

Environmental Transport and Fate

Chapter 2

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Diffusion – Part 2: Other initial & boundary conditions

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Problems with other conditions

Not every instance of a contaminant in the environment is the result of an localized and instantaneous release in a virtually infinite domain. We thus need to consider other initial and boundary conditions, namely:

- What happens if the release occurs over a finite area?
- How should we handle a finite domain?

To tackle these variations, we capitalize on the fact that the diffusion equation is linear in its variable, the concentration c . This allows us to use the superposition principle: The sum of solutions make a new solution.

First, consider the case of an initial (still instantaneous) release over a finite area. For this, we simply say that the outcome is the same as if there were very many tiny localized releases close to one another filling a finite interval.

To begin, suppose that we have a localized, instantaneous release no longer at position $x = 0$ but now at $x = \xi$. To accommodate this, we simply shift the prototypical solution by measuring distance now from $x = \xi$.

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

Suppose next that there are two releases, one of amount $M(\xi_1)$ at $x = \xi_1$ and another of amount $M(\xi_2)$ at $x = \xi_2$. The solution is then the superposition of two individual solutions:

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

From two releases, we can proceed to a very large number of them by summation. As an infinite sum of many small pieces becomes an integral, we have

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

in which $dM(\xi)$ is the small release occurring in the narrow zone extending from ξ to $\xi+d\xi$. This small release can be written for convenience as

$$dM(\xi) = \frac{dM(\xi)}{d\xi} d\xi = c_0(\xi) d\xi$$

and the preceding solution becomes

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

In this expression, the quantity $c_0(\xi)$ is none other than the initial concentration distribution, a given.

The preceding form of superposition

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

is called a *convolution*.

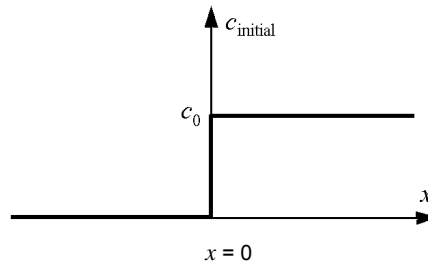
A convolution is none other than the use of an intermediate function (called kernel) to transform an input function into a different, output function.



In the present case, the kernel function is $\frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x-\xi)^2}{4Dt}\right]$ which is none other than the unit prototypical solution

A particular case

As an application, consider the problem of an infinite domain clean on one side ($c = 0$) and uniformly dirty ($c = c_0 = \text{constant}$) on the other.



The solution is

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

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

The integral cannot be expressed in terms of simple function, but the same integral arises in statistics, and statisticians have defined for their convenience the so-called *error function*, as follows

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\zeta^2} d\zeta$$

which represents twice the area under the normalized bell curve, starting from the middle. Key properties of the error function are:

$$\begin{aligned} \operatorname{erf}(0) &= 0, & \operatorname{erf}(+\infty) &= 1 \\ \operatorname{erf}(-z) &= -\operatorname{erf}(z) \end{aligned}$$

Sample values are:

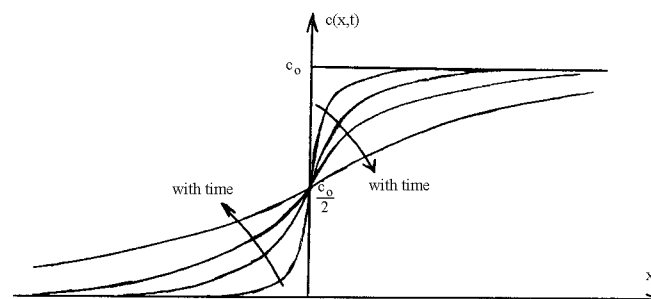
z	$\operatorname{erf}(z)$
0.0	0.0000
0.2	0.2227
0.4	0.4284
0.6	0.6309
0.8	0.7421
1.0	0.8427
1.2	0.9103
1.4	0.9523
1.6	0.9763
1.8	0.9891
2.0	0.9953
3.0	$1 - 2.32 \times 10^{-5}$
4.0	$1 - 1.59 \times 10^{-8}$
5.0	$1 - 1.57 \times 10^{-12}$
6.0	$1 - 2.18 \times 10^{-17}$
7.0	$1 - 2.10 \times 10^{-45}$
$+\infty$	1.0000

(see additional values in written notes, page 44)

In terms of the error function, the solution to the diffusion problem at hand is:

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

and looks like

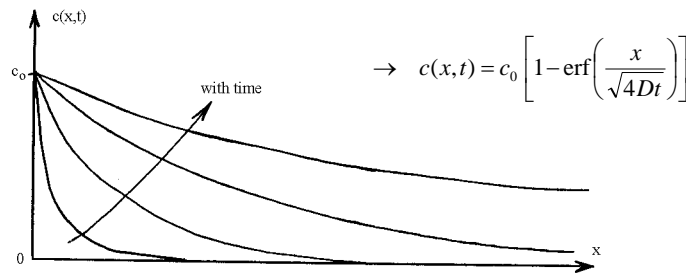


A variation on the previous case

Since the middle value remains constant (at $c_0/2$) in the previous solution, we may remove half of the domain and consider the problem of diffusion in a semi-infinite domain from a boundary where the concentration is held at a constant value.

To make this more practical, replace $c_0/2$ by c_0 and reverse the x -axis.

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \quad \text{with} \quad c(0) = c_0 \quad \text{and} \quad c(+\infty) = 0$$

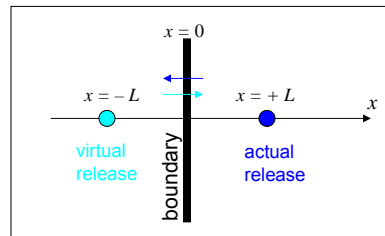


Effect of an impermeable boundary

Because physical boundaries are generally impermeable (such as the bank of a river), problems with domain boundaries requiring the implementation of a no-flux condition are quite common.

If $x = 0$ designates the location of a boundary, we impose there $q = -D \frac{\partial c}{\partial x} = 0$

The earlier, prototypical solution 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.



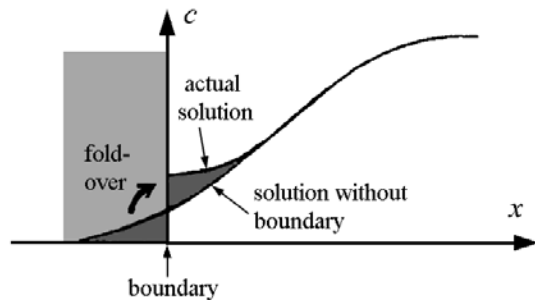
In other words, the situation with one release and a boundary is equivalent to another with two releases and no boundary. The solution is thus

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

From actual release at $x = +L$

From virtual release at $x = -L$

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.

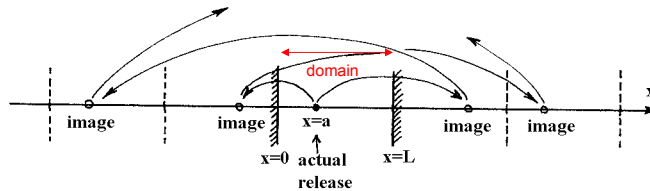


As time goes on, the piling up along the boundary ($x = 0$) starts to overtake the decreasing peak at the release location ($x = L$), and thereafter the concentration is maximal at the boundary and decreasing inward.

And what happens when there are 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:

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



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 $x = +4L - a$, etc. 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.

The solution for a release at position $x = a$ in the finite domain $0 \leq x \leq L$ is then:

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

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.

Application

We return to the previous example with the Chicago Ship Canal. This time, however, we shall be concerned with the earlier-time evolution of the benzene spill ($m = 87.9$ kg), namely when diffusion proceeds vertically in the canal (through depth $H = 8.07$ m), 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 $A = 2$ m², and the vertical diffusion coefficient is $D = 0.010$ m²/s.

The spill takes place at the surface ($x = H$) and diffusion proceeds downward, down to the bottom ($x = 0$). Thus, in this problem, $L = H$, and $a = H$. The solution is:

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

Note that at $x = H$, there is both the actual release and the first image, because the release occurs right at the boundary. Hence, factor 2 in front of the entire expression.

where $M = m/A = (87.9 \text{ kg}) / (2 \text{ m}^2) = 43.95 \text{ kg/m}^2$.

From this solution, consider the concentrations at the extremities

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

$$\text{Bottom } (x = 0): c_{\text{bottom}}(t) = \frac{M}{\sqrt{\pi Dt}} \left[2 \exp\left(-\frac{H^2}{4Dt}\right) + 2 \exp\left(-\frac{9H^2}{4Dt}\right) + \dots \right]$$

Sample values

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 hour	5.493 g/L	5.400 g/L
1.5 hours	5.449 g/L	5.443 g/L
2 hours	5.446 g/L	5.446 g/L

We note that there is a tendency toward homogenization, which makes c at surface and bottom become equal over time. QUESTION: By what time is domain well mixed?

Final concentration and 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.*

$$c_{\text{ultimate}} = c_{\text{average}} = \frac{M}{L}$$

We define the time T until nearly complete homogenization as the time it takes to reach the point when the maximum concentration in the domain has fallen to just 1% over the ultimate, average value.

This is a complicated mathematical problem, and we only give here the solution.

➤ If release occurs in the middle ($a = L/2$): $T = 0.134 \frac{L^2}{D}$

➤ If release occurs at one of the boundaries ($a = 0$ or L): $T = 0.536 \frac{L^2}{D}$

For the Chicago Ship Canal, the value is $T = (0.536)(8.07 \text{ m})^2 / (0.01 \text{ m}^2/\text{s}) = 3491 \text{ s} = 58 \text{ min}$. This compares favorably with the concentrations at the surface and bottom, which are within 1% of their ultimate values 1 hour after the spill.