benzene and parked along the side of the canal has been leaking over the last few weeks at the estimated rate of 2.5 liters per day, what is the benzene concentration in the canal water near the barge, and how far along the canal is the concentration in excess of the drinking-water standard of 0.005 mg/L? Assume steady state and uniformity of the benzene concentration across the canal and in the vertical. (Recall: canal width= 48.8 m, depth= 8.07 m, along-canal diffusivity= 3.0 m²/s, and benzene density= 0.879 g/cm³.)

To solve this problem, we first need to determine \dot{M} , the rate of input per cross-area:

$$\dot{M} = \frac{(2.5 \text{ L/day}) \times (879 \text{ g/L})}{(48.8 \text{ m}) \times (8.07 \text{ m}) \times (86,400 \text{ s/day})} = 6.458 \cdot 10^{-5} \frac{\text{g}}{\text{m}^2 \cdot \text{s}}.$$

We also establish the value of the decay constant:

$$K = \frac{0.11 \text{ /day}}{86,400 \text{ s/day}} = 1.273 \cdot 10^{-6} \text{ /s.}$$

Then, solution (2.38) provides the benzene concentration in the canal section at the position of the leaky barge:

$$c_{\max} = \frac{\dot{M}}{2\sqrt{DK}} = 0.0165 \text{ g/m}^3 = 0.0165 \text{ mg/L.}$$

The concentration equals the drinking standard $c_{\text{std}} = 0.005 \text{ g/m}^3$ at a distance x obtained by inverting (2.37):

$$x = -\sqrt{\frac{D}{K}} \ln \left(\frac{2c_{\text{std}}\sqrt{DK}}{\dot{M}} \right),$$

which yields $x = 1,835 \text{ m}$. Thus, the benzene concentration exceeds the drinking standard in a zone of 3.67 kilometers along the canal.

Continuous release over a finite distance

Let us now consider the case when the continuous release occupies a finite interval, say from $x = -L$ to $x = +L$ (Figure 2-15). The governing equation again during steady state is:

$$0 = D \frac{d^2c}{dx^2} - Kc + s,$$

where the rate of release per unit cross-area, per unit distance along the axis of diffusion, and per unit time is: $s = s_0$ in $-L < x < +L$ and $s = 0$ elsewhere. The solution is:

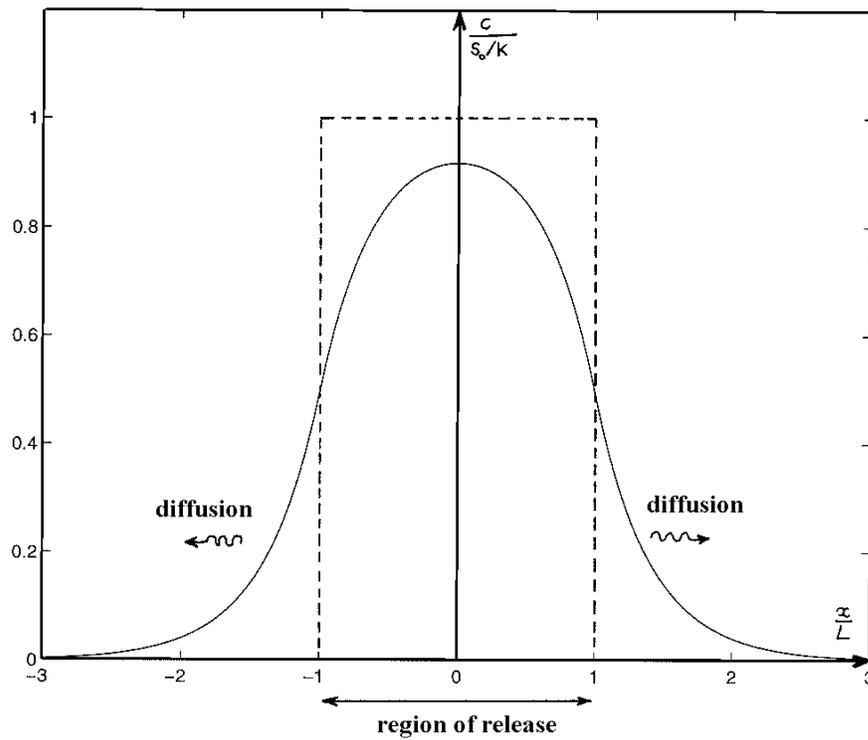


Figure 2-15. Steady-state concentration distribution created by a continuous release over a finite distance ($-L < x < +L$) and in the presence of decay, according to (2.40)–(2.42).

$$\begin{aligned}
x < -L: \quad c &= A e^{\lambda x} \\
-L < x < +L: \quad c &= B e^{\lambda x} + C e^{-\lambda x} + \frac{s_0}{K} \\
+L < x: \quad c &= D e^{-\lambda x}.
\end{aligned}$$

Matching the concentration and flux values at $x = \pm L$ determines the four constants of integration. The final solution is:

$$x < -L: \quad c = \frac{s_0}{K} \sinh \lambda L e^{+\lambda x} \quad (2.40)$$

$$-L < x < +L: \quad c = \frac{s_0}{K} (1 - e^{-\lambda L} \cosh \lambda x) \quad (2.41)$$

$$+L < x: \quad c = \frac{s_0}{K} \sinh \lambda L e^{-\lambda x}. \quad (2.42)$$

The maximum concentration is at the center of the patch ($x = 0$) and equals

$$c_{\max} = \frac{s_0}{K} (1 - e^{-\lambda L}). \quad (2.43)$$

For a narrow release area ($\lambda L \ll 1$), we can approximate $\exp(-\lambda L)$ by $1 - \lambda L$, to find $c_{\max} \simeq s_0 \lambda L / K$. Then defining the total rate of release $\dot{M} = 2Ls_0$, we obtain $c_{\max} \simeq \dot{M} / 2\sqrt{DK}$, which is identical to (2.38). This shows that a release over a small but finite distance can be approximated by a punctual release as long as $\lambda L = \sqrt{KL^2/D}$ is much less than unity.

In the opposite limit of a very wide release ($\lambda L \gg 1$), we find $c_{\max} \simeq s_0 / K$, which is the value obtained by neglecting diffusion and stating that source and decay locally cancel out. This occurs because diffusion is relegated to the edges of the release interval and does not affect the concentration in the middle.

Continuous punctual release near a boundary

We now consider a continuous release, at $x = 0$ and of rate \dot{M} , at a distance L from a boundary ($x = -L$), as depicted on Figure 2-16. The solution proceeds as previously, with the boundary conditions: No flux ($-Ddc/dx = 0$) at the boundary ($x = -L$), continuity of concentration [$c(x = 0-) = c(x = 0+)$] and a balance of fluxes [$q(x = 0+) - q(x = 0-) = \dot{M}$] at the release point. This solution is:

$$-L < x < 0: \quad c = \frac{\dot{M}}{\sqrt{DK}} e^{-\lambda L} \cosh[\lambda(x + L)] \quad (2.44)$$

$$0 < x: \quad c = \frac{\dot{M}}{\sqrt{DK}} \cosh \lambda L e^{-\lambda(x+L)}. \quad (2.45)$$

The concentrations of interest are those at the wall and at the point of release:

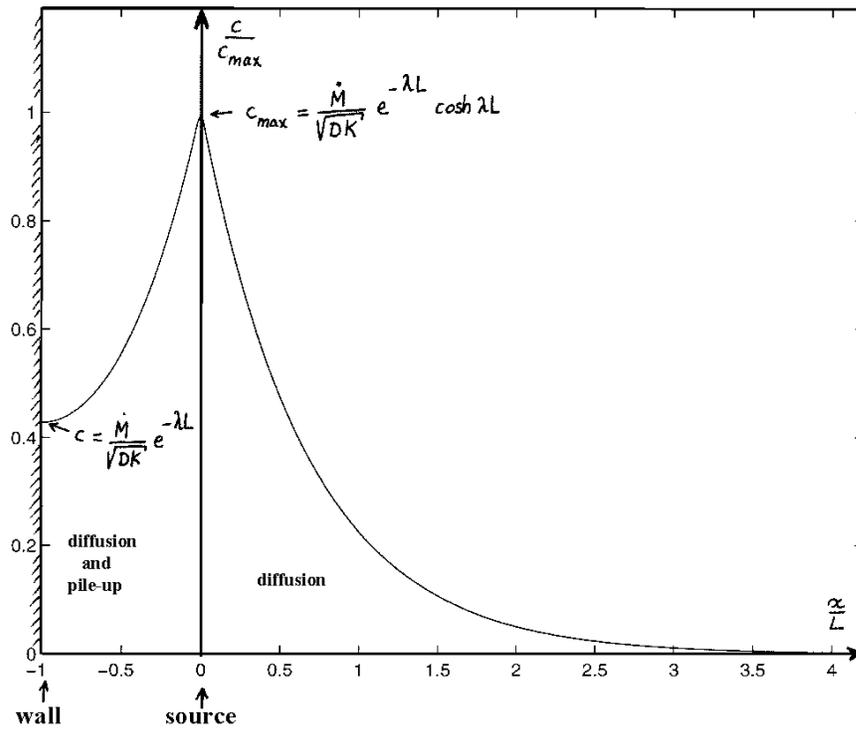


Figure 2-16. Steady-state concentration distribution due to a continuous punctual release in the proximity of a boundary and in the presence of decay, according to (2.44)–(2.45).

$$c_{\text{wall}} = \frac{\dot{M}}{\sqrt{DK}} e^{-\lambda L}$$

$$c_{\text{source}} = \frac{\dot{M}}{\sqrt{DK}} e^{-\lambda L} \cosh \lambda L.$$

Naturally, the concentration at the source is the largest of the two. Note that in the limit $\lambda L \rightarrow \infty$, we recover solution (2.36-2.37) of the punctual release away from boundaries.

2.7 Generalization to Three Dimensions

Introduction

Although the analysis of one-dimensional problems can find applications to spatially elongated systems that, in first approximation, may be modeled as one-dimensional (such as a pipe or a river), it remains that most engineering problems are two- or three-dimensional. We therefore need to extend our previous analysis to higher dimensions.

Formulation

For the time being, let us continue to assume that there is no mean fluid velocity, namely there is no advective component and the flux of substance is purely diffusive. The difference from the previous sections is that diffusion is now regarded as proceeding in all three directions of space. The flux quantity has three components (east-west, north-south and up-down – Figure 2-17) and is a vector. Thus, $\vec{q} = (q_x, q_y, q_z)$. Similar arguments as those outlined in Section 1-2, to arrive at Equation (1.5), can be replayed here to obtain:

$$q_x = -D \frac{\partial c}{\partial x}, \quad q_y = -D \frac{\partial c}{\partial y}, \quad q_z = -D \frac{\partial c}{\partial z}.$$

Putting it all together and using vectorial notation, we write:

$$\begin{aligned} \vec{q} &= -D \left(\frac{\partial c}{\partial x}, \frac{\partial c}{\partial y}, \frac{\partial c}{\partial z} \right) \\ &= -D \vec{\nabla} c, \end{aligned} \tag{2.46}$$

where $\vec{\nabla}$ is the so-called gradient operator.

Equipped with an expression for the flux, we can establish the three-dimensional mass budget. As before, we state that all mass of the substance must be accounted for:

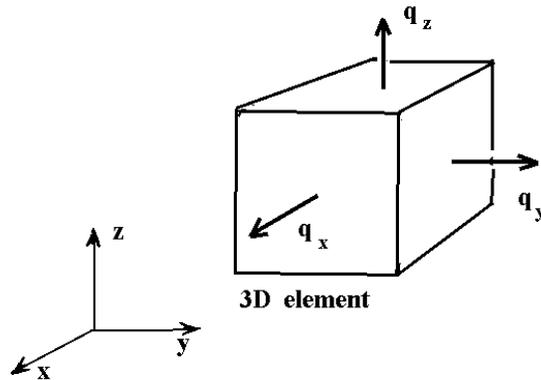


Figure 2-17. Flux components in the three-dimensional space.

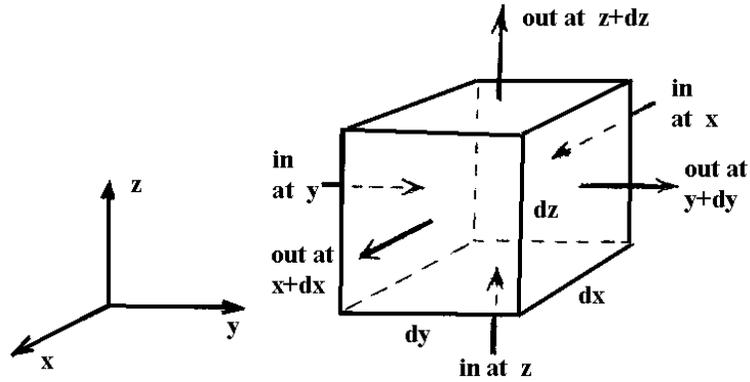


Figure 2-18. Mass budget for an infinitesimal 3D control volume.

$$\text{Rate of accumulation} = \sum \text{imports} + \sum \text{exports.}$$

For an infinitesimal 3D box of volume $dx dy dz$ (Figure 2-18), the statement becomes

$$\begin{aligned} \frac{\partial}{\partial t}(c \, dx dy dz) &= (q_x \text{ at } x) \, dy dz - (q_x \text{ at } x + dx) \, dy dz \\ &+ (q_y \text{ at } y) \, dx dz - (q_y \text{ at } y + dy) \, dx dz \\ &+ (q_z \text{ at } z) \, dx dy - (q_z \text{ at } z + dz) \, dx dy, \end{aligned}$$

or

$$dx dy dz \frac{\partial c}{\partial t} = - \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} \right) dx dy dz.$$

Simplification yields

$$\frac{\partial c}{\partial t} = - \vec{\nabla} \cdot \vec{q}, \quad (2.47)$$

where $\vec{\nabla} \cdot$ is the so-called divergence operator. With the flux \vec{q} given by the diffusion law (2.46), we can write a single equation for the concentration c :

$$\frac{\partial c}{\partial t} = + \vec{\nabla} \cdot (D \vec{\nabla} c). \quad (2.48)$$

With D taken as a constant, this reduces to:

$$\frac{\partial c}{\partial t} = D \nabla^2 c, \quad (2.49)$$

where ∇^2 is called the Laplace operator or laplacian. It is defined as

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$

[Exercise: Show that the 2D random-walk process described at the beginning of Section 2-2 leads, in the continuous limit, to the 2D version of the above diffusion equation.]

Instantaneous localized release

It is straightforward to verify that the product of three prototypical solutions, with spatial variables x , y and z , respectively,

$$c(x, y, z, t) = \frac{M}{(\sqrt{4\pi Dt})^3} \exp\left(-\frac{x^2 + y^2 + z^2}{4Dt}\right) \quad (2.50)$$

is a solution to the 3D equation (2.41). Obviously, this is the solution to the case of a localized and instantaneous release, at location (0,0,0) and at time $t = 0$ of a quantity M of the substance. In contrast to the 1D situation, where M was expressed in units of substance per unit cross-section, the quantity M here is in units of substance (example: in grams).

Since $r = \sqrt{x^2 + y^2 + z^2}$ is the distance to the point of release, the concentration c depends on that distance and time only. It does not depend on the direction with respect to the coordinate axes. Physically, the spreading is identical in all directions of space; diffusion is said to be isotropic. The size of the 3D ‘cloud’ is measured by the diametrical span

$$4\sigma = 4\sqrt{2Dt}. \quad (2.51)$$

Anisotropic medium

In most environmental systems (atmosphere, rivers, lakes and oceans), turbulence in the vertical direction differs greatly from that in the two horizontal

directions, chiefly because of gravity. As a result, diffusion does not proceed at the same rates in the horizontal and vertical directions.

If we generalize and imagine that all three directions are different from one another, then we are brought to define three distinct diffusion coefficients:

$$D_x \text{ for diffusion in the } x\text{-direction: } q_x = - D_x \frac{\partial c}{\partial x}$$

$$D_y \text{ for diffusion in the } y\text{-direction: } q_y = - D_y \frac{\partial c}{\partial y}$$

$$D_z \text{ for diffusion in the } z\text{-direction: } q_z = - D_z \frac{\partial c}{\partial z},$$

the diffusion equation becomes

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(D_z \frac{\partial c}{\partial z} \right), \quad (2.52)$$

and the solution to an instantaneous ($t = 0$) and localized ($x = y = z = 0$) release is:

$$c(x, y, z, t) = \frac{M}{(\sqrt{4\pi t})^3 \sqrt{D_x D_y D_z}} \exp \left(- \frac{x^2}{4D_x t} - \frac{y^2}{4D_y t} - \frac{z^2}{4D_z t} \right). \quad (2.53)$$

The spatial dimensions of the corresponding 3D cloud are measured by

$$4\sigma_x = 4\sqrt{2D_x t} \text{ in the } x\text{-direction}$$

$$4\sigma_y = 4\sqrt{2D_y t} \text{ in the } y\text{-direction}$$

$$4\sigma_z = 4\sqrt{2D_z t} \text{ in the } z\text{-direction.}$$

Solutions corresponding to releases over finite regions or near boundaries can be constructed following the same principles as outlined in Section 2-5.

Presence of a horizontal boundary

As for 1D problems, the preceding solution can serve as a building block for the construction of more realistic 3D applications. An important problem is that of a 3D instantaneous and punctual release near a boundary, such as an explosion in the air at some height (say $z = H$) above the ground (say $z = 0$). The ground, which we take to be flat and horizontal for simplification, acts as an impermeable horizontal boundary and requires that the vertical component of the diffusive flux be zero at that level ($q_z = 0$ at $z = 0$). This condition is accommodated by introducing a virtual release of the same amount at the same

time and at a symmetric position below the ground ($z = -H$). The solution then consists in the sum of two prototypical solutions, one caused by the actual release at ($x = 0, y = 0, z = +H$) and the other due to the image at ($x = 0, y = 0, z = -H$):

$$c(x, y, z, t) = \frac{M}{(\sqrt{4\pi t})^3 \sqrt{D_x D_y D_z}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t}\right) \times \left[\exp\left(-\frac{(z-H)^2}{4D_z t}\right) + \exp\left(-\frac{(z+H)^2}{4D_z t}\right) \right],$$

where M is the amount released (e.g., mass) at time $t = 0$. The horizontal coordinates x and y are measured along the ground, with the origin at the vertical below the point of release. Of interest is the ground concentration, $c_{\text{ground}} = c(x, y, z = 0, t)$, which is:

$$c_{\text{ground}}(x, y, t) = \frac{2M}{(\sqrt{4\pi t})^3 \sqrt{D_x D_y D_z}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t} - \frac{H^2}{4D_z t}\right). \quad (2.54)$$

The ground concentration is highest at the vertical below the release location ($x = y = 0$) and decreases away with distance from there. Only when D_x and D_y are equal is this decrease 2D isotropic. At any time t , the maximum ground concentration is thus:

$$c_{\text{center ground}}(t) = \frac{2M}{(\sqrt{4\pi t})^3 \sqrt{D_x D_y D_z}} \exp\left(-\frac{H^2}{4D_z t}\right). \quad (2.55)$$

This maximum concentration evolves over time from zero at the initial time (nothing has yet diffused from the level of the release down to the ground), to a maximum (after vertical diffusion has brought some of the substance near the ground), and back down to zero (because continuous lateral diffusion acts to dilute the substance and thus to decrease concentrations everywhere). The time of the maximum is obtained by setting the time derivative of $c_{\text{center ground}}(t)$ to zero. The result is:

$$\begin{aligned} c_{\text{max center ground}} &= \frac{D_z}{(\sqrt{2\pi/3})^3 \sqrt{D_x D_y}} \frac{2M}{H^3} \exp\left(-\frac{3}{2}\right) \\ &= 0.1472 \frac{D_z}{\sqrt{D_x D_y}} \frac{M}{H^3}, \end{aligned} \quad (2.56)$$

which occurs at

$$t_{\text{max}} = \frac{H^2}{6D_z}. \quad (2.57)$$

2.8 Combination of Advection and Diffusion

Oftentimes, the fluid within which diffusion takes place is also moving in a preferential direction. The obvious cases are those of a flowing river and of a smokestack plume being blown by the wind.

Formulation

We now retain the advective flux and combine it with the diffusive flux. Recall that in one dimension we established the total flux as [see Equations (1.4)–(1.5)]:

$$q = cu - D \frac{\partial c}{\partial x}, \quad (2.58)$$

which we can immediately generalize to three dimensions:

$$\vec{q} = c\vec{u} - D \vec{\nabla} c. \quad (2.59)$$

The vector \vec{u} is the three-dimensional vector velocity of the fluid medium transporting the substance. We here assume isotropy in diffusion (single D value) but allow for anisotropy in advection. (The \vec{u} vector introduces a preferential direction, that of the transporting flow.)

The three-dimensional mass budget (2.47) is true regardless of the composition of the flux vector \vec{q} and thus continues to hold. Replacement of \vec{q} by use of (2.59) yields the following equation for the concentration distribution:

$$\frac{\partial c}{\partial t} = - \vec{\nabla} \cdot (c\vec{u}) + \vec{\nabla} \cdot (D\vec{\nabla}c).$$

In environmental problems, it is usual to make the assumption of an incompressible medium. This is easily justified for water. It is also accurate for air, because the atmospheric motions responsible for advection (winds) and diffusion (turbulence) occur at velocities much less than the speed of sound, and compressibility effects are negligible. Writing the budget for the containing fluid itself, we take $c = \rho$, the constant density of the fluid (mass per volume), and the above equation reduces to

$$0 = - \rho \vec{\nabla} \cdot \vec{u} + 0,$$

or

$$\vec{\nabla} \cdot \vec{u} = 0. \quad (2.60)$$

In other words, the entraining motions must be non-divergent. What converges in one direction must diverge in another. Together with the usual assumption of uniform diffusion (constant value of diffusion coefficient D), the mass-budget equation for the contaminant reduces to the so-called advection-diffusion equation:

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \vec{\nabla} c = D \nabla^2 c. \quad (2.61)$$

This equation consists of three terms, representing respectively the local accumulation or depletion, the movement by the carrying fluid, and the effect of diffusion (movement by random motions in the fluid).

In one dimension, the advection-diffusion equation simplifies to:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2}. \quad (2.62)$$

The solution corresponding to an instantaneous and localized release, in the absence of a continuous source and decay, is:

$$c(x, t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x - ut)^2}{4Dt}\right).$$

Exercise: Show that an analogous random-walk process can be constructed by the inclusion of a directional bias in a particular direction (asymmetric probabilities). How does the entraining velocity relate to the various probabilities, spacing and time step?

Since the above advection diffusion equation, in 3D or 1D, includes a combination of two physical processes (advection and diffusion), we are prompted to ask the following questions:

1. How do the processes of advection and diffusion differ?
2. Under which condition(s) is one more important than the other?
3. How could we easily tell which one dominates?

To answer these questions, it is simpler to work with the 1D formulation and then generalize the conclusions. The advection process is represented in (2.62) by the term $u\partial c/\partial x$, which has a first-order derivative, while diffusion is represented by $D\partial^2 c/\partial x^2$, which is of second-order. Upon replacing x by $-x$, the former changes sign while the latter does not. Therefore, advection is skewed (going one way, in the direction of the flow) while diffusion is symmetric (going both ways). For an insightful illustration of this difference, see the example at the end of the present section. The other two questions are answered in the following subsection.

Relative importance of advection and diffusion

To facilitate the derivation of a practical criterion that would tell us which of the two processes dominates, we introduce SCALES for the relevant quantities. A scale is a quantity of dimension identical to the variable to which it refers and the value of which gives a practical estimate of the magnitude of that variable. Examples are: The scale for the width of the Mississippi River is $L = 100$ m, the scale for mid-ocean depths is $H = 3000$ m, the scale of the prevailing winds in the atmosphere is $U = 10$ m/s, and the scale for the concentration of a substance in a finite domain could be taken as the average or maximum

concentration value. To make matters easy, scales are usually taken as pure constants (independent of space and time), and their values are rounded to just a few digits. See table 2-3.

VARIABLE	SCALE	CHOICE OF VALUE
c	C	Typical concentration value, such as average, initial or boundary value
u	U	Typical velocity value, such as maximum value
x	L	Approximate domain length or size of release location

Table 2-3. Scales and their choices.

Using the preceding scales, we can derive estimates of the sizes of the different terms. Since the derivative $\partial c/\partial x$ is expressing, after all, a difference in concentration over a distance (in the infinitesimal limit), we can estimate it to be approximately (within 100% or so, but certainly not completely out of line with) C/L , and the advection term $u\partial c/\partial x$ to be about UC/L . Similarly, the second derivative $\partial^2 c/\partial x^2$ represents a difference of the gradient over a distance and is estimated at $(C/L)/L = C/L^2$. The diffusion term $D\partial^2 c/\partial x^2$ thus scales as DC/L^2 .

Equipped with these estimates, we can then compare the two processes by forming the ratio of their scales:

$$\frac{\text{advection}}{\text{diffusion}} = \frac{UC/L}{DC/L^2} = \frac{UL}{D}.$$

This ratio is obviously dimensionless; traditionally, it is called the Peclet number and is denoted by Pe :

$$Pe = \frac{UL}{D}. \quad (2.63)$$

The Peclet number leads to an immediate criterion, as follows.

If $Pe \ll 1$ (in practice, if $Pe < 0.1$): then the advection term is significantly smaller than the diffusion term. Physically, diffusion dominates and advection is negligible. Spreading occurs almost symmetrically despite the directional bias of the (weak) flow. If we wish to simplify the problem, we may drop the $u\partial c/\partial x$ term, as if u were nil. The relative error committed in the solution by so doing is expected to be on the order of the Peclet number, and the smaller Pe , the smaller the error. The solutions established in the few preceding sections were based on such simplification and are thus valid whenever $Pe \ll 1$.

If $Pe \gg 1$ (in practice, if $Pe > 10$): then the advection term is significantly bigger than the diffusion term. Physically, advection dominates and diffusion is negligible. Spreading is almost inexistent, and the patch of pollutant is simply moved along by the flow. If we wish to simplify the problem, we may drop the $D\partial^2 c/\partial x^2$ term, as if D were nil. The relative error committed in the solution

by so doing is expected to be on the order of the inverse of the Peclet number ($1/Pe$), and the larger Pe , the smaller the error. [Note that the neglect of the term with the highest-order derivative reduces the need of boundary conditions by one. No boundary condition may be imposed at the downstream end of the domain, and what happens there is whatever the flow brings.]

The prototypical solution of the 1D advection only equation is:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = 0 \quad \rightarrow \quad c(x, t) = c_0(x - ut),$$

since a divergence-free flow requires $\partial u / \partial x = 0$ and thus u constant; $c_0(x)$ is the initial concentration distribution. For non-uniform flows at 2D and 3D, there is no prototypical solution of general interest and simultaneously expressible in convenient mathematical terms. Physically, a three-dimensional flow can cause not only translation but also rotation, strain and shear.

If $Pe \simeq 1$ (in practice, if $0.1 < Pe < 10$): then the advection and diffusion terms are not significantly different, and neither process dominates over the other. No approximation to the equation can be justified, and the full equation must be utilized.

Exercise: After adding decay and source terms in Equation (2.62) as done in (2.35),

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} - Kc + s, \quad (2.64)$$

derive the relevant dimensionless ratios. Show that only three independent ratios can exist. Discuss in the framework of these dimensionless ratios under which conditions one or more processes are negligible. Finally, show that for $s = 0$, the solution corresponding to an instantaneous and localized release is:

$$c(x, t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x - ut)^2}{4Dt} - Kt\right).$$

Steady state with advection and diffusion

Let us consider the steady release of a contaminant in a one-dimensional stream, as depicted in Figure 2-19. The concentration is assumed to be vertically and laterally homogenized, in order to justify the 1D simplification. It is of sufficient interest to restrict our attention to the steady state (which does exist) by setting $\partial c / \partial t = 0$. The equation reduces to:

$$u \frac{dc}{dx} = D \frac{d^2c}{dx^2}.$$

(The steady-state assumption is equivalent to imagining that the source of pollution has been there since ever. In practice, a long time compared to D/u^2 suffices.)

Since the coefficients u and D are constant, we can rewrite the equation as

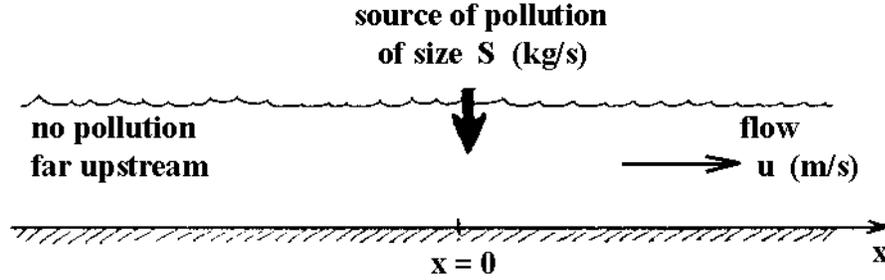


Figure 2-19. Steady punctual release in a one-dimensional stream.

$$\frac{d}{dx} \left(uc - D \frac{dc}{dx} \right) = 0,$$

which can be readily integrated to yield:

$$q = uc - D \frac{dc}{dx} = \text{constant.}$$

In retrospect, this equality is obvious: In a steady-state regime, there is no local accumulation/depletion of pollutant anywhere and thus what arrives at one location must also depart from it, and the flux is uniform all along the stream, except of course for a discontinuity at the location of the source.

Far away on the upstream side, the concentration must vanish, and therefore both c and dc/dx must tend toward zero as $x \rightarrow -\infty$. This implies $q = 0$ far away upstream (no pollution, no transport thereof), and since q is constant for all values of x upstream ($x < 0$) we have

$$uc - D \frac{dc}{dx} = 0 \quad \text{for } x < 0,$$

with solution

$$c = c_0 \exp\left(\frac{ux}{D}\right),$$

where c_0 is a constant of integration to be determined later.

On the downstream side, we must expect a non-zero transport ($q \neq 0$). The value of this transport is obtained from a consideration of the vicinity of the source: $q(x = 0+) = \dot{M}$, where \dot{M} is the amount of substance released per unit time and cross-sectional area of the stream. [If S is the discharge rate, in amount per time, and A is the cross-sectional area, then $\dot{M} = S/A$.] We have

$$uc - D \frac{dc}{dx} = \dot{M} \quad \text{for } x > 0,$$

with solution

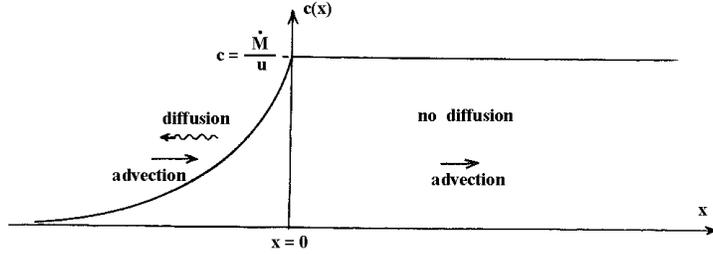


Figure 2-20. Concentration distribution in a one-dimensional stream in the vicinity of a steady and punctual release, according to (2.65)–(2.66).

$$c = c_1 \exp\left(\frac{ux}{D}\right) + \frac{\dot{M}}{u},$$

where c_1 is a new constant of integration.

Far downstream, we do not expect infinitely large concentrations, and thus the limit of c for $x \rightarrow +\infty$ must be finite, which implies that c_1 must be zero. This leaves a uniform concentration all along the downstream portion of the stream:

$$c = \frac{\dot{M}}{u} \quad \text{for } x > 0. \quad (2.65)$$

Continuity of the concentration values near the source requires matching the upstream and downstream solutions at $x = 0$, which yields $c_0 = \dot{M}/u$. The concentration distribution on the upstream portion of the stream is thus:

$$c = \frac{\dot{M}}{u} \exp\left(\frac{ux}{D}\right) \quad \text{for } x \leq 0. \quad (2.66)$$

Graphically (Figure 2-20), the solution displays a wedge upstream and a plateau downstream.

It is interesting to discuss the above solution in some details, especially from the point of view of the separate processes of advection and diffusion. On the downstream side, the concentration is uniform and thus has no gradient; diffusion is nil, and the pollutant is simply transported with the flow. We could qualify this as flushing. For increasing \dot{M} values, $c = \dot{M}/u$ also increases, as a greater input leads to a proportionally higher concentration. For increasing u values, c decreases, because a faster current implies a greater dilution.

On the upstream side, the concentration decays exponentially away from the source, and the gradient indicates active diffusion. Since diffusion proceeds downgradient (from higher to lower values), the diffusive flux is upstream. Advection, by contrast, is directed downstream. The two processes act against each other and, in fact, negate each other exactly leaving no net flux of contaminant.

We may well ask: How far does the concentration tail extend upstream? Since the exponential function has non-zero values all the way to infinity, we need to set a practical criterion. Placing the arbitrary limit where the concentration has dropped to 5% of its maximum value at the source, we obtain:

$$\exp\left(\frac{ux}{D}\right) = 0.05 \quad \rightarrow \quad \frac{ux}{D} = -3.00, \quad (2.67)$$

and a practical answer is: The concentration is less than 5% of its maximum value beyond the distance $3D/u$ upstream of the source. Note how this distance increases with D (and thus the level of turbulence) and decreases with u (and thus the speed of the flow). Since the level of turbulence typically increases with the speed of the flow, it is not immediately clear which way the tendency is.

[Exercise: Taking the diffusion coefficient D as the product of a turbulent velocity u_* and an eddy diameter scale d – see end of Section 1-2 –, taking u_* as one tenth of the mean speed u and d as the stream depth H , what is the upstream extent of the pollution?]

Steady state with advection, diffusion and decay

Let us now consider the same situation but in the presence of decay. In this case, the pollutant is continuously discharged at $x = 0$, is advected downstream with speed u , is diffused in both upstream and downstream directions with diffusivity D , and is continuously withdrawn from the carrying fluid at rate K . The governing differential equation is:

$$u \frac{dc}{dx} = D \frac{d^2c}{dx^2} - Kc. \quad (2.68)$$

Looking for a solution of the form $\exp(\lambda x)$, we find that the coefficient λ must be a root of the algebraic equation

$$D\lambda^2 - u\lambda - K = 0,$$

of which there are two solutions:

$$\lambda_+ = \frac{u + \sqrt{u^2 + 4DK}}{2D}$$

$$\lambda_- = \frac{u - \sqrt{u^2 + 4DK}}{2D}.$$

The first root is positive while the second is negative. Since it would be unrealistic if concentration values grew without bound at large distances from the source, we must retain on each side of the source only the decaying exponential, that is, λ_+ on the upstream side ($x < 0$) and λ_- on the downstream side ($x > 0$). Since furthermore the concentration must have a unique value at the $x = 0$, we have:

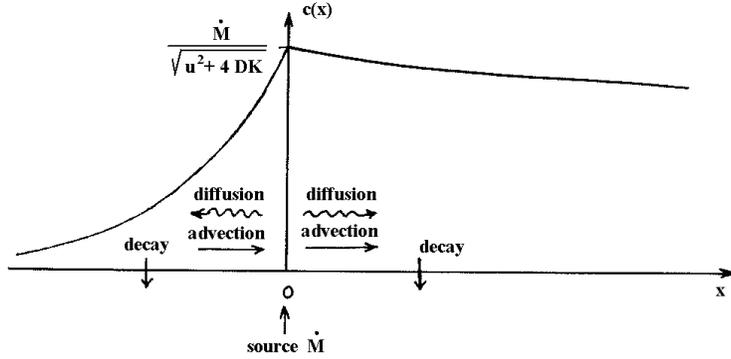


Figure 2-21. Concentration distribution in a one-dimensional stream around the vicinity of a steady and punctual discharge in the presence of diffusion and decay.

$$c(x) = A e^{\lambda_+ x} \quad \text{for } x < 0$$

$$c(x) = A e^{\lambda_- x} \quad \text{for } x > 0,$$

where the constant of integration A is the same in both expressions.

The balance of fluxes in the vicinity of the source, which stipulates that what comes from the upstream side plus what comes from the source is what goes downstream [$q(x = 0^-) + \dot{M} = q(x = 0^+)$ where $q = cu - D(dc/dx)$], yields:

$$(u - \lambda_+ D)A + \dot{M} = (u - \lambda_- D)A,$$

or

$$A = \frac{\dot{M}}{(\lambda_+ - \lambda_-)D} = \frac{\dot{M}}{\sqrt{u^2 + 4DK}}.$$

The final solution is then (Figure 2-21):

$$c(x) = \frac{\dot{M} e^{\lambda_+ x}}{\sqrt{u^2 + 4DK}} \quad \text{for } x \leq 0 \quad (2.69)$$

$$c(x) = \frac{\dot{M} e^{\lambda_- x}}{\sqrt{u^2 + 4DK}} \quad \text{for } x \geq 0. \quad (2.70)$$

The concentration is naturally maximum at the source ($x = 0$), with value equal to:

$$c_{\max} = \frac{\dot{M}}{\sqrt{u^2 + 4DK}}. \quad (2.71)$$

We note that in the absence of advection ($u = 0$) this solution reduces to (2.38), while in the absence of decay ($K = 0$) it reduces to (2.65).

Exercise: Explain physically why the peak concentration decreases with increasing u , D and K .

2.9 Highly Advective Situations

Distance as time

Consider now a two-dimensional system in which the flow is uniform and therefore unidirectional. Choosing the x -axis to point in that direction and noting the flow speed u , we write the advection-diffusion equation, (2.61), as

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right). \quad (2.72)$$

Making the further assumptions of a steady state and of a very large Peclet number ($Pe = UL/D \gg 1$, as for a swift flow or a long patch), we can discard the terms $\partial c/\partial t$ and $D\partial^2 c/\partial x^2$, reducing the equation to:

$$u \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial y^2}. \quad (2.73)$$

In such a system, advection proceeds in one direction (downstream) while diffusion proceeds in the transverse direction. An example is the confluence of two streams, one being polluted, the other not. Downstream of the confluence point, the two kinds of water flow side by side with approximately the same speed but uneven transverse concentration. With downstream distance, cross-flow diffusion acts to homogenize gradually the cross-section concentration distribution (Figure 2-22). The further downstream we go, the more spreading and homogenization we observe, because the two fluid masses have been in contact longer. Thus, downstream distance plays the role of time.

Let us exploit this remark and define the travel time

$$\tau = \frac{x}{u}, \quad (2.74)$$

which is the time taken by the fluid to cover the distance x at the speed u . Then, the x -derivative can be transformed as follows:

$$\frac{\partial c}{\partial x} = \frac{\partial c}{\partial \tau} \frac{\partial \tau}{\partial x},$$

which yields

$$u \frac{\partial c}{\partial x} = \frac{\partial c}{\partial \tau}.$$

Equation (2.73) then becomes

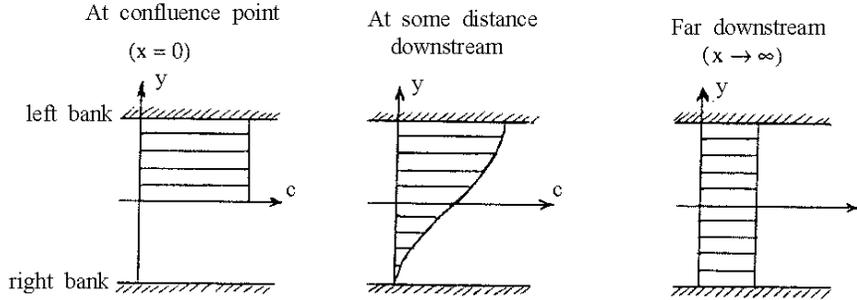


Figure 2-22. Gradual homogenization of the concentration in a river downstream of a confluence. Downstream distance acts as time.

$$\frac{\partial c}{\partial \tau} = D \frac{\partial^2 c}{\partial y^2},$$

which is morphologically identical to (2.4), with the travel time τ replacing the true time t and the transverse coordinate y replacing the canonical coordinate x . The ‘initial’ condition is now the specification of the concentration $c_0(y)$ at the upstream end (say $x = 0$), while the two boundary conditions are to be applied at the edges of the y -interval.

As an example, let us return to the prototypical solution derived in Section 2-1, that corresponding to an instantaneous and localized release. Translated to the case of a wind blowing at speed u , it corresponds to the cross-wind diffusion that proceeds downwind of a release point (e.g., a smokestack) at location $x = 0$ and cross-wind position $y = 0$. Solution (2.12) becomes

$$c(x, y) = M \sqrt{\frac{u}{4\pi Dx}} \exp\left(-\frac{uy^2}{4Dx}\right). \quad (2.75)$$

The quantity M is here to be interpreted as the amount of the contaminant released per unit height and per unit downwind length of fluid (i.e., per unit cross-section perpendicular to the direction in which the diffusion occurs – dimensions M/L^2). Because in such problem the release would typically be expressed in amount per unit height and per unit time, we define the input rate $S = Mu$ (dimensions M/LT), and rewrite the preceding solution:

$$c(x, y) = \frac{S}{\sqrt{4\pi Dux}} \exp\left(-\frac{uy^2}{4Dx}\right). \quad (2.76)$$

The patch width, a function of the downwind distance, can be defined as

$$\text{Width} = 4\sigma = 5.66 \sqrt{D\tau} = 5.66 \sqrt{\frac{Dx}{u}}. \quad (2.77)$$

As a second example, let us consider the case described above of transverse river diffusion downstream of a confluence. The upstream condition (at $x = 0$)

corresponding to a polluted stream (concentration $c = c_0$ for $y > 0$) coming into contact with a clean river (concentration $c = 0$ for $y < 0$) is the step function pictured in Figure 2-9, and the solution is given by (2.25) with time being x/u and the diffusion coordinate being y :

$$c(x, y) = \frac{c_0}{2} \left[1 + \operatorname{erf} \left(y \sqrt{\frac{u}{4Dx}} \right) \right]. \quad (2.78)$$

Note that this solution ignores the presence of boundaries at the river banks, and its validity is thus limited to the immediate downstream vicinity of the confluence point. The generalization of the solution to include boundary effects is left as an exercise for the reader.

Remarks

In closing this section, we recall that the substitution of time for distance is justified only if two conditions are satisfied:

1. The fluid velocity is uniform across the flow (to avoid ambiguity in the distance-time relationship), and
2. The Peclet number is very large (to permit the neglect of diffusion in the stream direction).

When the fluid velocity is not uniform across the flow, diffusion can be greatly enhanced by a special effect called 'shear dispersion'. This is the object of the following chapter.

Chapter 3

NEXT CHAPTER

THIS IS TO ENSURE THAT CHAPTER 2 ENDS ON AN EVEN PAGE SO THAT CHAPTER 3 CAN BEGIN ON AN ODD PAGE.