Numerical Methods in Mechanics and <u>Environmental Flows</u>

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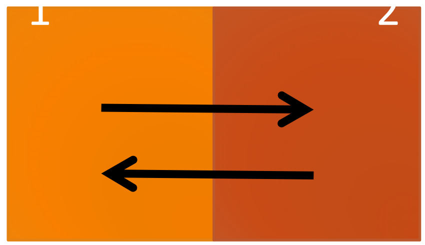
1-D DIFFUSION DETAILS

Deriving gradient relationship (Fick’s law)

The problem of randomness allows us to approach diffusion from a statistical approach



$$q = -D\frac{dc}{dx}$$

A simple budget allows us to derive a diffusive flux equation:

- With the following assumptions
- 1. No net flow from one box to another → if there is a flow from 1-2 there must be a compensating and equal flow from 2 – 1.
- 2. Multiply by dx and take limit to infinitestimal

What is D and what units for D?

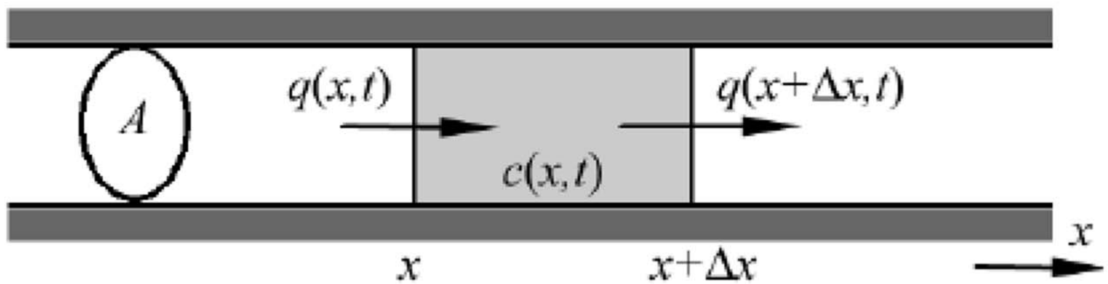
- D is diffusion coefficient or diffusivity (m2/s)

An important point: $q \propto \frac{dc}{dx}$ → what does this imply?

- No gradient, no flux. Larger gradient, larger flux.

Analogous to Fourier’s law of heat conduction

If we then use a mass budget



Budget: $$V\frac{dc}{dt} = Q_i - Q_o = q_i A - q_o A = q_{(x,t}) A - q_{(x+\Delta x,t)} A$$

Dividing by V; $$\frac{dc}{dt} = -\frac{q_{(x+\Delta x,t)} - q_{(x,t)}}{\Delta x}$$

Taking limits: $$\frac{\partial c}{\partial t} = -\frac{\partial q}{\partial x}$$

Putting it all together

From mass budget, $$\frac{\partial c}{\partial t} = -\frac{\partial q}{\partial x}$$

From Fick's $$q = -D\frac{dc}{dx}$$

This results in $$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right)$$

- This is the 1D diffusion equation.
- Most times the equation is simplified by treating D as constant in space → Is this realistic?

What do we need to solve this?

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

Initial conditions

- How many and what?

Boundary conditions

- How many and what?

Similarity Solution to the 1D Diffusion Equation

First recognize that this is a linear Equation

- → Possible to add solutions!

Therefore start with a simple (elementary) problem:

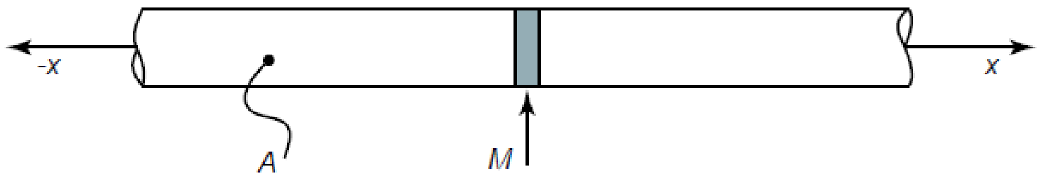
- Instantaneous
- Localized release
- Infinite Domain free of the concentration
- Constant D

Solution can be derived through a combination of

- Dimensional analysis
- Pure mathematical solution

The Simple Problem

Problem



- 1D Narrow, Infinite Pipe (r = a)
- Impose C at +/- infinity = 0 [2 B.C] $C(\pm\infty, t) = 0$
- Point source of Mass M is injected uniformly across at x, point=0 [1 I.C]
  - Thus total injected mass is

$$C(x,0) = (\frac{M}{A})\delta(x)$$

Solution Step (1)

Dimensional analysis [revise on your own].

Essentially one ends up with 2 dimensionless groups

-
- And $\pi_1 = f(\pi_2)$

Which implies our solution for C is $c(x,t) = \dfrac{M}{A\sqrt{Dt}} f\left(\dfrac{x}{Dt}\right)$

To solve this we will use similarity solution method

Solution Step (2)

First create a variable, $\eta = x/\sqrt{Dt}$

Create two derivatives $\frac{\partial \eta}{\partial t} = -\frac{\eta}{2t'};\qquad \frac{\partial \eta}{\partial x} = \frac{1}{\sqrt{Dt}}$

Use chain rule to then obtain $\frac{\partial C}{\partial t}$ and $\frac{\partial^2 C}{\partial x^2}$

Substituting results in an ODE

$$\frac{\partial^2 f}{\partial \eta^2} + 0.5\left(f + \eta \frac{\partial f}{\partial \eta}\right) = 0$$

Solution Step (3)

Using identity, we obtain $\frac{\partial}{\partial\eta}\left[\frac{\partial f}{\partial\eta} + 2f\eta\right] = 0$

Integrating twice, taking C_0=0 at both ends leads us to $f = C_1 \exp(-\eta^2/4)$

Using coordinate transformation and solving for C1 gives us

$$C_1 = \frac{1}{\int_{\infty}^{\infty} \exp(-\tfrac{1}{4}\eta^2)\,d\eta}$$

- Which can be found to be $C_1 = 1/\left(2\sqrt{\pi}\right)$

Which then becomes our final solution

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

Solving for spread (1)

Diffusion → spread → spatial extent grows with time

- This is really what we want. How do we quantify this?

Can the solution $c(x,t) = \frac{M}{A\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$ give us the answer?

Solving for spread (2)

To proceed we resort to integral quantities, the first 3 moments (revise mathematics please):

$$\int_{-\infty}^{+\infty} c\,dx = M / A = const$$

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

$$\int_{-\infty}^{+\infty} (x - \bar{x})^2 c\,dx = 0$$

The first moment gives us the total amount.

The second moment gives us the mean position.

The issue of spreading (3)

Focusing on the third moment:

$$\int_{-\infty}^{+\infty} (x-\bar{x})^2 c\,dx = 0$$

For ease we define:

$$\sigma^2 = \frac{1}{M/A}\int_{-\infty}^{+\infty} (x-\bar{x})^2 c\,dx = 0 \qquad M/A = \int_{-\infty}^{+\infty} c\,dx; \qquad \bar{x} = \frac{1}{M/A}\int_{-\infty}^{+\infty} xc\,dx$$

This results in:

$$\sigma = \sqrt{2Dt}$$

- The implication is that the distance grows with the square root of time; never stopping but gradually slowing

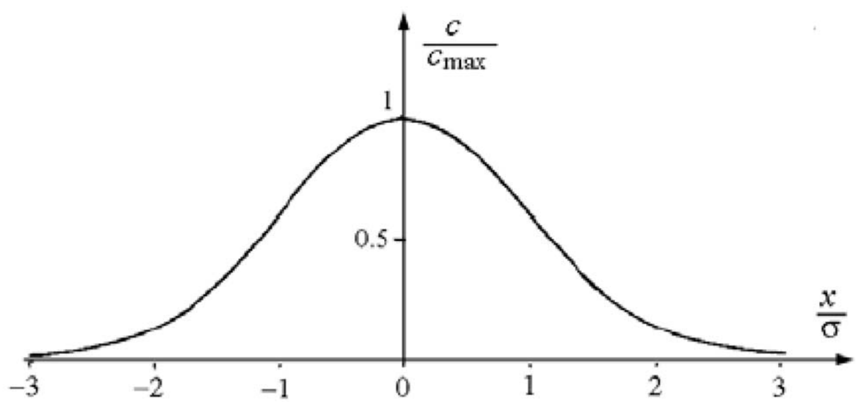
The issue of spreading (4)

How wide is wide? $\sigma = \sqrt{2Dt}$

The *c(x,t)* essentially obeys the Bell Curve

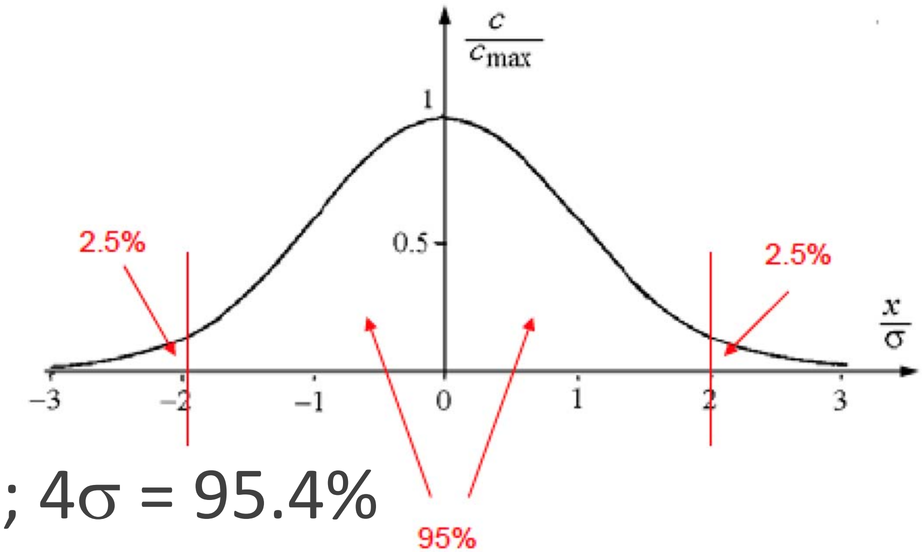
So if we normalize the distribution we obtain this distribution:

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



Spreading (5)

Since it's Gaussian



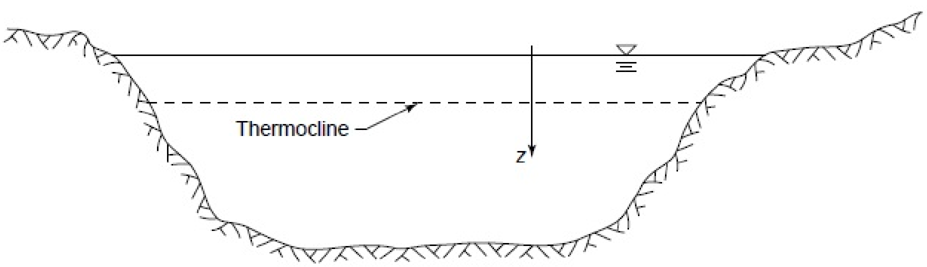
We know that 2σ = 64.2%; 4σ = 95.4%

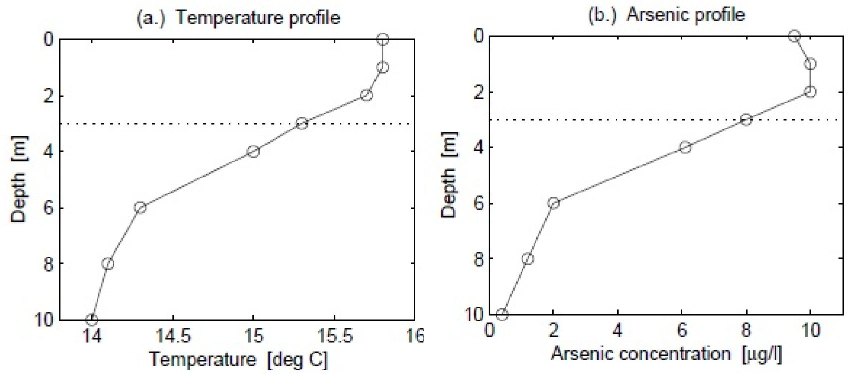
→ For practical purposes we use 4.

Application Example - Lake

Mildly stratified, thermocline of 3 m depth, contaminated by arsenic

Determine magnitude and direction of mass flux of arsenic through thermocline due to molecular diffusion if $A = 2 \times 10^4\ m^2$ and $D = 1 \times 10^{-10}$ m2/s





Application Example – Lake (2)

Solution steps

- Calculate concentration gradient at $z = 3$. How?
- Use 1D Fick's Law
- Mass flux from multiplying over the area

Application example - Spill

Ship leaks in a narrow straits

100l of pollutant that has a density of 0.879kg/L

Assume rapid mixing across the straits (10m deep, 50m wide) and D = 3m^2/s

What are the concentrations of the pollutant 0.5,2, 4, and 8 hours; 350m away?

What is the time at x = 350m when concentration is maximum?

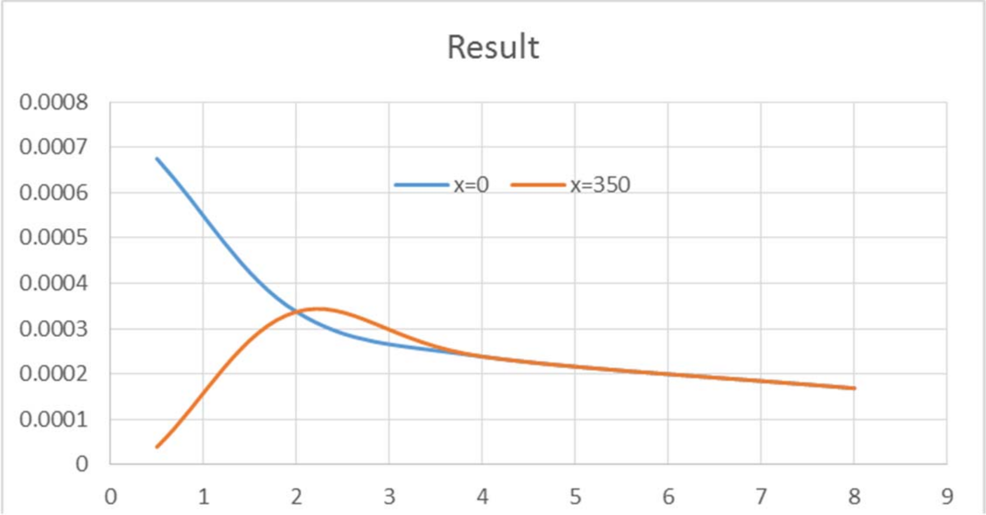
Solution steps

Find mass of spill

Find mass of spill over channel cross-section

Find at x = 0, c = m/sqrt(4πDt) this will become c_{max}

Then use $\sigma = \sqrt{2Dt}, \frac{c}{c_{max}} = \exp\left[-\frac{1}{2}\left(\frac{x}{\sigma}\right)^2\right]$ to find at x = 350,



More realistic Diffusion Cases

More realistic cases

Finite area release (instead of point)?

Finite domain

Sources

Decay

Can we solve these cases?

→ Remember this is a linear equation therefore we can superposition solutions.

Finite Area release (1)

Assume many infinitely small releases, we can accommodate by

- shifting x and having smaller M quantities, allows us to set

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

- If we now say

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

- We can then rewrite

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

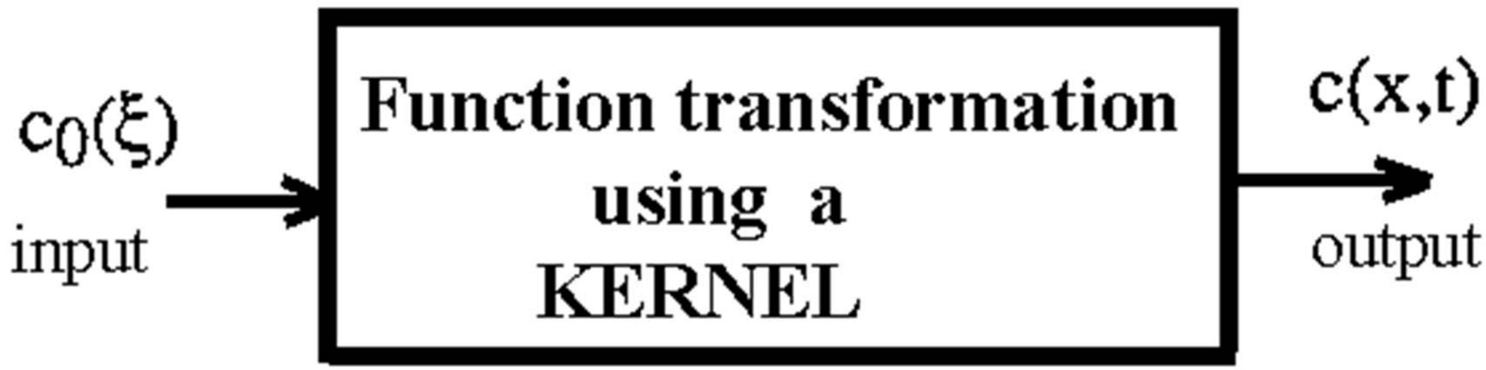
  - This is called a convolution

Finite Area release (2)

Mathematically this process of superposition is called a

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

convolution.



Finite Area Release (3)

However even for a simple problem like this,

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

We have a solution of the form:

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

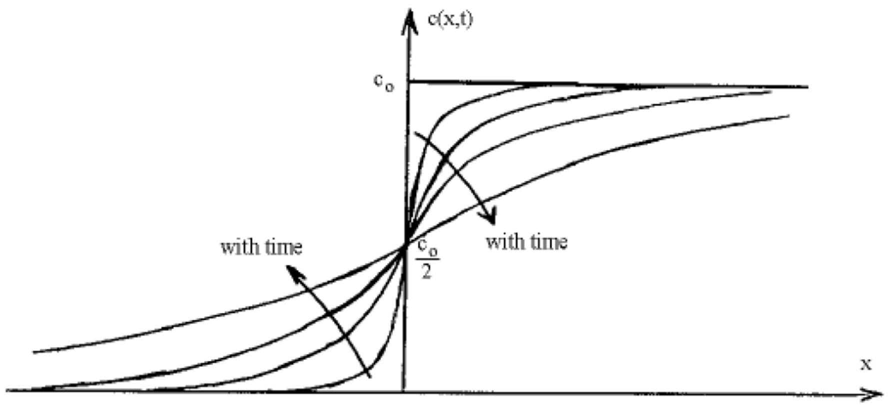
Which can only be solved through a function called the error function:

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

This results in the final solution: $c(x,t) = \frac{c_0}{2}\left[1 + \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right]$

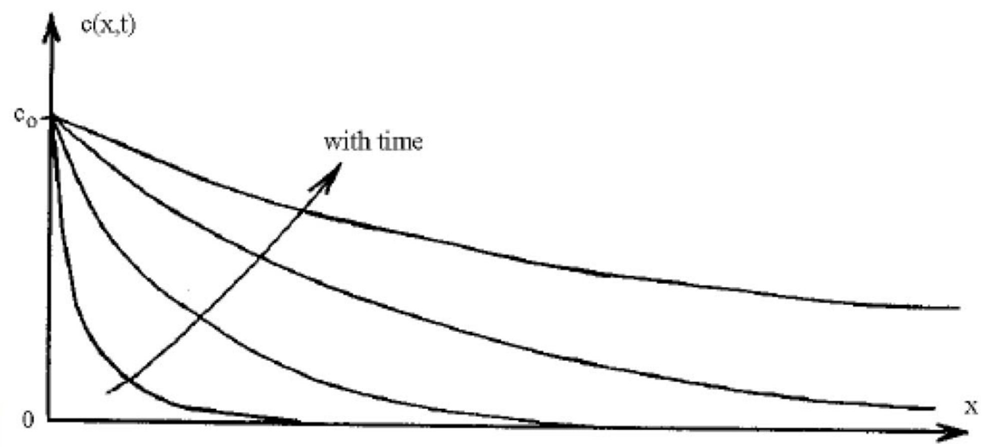
Finite Area Release (4)

Final solution:



Technically you can solve a semi-infinite domain with a continuous release with this solution by adapting it, resulting in the following solution:

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



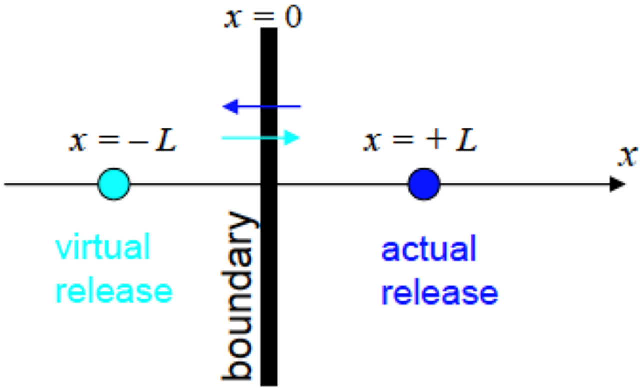
Finite domain (1)

Why do we need to consider this? [Think!]

Impermeable boundary → flux = 0,

- $$q_{(x=0)} = -D\frac{\partial c}{\partial x} = 0$$

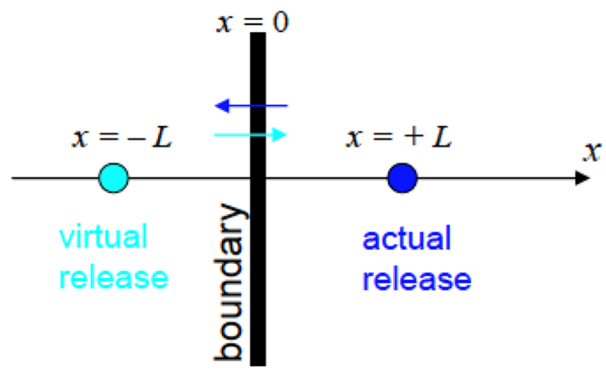
Create an equal and opposite flux at a symmetric distance away



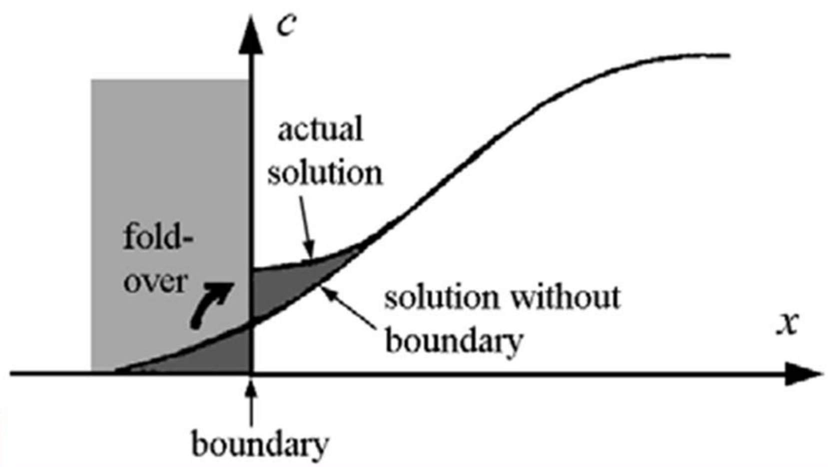
Resulting in the solution

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

Finite domain (2)

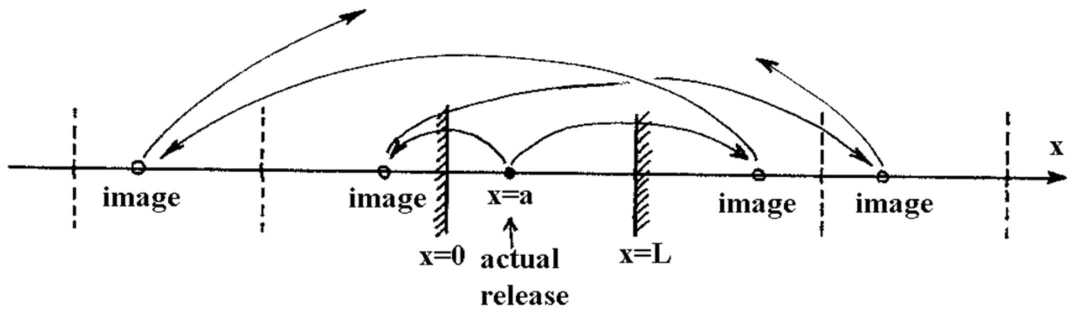
What does this →  do?

Physically prevents leakage, confines the substance
→ practically adds to the solution in the boundary



Finite domain (3)

For two boundaries the same method with care, can be used:



Resulting in:

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

- Normally we only go out to the first 5 – 7 terms

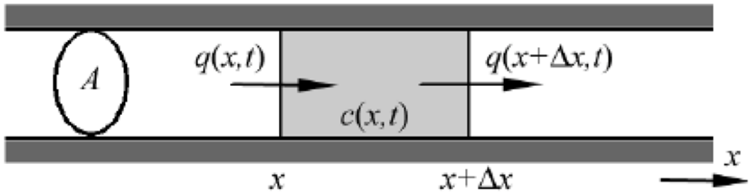
Final Concentration and Required Mixing Time

We can now proceed to get the required mixing time in a limited domain to obtain

$$c_{final} = c_{average} = M / L$$

- T (for release in the middle of the domain; L/2) = 0.134 L^2/D
- T (for release at x=0 ot x=L) = 0.536 L^2/D

Source and Decay (1)



Budget:

$$V\frac{dc}{dt} = Q_i - Q_o = q_i A - q_o A \boxed{+ S - KVc}$$

$$\frac{dc}{dt} = -\frac{q_{(x+\Delta x,t)} - q_{(x,t)}}{\Delta x} + \frac{S}{V} - Kc$$

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + s - Kc$$

→ Solution for decay is simple.

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

Source and Decay (2)

Continuous release at a fixed location or source.

- Difficult to solve

To solve, assume steady-state → simplifying the equation and reduces the solution to the form:

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

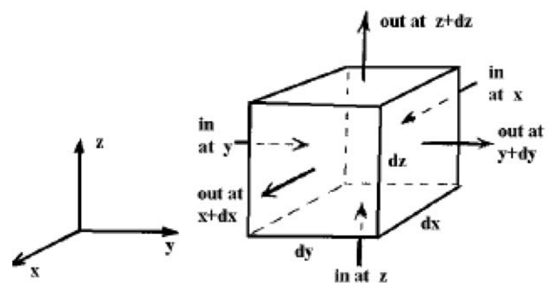
$$c(x) = \frac{\dot{M}}{2\sqrt{DK}} \exp\left(-\sqrt{\frac{K}{D}}x\right) for \quad 0 < x$$

Where $\quad c(\max) = \frac{\dot{M}}{2\sqrt{DK}}$

2-D / 3-D Diffusion

The real-world

While some systems can be modeled as 1-D, most real-world systems are 2-D (vertical or horizontal) or 3-D.



Therefore starting with

- Flux $$q_i = -D\frac{\partial c}{\partial x_i}$$
- Budget $$\frac{\partial c}{\partial t} = -\frac{\partial q_i}{\partial x_i}$$
- Results in $$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x_i^2}$$

Rate of accumulation =
Σ imports + Σ exports

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

$$dxdydz\frac{\partial c}{\partial t} = -\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right)dxdydz \longrightarrow \frac{\partial c}{\partial t} = -\vec{\nabla}\cdot\vec{q}$$

Solution?

Actually quite simple for the elemental solution → Just super position

And if D is same in all directions →

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