4. Boundary Conditions

This section discusses the evolution of a diffusing cloud once it encounters a boundary. Emphasis is placed on two common types of boundaries, namely those that are perfectly absorbing and those through which there is no flux. The theory section describes how the use of image sources allows us to correctly model the concentration profile of the cloud in the presence of a boundary. The animation compares the effect that no-flux and perfectly absorbing boundaries have on a diffusing cloud, highlighting the progression to a well-mixed condition in the presence of parallel no-flux boundaries.

4. Boundary Conditions

When a diffusing cloud encounters a boundary, its further evolution is affected by the condition of the boundary. The mathematical expressions of four common boundary conditions are described below.

Specified Flux: In this case the flux per area, $(q/A)_n$, across (normal to) the boundary is specified. The subscript 'n' indicates the direction of the outward facing normal, such that $(q/A)_n$ is understood as the flux leaving the fluid domain. The specified flux boundary condition is then written,

(1) $[CV_n - D_n\partial C/\partial n]_{\text{at the boundary}} = (q/A)_n$ = flux leaving fluid domain at boundary

Specified Constant Concentration: In this case the concentration at the boundary is given.

(2) $C_{\text{at the boundary}} = \text{constant}$

No-flux boundary: This is a special case of the specified flux condition given above, with $(q/A)_n = 0$. The most general condition is,

(3a) $[CV_n - D_n\partial C/\partial n]_{\text{at the boundary}} = 0.$

Again, the subscript 'n' indicates the outward facing normal. For no flux, the advective and diffusive fluxes must exactly balance. If the boundary is solid, then the velocity normal to it is zero, and the constraint is reduced to,

(3b) $\partial C/\partial n = 0$ at boundary.

When the source is located on the boundary (3b) is somewhat misleading, because the symmetry of the Gaussian curve about its center allows (3b) to be satisfied even as mass leaves the real domain. This exception is explained below.

Perfectly Absorbing: Any chemical molecule that touches this boundary is instantly absorbed, and thus removed from the fluid. The concentration in the fluid at this boundary must be zero.

(4) $C_{\text{at the boundary}} = 0$

No-Flux Boundary Condition:
Analytical solutions that satisfy the no-flux boundary condition are found using the principle of superposition. The method requires that the transport equation,

(5) $$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} \pm S$$

be linear. This is generally the case, unless the specific form of the source or sink (±S) is non-linear. If the equation and boundary conditions are linear, then one can superpose (add together) any number of individual solutions to create a new solution that fits the desired initial or boundary condition. The method is demonstrated here for a one-dimensional system in x, into which mass, M, is released at x = 0 and t = 0. For simplicity, velocity is assumed to be zero everywhere in the system. The cross-sectional area perpendicular to the x-direction is A_{yz}. A solid boundary exists at x = -L. Specifically, we wish to solve:

(6a) $$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

(6b) Initial Condition (t = 0): $C(x) = M\delta(x)$
Boundary Condition: $\partial C/\partial x = 0$ at x = -L.

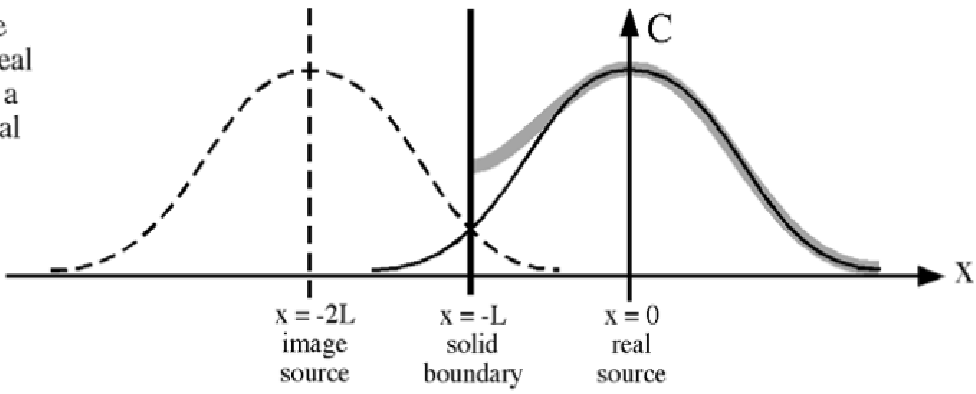
The system's transport equation and initial condition are satisfied by the one-dimensional solution for an instantaneous, point release located at the real source position:

(7) $$C_{real}(x, t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}}\exp\left(-x^2/4Dt\right).$$

However, this solution, shown as a solid black line in the following figure, does not satisfy the no-flux condition at x = -L. Specifically, $\partial C/\partial x > 0$ at x = -L. In addition, (7) allows the mass $\int_{-\infty}^{-L} C(x)dx$ to cross the boundary x = -L. This mass can be exactly replaced within the real domain (x > -L) by adding a new, identical source at x = -2L. The additional source is located at the mirror image to the original source, with the mirror located at the no-flux boundary x = -L. So, we call the added source an image source. The mass distribution for the image source, $C_i(x,t)$, is shown as a dashed line. Its shape is identical to the original source, C(x,t), but its peak is shifted from x = 0 to x = -2L. The shift is accomplished by forcing the exponential term to be one at x = -2L, *i.e.* making the argument zero at x = -2L.

(8) $$C_{image}(x, t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}}\exp\left(-(x+2L)^2/4Dt\right)$$

Figure 1. Add an image source (dashed) to the real source (black) to create a solution (gray) in the real domain (x > -L) that satisfies the boundary condition, $\partial C/\partial x = 0$ at x = -L.



The superposition (sum) of the original and image sources is shown within the flow domain ($x > -L$) as a thick, gray line. Note, specifically that this curve satisfies the condition $\partial C/\partial x = 0$ at $x = 0$, as stated in (6). The solution is thus the sum of (7) and (8),

$$(9) \qquad C(x,t) = C_{real} + C_{image} = \frac{M}{A_{yz}\sqrt{4\pi\, Dt}}\left(\exp\left(-x^2/4Dt\right) + \exp\left(-(x+2L)^2/4Dt\right)\right)$$

Perfectly Absorbing Boundary Condition:
The method of superposition can also be used to satisfy a perfectly absorbing boundary condition. Consider again the one-dimensional system described above, with the boundary at $x = -L$ acting as a perfect absorber. We then seek a solution to,

$$(10a) \qquad \frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

(10b) Initial Condition ($t = 0$): $C(x) = M\delta(x)$
Boundary Condition: $C(x=-L, t) = 0$.

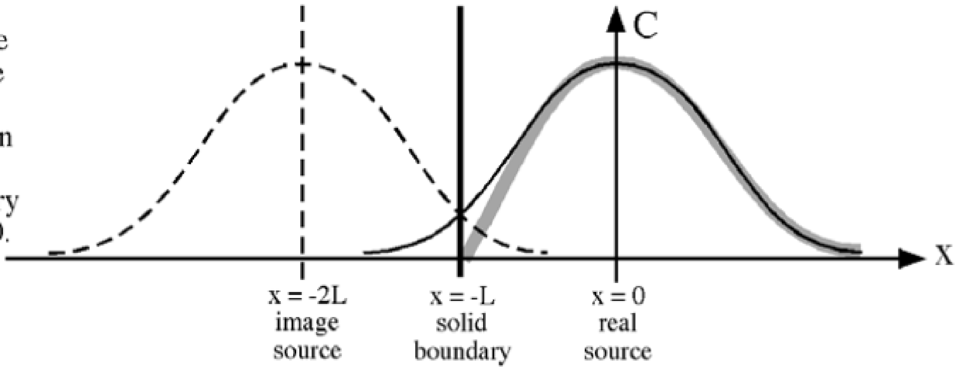
As above, the basic solution within the flow domain will be that for an instantaneous release of mass at a discrete point, namely (7). To satisfy the boundary condition, we now subtract, rather than add, the image source.

$$(11) \qquad C(x,t) = C_{real} - C_{image} = \frac{M}{A_{yz}\sqrt{4\pi\, Dt}}\left(\exp\left(-x^2/4Dt\right) - \exp\left(-(x+2L)^2/4Dt\right)\right).$$

By subtracting the image source (dashed line) from the real source (solid black line), the concentration at the boundary is fixed at zero. Note that the superposed solution (heavy gray line) indicates a flux into the boundary at $x = -L$, i.e. $\partial C/\partial x > 0$, which is consistent with an absorbing boundary. Also note that the solution (11) gives negative concentrations for the region $x < -L$, which is physically unrealistic. However, this region is outside the real flow domain ($x > -L$), so that the unrealistic values are

unimportant. We only require the solution within the real domain ($x > -L$) to be physically reasonable, and it is.

Figure 2. Subtract image source (dashed) from the real source (black) to create a solution (gray) in the real domain (x > -L) that satisfies the boundary condition, C(x= -L,t) = 0.



Multiple Boundaries:

If there is more than one boundary, additional image sources will be required. Continuing with the same one-dimensional system describe above, we now consider boundaries at both x = -L and x = +L.

(12a) $$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

(12b) Initial Condition (t = 0): C(x) = Mδ(x)

Boundary Condition: ∂C/∂x = 0 at x = -L and x = +L

To satisfy a no-flux condition at x = -L, we add an image source at x = -2L, as above. To satisfy a no-flux condition at x = +L, we need an image source at x = +2L. These two image sources are depicted in figure 3.

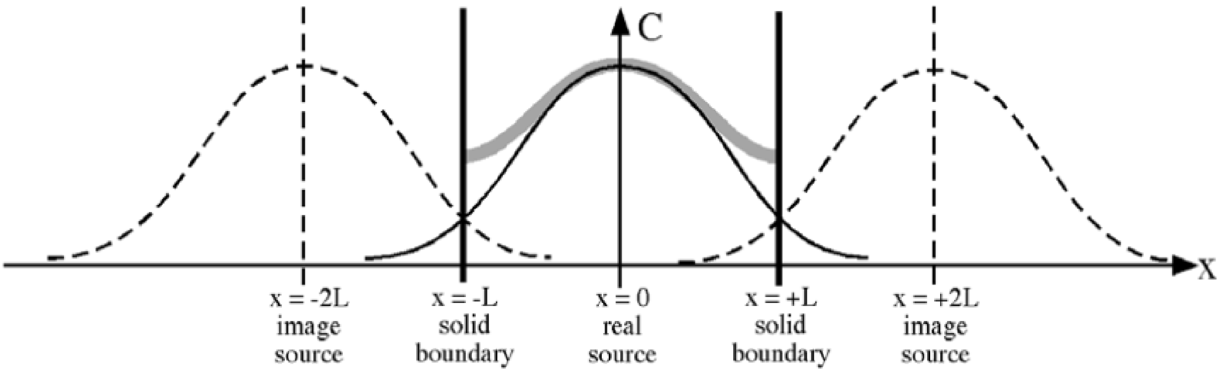


Figure 3. To satisfy the no-flux condition at both boundaries, two image sources (dashed) are added to the real source (black). For short time, the sum of these three sources (gray) is sufficient to satisfy ∂C/∂x = 0 at x = ±L. However, at later time each image source will begin to lose mass across its opposite boundary, and the no-flux condition will no longer be satisfied. Ultimately, images will be needed at x = ± 2nL, for all integer n.

Figure 3 depicts the concentration field for small time. At longer time, one anticipates that, for example, the image source originating at x = -2L will reach and begin to cross the opposite boundary at x = +L and mass will again be lost from the real domain. To balance the loss, an additional image is needed at x = +4L, *i.e.* at the image of x = -2L across a 'mirror' located at the boundary x = +L. Similarly, the image source at x = +2L requires its own image across the x = -L boundary, *i.e.* at x = -4L. Taking this reasoning further, we ultimately need an infinite number of images, just as an object between parallel mirrors generates an infinite number of images. The solution to (12) is then,

$$(13) \qquad C(x,t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} \left(\exp\left(-(x+2nL)^2/4Dt\right)\right).$$

Similarly, if the boundaries at x = ±L are perfect absorbers, we must solve

$$(14a) \qquad \frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

(14b) Initial Condition (t = 0): C(x) = Mδ(x)
Boundary Condition: C = 0 at x = -L and x = +L.

Simple geometric reasoning will show that negative images are needed at x = ± 2L and positive images at x = ±4L, and continuing thusly in an alternating fashion. That is,

$$(15) \qquad C(x,t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} \left(\underbrace{-\exp\left(-\frac{(x+(4n-2)L)^2}{4Dt}\right)}_{\text{negative image}} + \underbrace{\exp\left(-\frac{(x+4nL)^2}{4Dt}\right)}_{\text{positive image}} \right).$$

Boundaries in two- and three-dimensional systems:
The method of superposition described above for one-dimensional systems is readily extended to two- and three-dimensional systems. As an example, consider a three-dimensional domain filled with a stagnant fluid (zero current). The system is bounded below by a solid plane at y = 0, such that the domain of interest occupies y ≥ 0. The system is unconstrained in the x-z plane. A slug of mass, M, is released at the point (x, y, z)=0 at the time t = 0. Diffusion is isotropic and homogeneous. Note that because the source is located on the boundary, the gradient condition (3b) is insufficient to inhibit loss of mass from the real domain (y≥0). A more general boundary condition is used,

$$(16a) \qquad \frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right)$$

(16b) Initial Condition (t = 0): C(x) = M δ(x) δ(y) δ(z)
Boundary Condition: no-flux out of fluid domain at y = 0.

A general solution that satisfies the stated transport equation and initial condition is given by equation (25) in chapter 3, and repeated here for convenience.

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

In fact, this solution also satisfies the gradient expression for a no-flux boundary condition, *e.g*. as given in (3b). However, this solution does not conserve mass within the real domain, but rather allows half of the mass to diffuse into the region $y < 0$, violating the no-flux boundary condition. To satisfy the no-flux condition at $y = 0$, we must add an image source. The image of the real source, located at $y = 0$, across the plane $y = 0$ will also be located at $y = 0$. Since the real and image sources are co-located, we need only add a factor of 2 to the solution given above. Additionally noting that the diffusion is isotropic ($D_x = D_y = D_z = D$), the solution to (16) is,

$$(17) \qquad C(x, y, z, t) = 2\,\frac{M}{(4\pi Dt)^{3/2}} \exp\left(-\frac{x^2 + y^2 + z^2}{4Dt} \right).$$

As a final case, we consider parallel boundaries in a three-dimensional system. The fluid domain is unconstrained in the x-z plane, but constrained in the y-direction by solid, planar boundaries located at $y = \pm L$. There is no current and the diffusion is isotropic and homogeneous. An instantaneous release of mass, M, occurs at $x = y = z = t = 0$. The appropriate transport equation and initial conditions are,

$$(18) \qquad \frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right), \text{ with } C(x, y, z, t{=}0)) = M\,\delta(x)\,\delta(y)\,\delta(z).$$

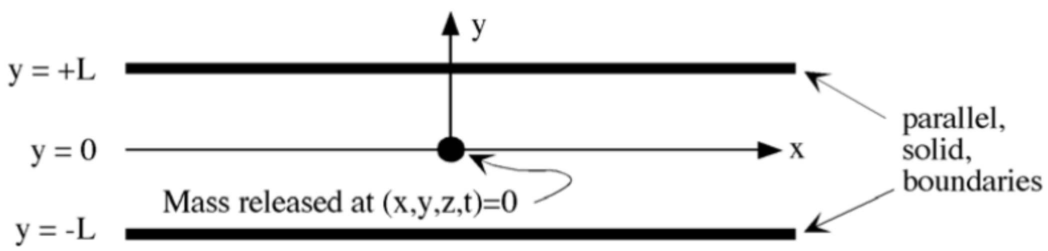


Figure 4. Mass released mid-way between parallel, solid boundaries. System is unconfined in x and z.

To satisfy either a no-flux or perfectly absorbing boundary condition, we will add image sources at positions corresponding to the mirror images of the real source across the planes $y = \pm L$. The real source is located at (x=0, y=0, z=0). The image sources must be then be located at (x=0, y=2nL, z=0) with $n = \pm 1, \pm 2, \pm 3$ upward to $\pm$ infinity. If the boundaries at y = ± L permit no flux, the image sources will all be positive, and the concentration field is described by,

$$(19) \qquad C(x, y, z, t) = \frac{M}{(4\pi\, Dt)^{3/2}} \sum_{n=-\infty}^{\infty} \exp\left(-\frac{x^2 + (y + 2nL)^2 + z^2}{4Dt}\right)$$

If the boundaries at y = ± L are perfect absorbers, both positive and negative image sources will be needed. The concentration field is can then be described by,

$$(20) \qquad C(x, y, z, t)=$$

$$\frac{M}{(4\pi\, Dt)^{3/2}} \sum_{n=-\infty}^{\infty} \left(-\exp\left(-\frac{x^2 + (y + (4n-2)L)^2 + z^2}{4Dt}\right) + \exp\left(-\frac{x^2 + (y + 4nL)^2 + z^2}{4Dt}\right)\right).$$

Animation to Compare Perfectly Absorbing and No-Flux Boundaries -
The animation on the chapter homepage examines the evolution of concentration after a slug mass is released mid-way between solid, parallel boundaries, as in Figure 4. Two scenarios are shown, perfectly absorbing and no-flux boundaries, using the solutions (19) and (20) above. For each system the concentration field is displayed in the plane z = 0. In addition, the concentration profile C(x=0, y, z=0) for each system is plotted for comparison on a single graph.

Before you view the animation answer the following questions.

1. The parallel boundaries are located at y = ± 70 cm, and the diffusivity is $D = 1\ cm^2s^{-1}$. Estimate the time at which the boundaries will begin to impact the evolution of the diffusing cloud.
2. For which boundary condition will peak concentrations decrease more rapidly? Why?
3. What will be the final concentration in each system?

As you view the animation consider the following.

4. Based on the profiles at (x=0, y, z=0), at what time do the boundary conditions begin to impact the concentration field? How does this compare to your prediction in 1)?
5. If the two profiles C(x=0, y, z =0) were not labeled, how would you identify the profile evolving with a no-flux boundary? with an absorbing boundary?
6. Finally, consider the system with no-flux boundaries. Note that over time the profile perpendicular to the boundaries, C(y), becomes increasingly uniform. Eventually, this profile will be sufficiently uniform to consider the system well mixed in this dimension. Evolution of the cloud beyond this point in time will proceed as if the system were two-dimensional in x and z. This is discussed in more detail below.

Answers

1. A common length scale for a diffusing patch defines the edge of the cloud at 2σ from the centroid (chapter 1). Based on this definition, the cloud edge touches the boundary when $L = 2\sigma = 2\sqrt{2Dt}$. With L = 70 cm and $D = 1 cm^2 s^{-1}$, t = 613 s. But, the 2σ delineation of the cloud edge encompasses only 95% of the total mass in the cloud, such that at t = 613 s 5% of the mass has already reached and passed the boundary. A more conservative estimate would define the cloud edge at 3σ, for which the edge of the cloud will touch the boundary at $t = L^2/(18D) = 270$ seconds. At this time, only 0.3% of the mass has reached the boundary (chapter 1).
2. The peak concentration should decay more rapidly in the system with absorbing boundaries, because the boundaries permit flux, and thus additional dilution, compared to the no-flux boundaries.
3. Since each system is unconfined in x and z, the final concentration will be zero.
4. Based on the animation, the two curves begin to diverge at about 250 seconds. This reasonably agrees with the time estimated for $L = 3\sigma$.
5. The boundary conditions are reflected in the profile shape at the boundary. For the absorbing boundary condition, $\partial C/\partial y > 0$ at y = -L and < 0 at y = +L, both of which indicate flux into the boundary. For the no-flux boundary, $\partial C/\partial y = 0$ at both boundaries.

Time-scale for achieving a uniform condition between boundaries.

We saw in chapter 3 that the transport equation is simpler in systems that may be approximated in reduced dimensions, *e.g*. two rather than three dimensions. When one first considers a system, it is therefore useful to determine whether a reduction in dimensions is possible. To eliminate a given dimension, *e.g*. y, one must show that the concentration is uniform in y, that is $\partial C/\partial y = 0$. If $\partial C/\partial y = 0$, then both the diffusive flux ($D\, \partial^2 C/\partial y^2$) and the advective flux ($v\, \partial C/\partial y$) in y are eliminated,

$$(21) \qquad \frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + \cancel{v\frac{\partial C}{\partial y}} + w\frac{\partial C}{\partial z} = D\left[\frac{\partial^2 C}{\partial x^2} + \cancel{\frac{\partial^2 C}{\partial y^2}} + \frac{\partial^2 C}{\partial z^2}\right]$$

reducing the transport equation to two-dimensions in x and z. For example, consider the system represented in the above animation with parallel, no-flux boundaries at $y = \pm L$. Initially, the concentration field is three-dimensional with gradients in x, y, and z. Over time the profile perpendicular to the boundaries, C(y), becomes uniform. A temporal progression of C(y) is shown in Figure 5 below. The basic unit of time, L^2/D, is selected from dimensional reasoning. From Figure 5, one sees that the system is uniform in y, i.e. perpendicular to the boundaries, at $t = t_y = (2L)^2/4D$, which is called the mixing-time.

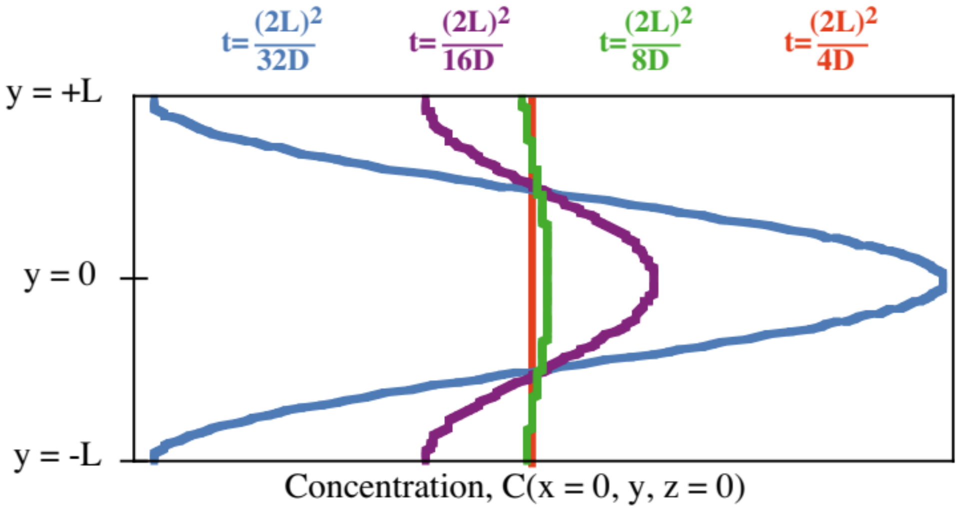


Figure 5. A slug of mass is released at (x, y, z, t)=0 into a fluid domain that is unconstrained in the x-z plane, but is constrained by parallel, no-flux boundaries at y = +L and -L. The profiles of concentration, C(x=0, y, z=0), are plotted for several times after the release. The system is fully mixed (uniform) across the y-domain in a time $t = (2L)^2/4D$.

At times greater than the mixing time $\partial C/\partial y = 0$, and the system can be considered in two-dimensions (x and z) only. That is, for $t > t_y$, the transport equation reduces to,

(22) $$\frac{\partial C}{\partial t} = D\left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2}\right],$$

and the evolution of concentration is described by the solution for an instantaneous, point-release in *two-dimensions* (see chapter 3), that is for $t > t_y$

(23) $$C(x,z,t) = \frac{M}{(2L)\, 4\pi D t}\exp\left(-\frac{x^2 + z^2}{4Dt}\right),$$

where (2L) is the length-scale of the now neglected dimension.

Definition of Mixing Time

For a generic system, we define the length-scale of interest as the full width of the domain in a given direction, e.g. L_x, L_y, L_z. If mass is released in the center of the domain, the time-scales required to achieve uniform conditions in each dimension is,

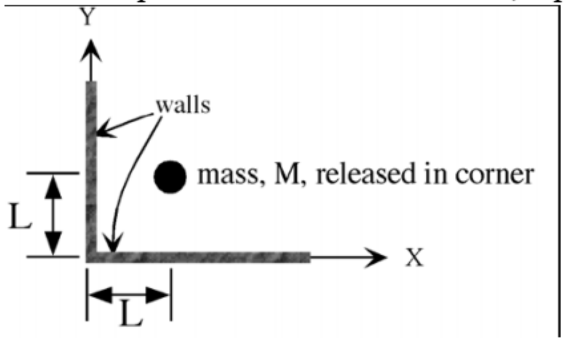
(24) Mixing Time $t_i = L_i^2/4D_i$, where i = x, y, z.

While the above time scale is a standard definition, from Figure 5, we can see that nearly uniform conditions are approximated at the shorter time $L_i^2/8D_i$.

CLASS EXERCISES WITH SOLUTIONS

Problem 4.1

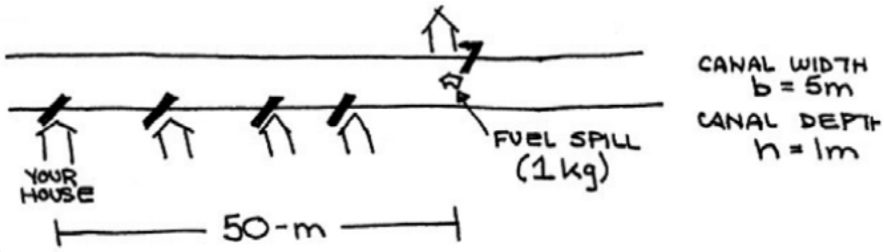
A slug of mass, M, is released instantaneously into the corner of a large, shallow box. The full width and length of the box are $L_X = L_Y = 100L$, and the height of the box is $L_Z = 0.01L$. Every wall of the box is a no-flux boundary. The mass is released a distance L from two adjacent walls, and mid-way between the top and bottom boundary.
Assume isotropic diffusion within the box, represented by diffusivity, D.



Describe the concentration field inside the box from t = 0 to $t = L^2/D$.

***Hint 1** When will the mass be mixed uniformly in the vertical?*
***Hint 2** Estimate when the mass will reach each vertical wall in the box*
***Hint 3** How will each boundary impact the solution in the time t = 0 to L^2/D ?*
***Hint 4** Place image sources to satisfy the no-flux boundary condition*

Problem 4.2



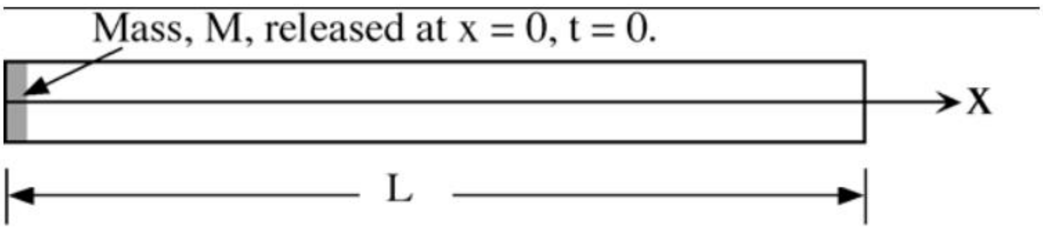
You own a house and dock along a boat canal, which ends 25 m upstream from you. One day, your neighbor has a small (1 kg) fuel spill. Due to the boat traffic, the diffusivity in the canal is quite high, $D = 0.01\ m^2/s$. The current in the canal is negligible, such that the fuel is transported to your house (x = -50 m) by diffusion only. Assume the fuel mixes rapidly across the width and depth, and that there is no flux through the canal walls.

(a) What is the concentration at your house 10 hrs after the spill?
(b) What is the maximum concentration at your house, and when does it occur?
(c) Suppose the safety limit is $0.2\ g/m^3$. At what time after the spill is this concentration reached?
(d) Repeat a, b & c assuming that the boundary at x = -75 m is totally absorbing.

Problem 4.3

A slug of dye, M = 1mg, is released at one end of a sealed tube and in such a way that it uniformly fills the cross-section y-z. Every boundary of the tube is a no-flux boundary.

The tube length is L = 10-cm, molecular diffusion is $D = 10^{-5}\ cm^2 s^{-1}$, and the cross-section of the tube is $A_{yz} = 1\ cm^2$. Assume 1-D diffusion.



a) Estimate the time scale, T, at which the dye will become uniformly distributed in x.
b) Confirm your estimate by plotting C(x) at the times t = T/10, T/4, T/2, T.

CLASS EXERCISES – SOLUTIONS

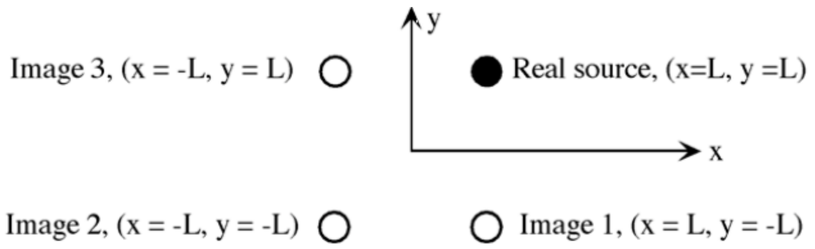
Answer 4.1 - Describe the concentration field inside the box from t = 0 to $t = L^2/D$.

Hint 1 - When will the mass be mixed uniformly in the vertical?
From equation 4.24 a mass released mid-way between two parallel boundaries a distance L_Z apart will be mixed to a uniform concentration between those boundaries in time $t = L_Z^2/4D$, where L_Z is the distance between the boundaries. The time for the concentration to become well-mixed in the vertical is then, $t = (0.01L)^2/D = 0.0001\ L^2/D$.

Hint 2 - Estimate when the mass will reach each vertical wall in the box.
We estimate the time that the cloud will first touch a boundary based on the standard deviation of the mass distribution. The cloud will touch the top and bottom walls when, $3\sigma = 3\sqrt{2Dt} = L$, or at the time $t = L^2/18D$. The cloud will touch the far wall when $3\sigma = 3\sqrt{2Dt} = 99L$, or at the time $t \approx 545L^2/D$.

Hint 3 - How will each boundary impact the solution in the time t = 0 to L^2/D?
Use the time scales determined in hint 1 and 2. Because the concentration field becomes uniform in the vertical very rapidly, within 1/10,000th of the time of interest, we will assume that the concentration is instantly uniform in z, i.e. $\partial C/\partial z = 0$ for all time. In the time of interest, the cloud will never reach the far walls ($545L^2/D >> L^2/D$), so these boundaries do not impact the solution. The cloud will reach the near walls ($L^2/18D < L^2/D$), and a correction must be made to satisfy the no flux condition at these walls.

Hint 4 - Place images sources to satisfy the no-flux boundary condition.
Image sources are needed at the following locations. Image 2 balances the loss of mass from Image 3 across the x-axis and the loss of mass from Image 1 across the y-axis.



Solution - The concentration in the box is described by a superposition of two-dimensional, instantaneous, slug releases (equation 3.23) at each of the above sources.

$$C(x, y, t) = \frac{M}{L_z 4\pi\, Dt} \bullet$$

$$\left(\exp\left(-\frac{(x-L)^2 + (y-L)^2}{4Dt}\right) + \exp\left(-\frac{(x-L)^2 + (y+L)^2}{4Dt}\right) + \exp\left(-\frac{(x+L)^2 + (y+L)^2}{4Dt}\right) + \exp\left(-\frac{(x+L)^2 + (y-L)^2}{4Dt}\right)\right)$$

real source image 1 image 2 image3

Solution 4.2

(a) An image source is needed at x = -150 m to account for the no-flux boundary at the end of the canal. The concentration of fuel in the canal is described by the superposition of these two instantaneous, 1-D sources.

$$C(x,t) = \frac{M}{A\sqrt{4\pi Dt}}\left[\underbrace{\exp\left(\frac{-x^2}{4Dt}\right)}_{REAL} + \underbrace{\exp\left(\frac{-(x+150)^2}{4Dt}\right)}_{IMAGE}\right]$$

Therefore, at x = -50 m, t = 10 hrs (= 36000 s),

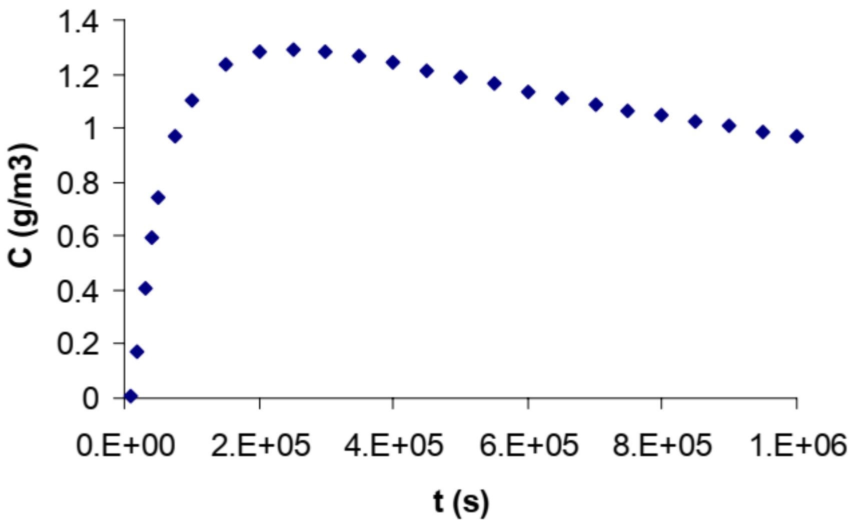
$$C = \frac{1000\text{ g}}{5\text{ m}^2\sqrt{4\pi(0.01\text{ m}^2\text{s}^{-1})(36000\text{ s})}}\left[\exp\left(\frac{-(-50\text{ m})^2}{4(0.01\text{ m}^2\text{s}^{-1})(36000\text{ s})}\right) + \exp\left(\frac{-(100\text{ m})^2}{4(0.01\text{ m}^2\text{s}^{-1})(36000\text{ s})}\right)\right]$$

$$= 2.97\text{ gm}^{-3}(0.176 + 0.001) = \mathbf{0.53\ gm^{-3}}$$

(b) This is best solved graphically. The plot of:

$$C(-50\text{ m}, t) = \frac{1000\text{ g}}{5\text{ m}^2\sqrt{4\pi(0.01\text{ m}^2\text{s}^{-1})t}}\left[\exp\left(\frac{-(-50\text{ m})^2}{4(0.01\text{ m}^2\text{s}^{-1})t}\right) + \exp\left(\frac{-(100\text{ m})^2}{4(0.01\text{ m}^2\text{s}^{-1})t}\right)\right]$$

is shown below.



From this plot, we can see that the maximum concentration at the house is approximately **1.3 gm^{-3}** (when $t \approx 2.4 \times 10^5$ s = 67 hrs)

(c) The easiest ways to solve the equation in (b) for C = 0.2 gm^{-3} are graphically, or by trial and error. As the above plot lacks detail in the early stages, we will use trial and error in our spreadsheet to solve

$$0.2\ \text{gm}^{-3} = \frac{1000\ \text{g}}{5\ \text{m}^2\sqrt{4\pi(0.01\ \text{m}^2\text{s}^{-1})t}}\left[\exp\left(\frac{-(-50\ \text{m})^2}{4(0.01\ \text{m}^2\text{s}^{-1})t}\right)+\exp\left(\frac{-(100\ \text{m})^2}{4(0.01\ \text{m}^2\text{s}^{-1})t}\right)\right]$$

for t. This yields a solution of ***t* = 21060 s = 5.8 hrs**.

Compare this solution to that of Problem 1.5 to see the effect that the no-flux boundary has on the concentration of fuel observed at your house.

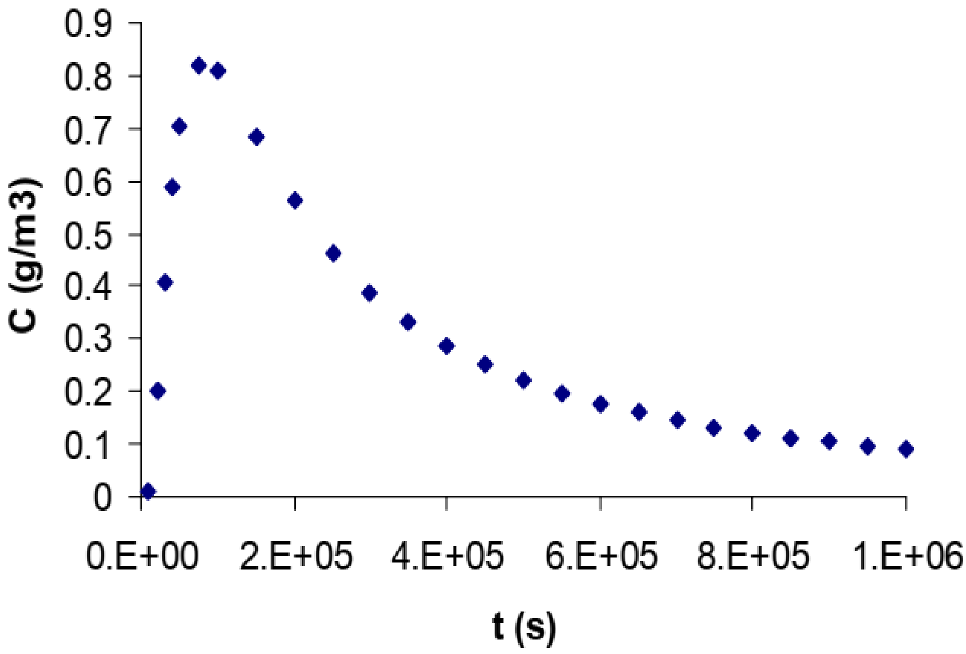
(d) An image **sink** is needed at x = -150 m to account for the perfectly absorbing boundary at the end of the canal (see Chapter 4 notes, p 4)

$$C(x,t) = \frac{M}{A\sqrt{4\pi Dt}}\left[\underbrace{\exp\left(\frac{-x^2}{4Dt}\right)}_{REAL} - \underbrace{\exp\left(\frac{-(x+150)^2}{4Dt}\right)}_{IMAGE}\right]$$

Repeating (a) – (c) is relatively simple, the results being:

- $C(x = -50\ \text{m}, t = 36000\ \text{s})$ = **0.52 gm^{-3}** (i.e. at this short time, the boundary has little/no effect).

- $C_{max}(x = -50\ \text{m})$ = **0.82 gm^{-3}** (i.e. at $t \approx 83000$ s = 23 hrs).

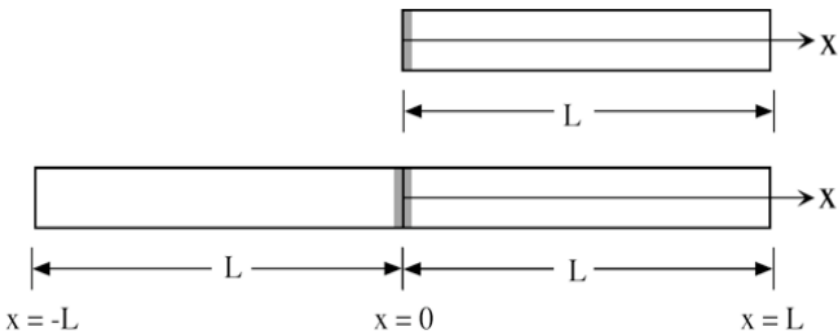


- $C = 0.2$ gm^{-3} when ***t* = 21060 s**. This is the same answer as in (c) – before the cloud encounters the boundary (i.e. for $2\sqrt{2Dt} < 75\,\text{m} \Rightarrow t < 70300\text{ s}$), the boundary has little/no effect.

Answer 4.3

a) Estimate the time scale, T, at which the dye becomes uniformly distributed in x.

The diffusion of dye released at the end wall (top figure) will be similar to the diffusion of dye released mid-way between end walls placed twice as far apart (bottom figure). This is because the diffusion in both systems proceeds as a function of $\exp(-x^2/4Dt)$, which is symmetric about x = 0. From this similarity we expect that the dye will be well mixed in both systems in the time-scale already established for the bottom system. Specifically, from eq. 4.24 applied to the bottom system, $T = (2L)^2/4D = L^2/D = 10^7$ sec.

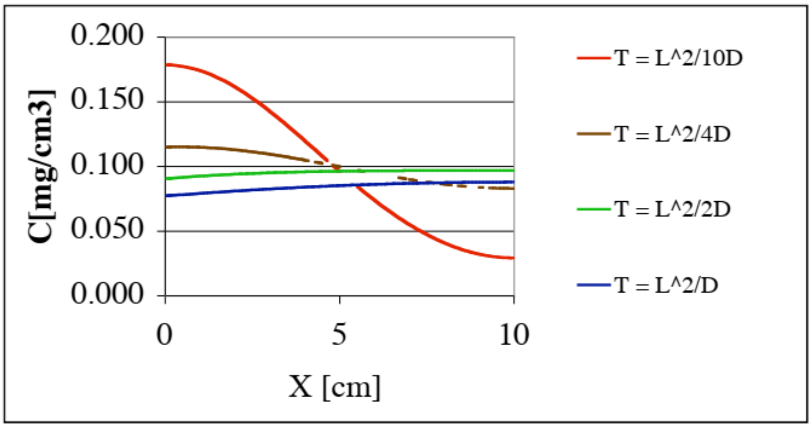


b) Confirm your estimate by plotting C(x) at the times t = T/10, T/4, T/2, T.

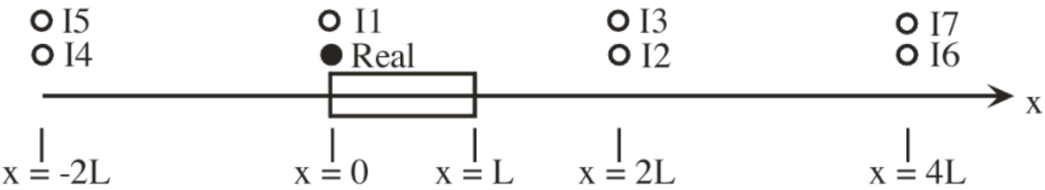
Theoretically an infinite number of images is needed to satisfy a no-flux boundary condition at two parallel boundaries. For simplicity we initially consider only one image position for each boundary. The boundary at x=0 requires image I1 at x=0, i.e. co-located with the source. The boundary at x=L requires image I2 at x=2L for the real source, as well as image I3 for the image source I1. The concentration field is,

$$C(x,t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}}\left(2\exp\left(-x^2/4Dt\right) + 2\exp\left(-(x-2L)^2/4Dt\right)\right)$$

Real + I1 I2+I3

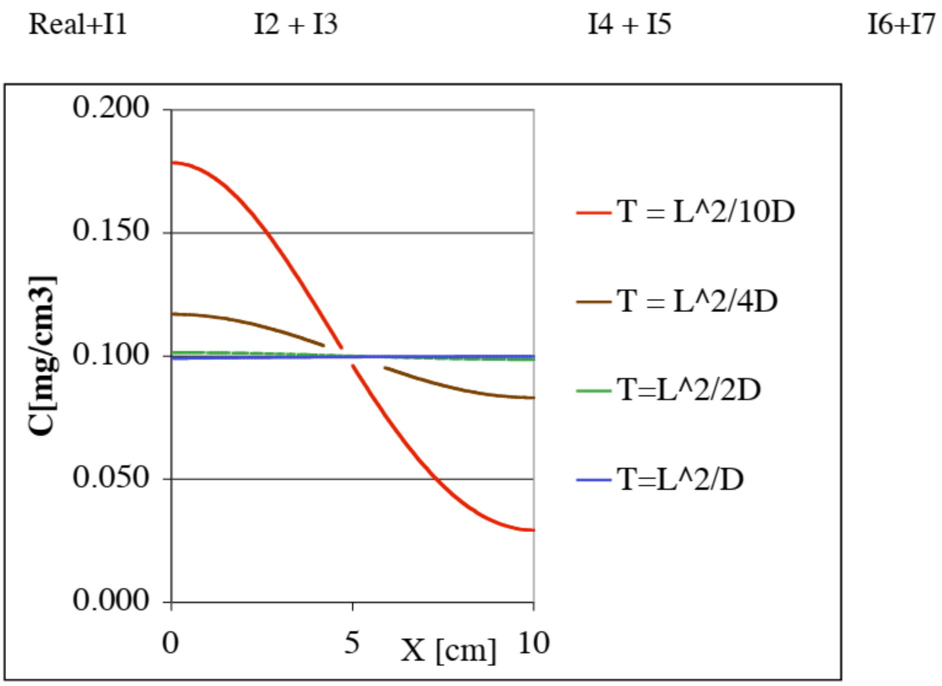


The solution indicates that three images are not sufficient, because mass is not conserved in the time of interest. The final concentration should be 1mg/(10cm^3) = 0.1 mg cm^{-3}, but the above solution yields 0.66 mg cm^{-3} at t =L^2/D. In addition, the gradient of concentration should be zero at the boundaries, $\partial C/\partial x = 0$, to satisfy the no-flux condition. This condition is not met at x = 10cm. For comparison, we now consider a solution with seven images, each denoted by I.



I1 balances the real source at boundary x = 0.
I2 and I3 balance the real source and I1 at boundary x = L.
I4 and I5 balance I2 and I3 across the boundary at x = 0.
I6 and I7 balance I4 and I5 across the boundary at x = L.

$$C(x,t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}}\left(2\exp\left(-x^2/4Dt\right) + 2\exp\left(-(x-2L)^2/4Dt\right) + 2\exp\left(-(x+2L)^2/4Dt\right) + 2\exp\left(-(x-4L)^2/4Dt\right)\right)$$



With seven images the concentration is correct at $T = L^2/D$. At longer times mass will still be lost due to unbalanced images and the concentration will decline. However, longer times hold no interest, because once the system is well mixed in x ($\partial C/\partial x = 0$ for all x), the solution may be ended as no further evolution of the true profile will occur. Note, the shape of the concentration profiles are similar with 2 and 6 images, and both solutions indicate a uniform distribution in x is achieved by $T = L^2/D$.