Heat (Diffusion) Equation

Derivation of Diffusion Equation

The fundamental mass balance equation is

$$\sum I + \sum P - \sum O - \sum L = \sum A \qquad (\textbf{1})$$
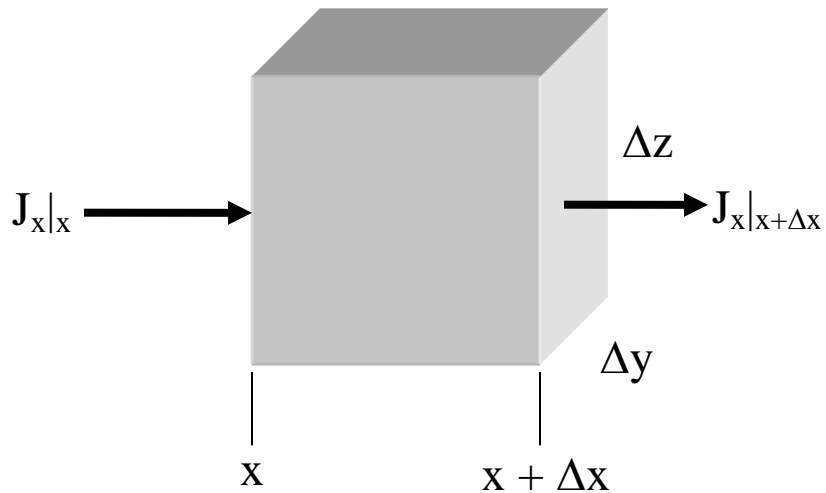
where:

- I = inputs
- P = production
- O = outputs
- L = losses
- A = accumulation

Assume that no chemical is produced or lost within the control volume and hence $\Sigma P = \Sigma L = 0$. So (**1**) simplifies to

$$\sum I - \sum O = \sum A \qquad (\textbf{2})$$

Considering a control volume cell where there is flux in the x direction only, we have

where $J_x|_x$ indicates the mass flux density $(ML^{-2}T^{-1})$ in the x direction at the point x.

In order to satisfy (**2**), we must have

$$\left(J_x\big|_x - J_x\big|_{x+\Delta x}\right)\Delta y\Delta z = \frac{\partial C}{\partial t}\Delta x\Delta y\Delta z \tag{3}$$

That is, the flux into the left wall times the area over which it occurs, minus the flux out of the right wall times its area in any interval of time Δt must equal the change in chemical mass in the control volume.

Diffusion occurs in response to concentration gradients (e.g., $\partial C/\partial x = 0.001$) in accordance with Fick's law:

$$J = -D\frac{\partial C}{\partial x} \tag{4}$$

where J is the areal flux ($ML^{-2}T^{-1}$) and D is the diffusion coefficient (L^2T^{-1}).

Incorporating Fick's law into equation (**3**), we have

$$\left(-D\frac{\partial C}{\partial x}\bigg|_x + D\frac{\partial C}{\partial x}\bigg|_{x+\Delta x}\right)\Delta y\Delta z = \frac{\partial C}{\partial t}\Delta x\Delta y\Delta z \tag{5}$$

Dividing both sides by $\Delta x\Delta y\Delta z$ gives

$$\frac{\left(-D\frac{\partial C}{\partial x}\bigg|_x + D\frac{\partial C}{\partial x}\bigg|_{x+\Delta x}\right)}{\Delta x} = \frac{\partial C}{\partial t} \tag{6}$$

Obviously, we are just taking the gradients of the gradients, and if we shrink Δx to differential size (and assume that D is constant in space) we have

$$D\frac{\partial\left(\frac{\partial C}{\partial x}\right)}{\partial x} = \frac{\partial C}{\partial t} \tag{7}$$

or equivalently,

$$D\frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t} \tag{8}$$

This is the 1-D version of the widely applicable Heat Equation.

Finite Difference Expression of Heat Equation

Most partial differential equations can not be solved analytically. Numerical solutions that reduce the problem to algebraic equations are often necessary. These equations can then be solved by direct or iterative methods.

The essence of numerical methods for PDEs lies in converting the differentials to 'finite differences'.

Consider the following concentration values on a linear domain from x to x + Δx.
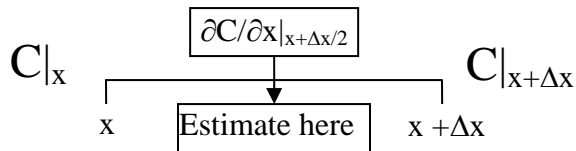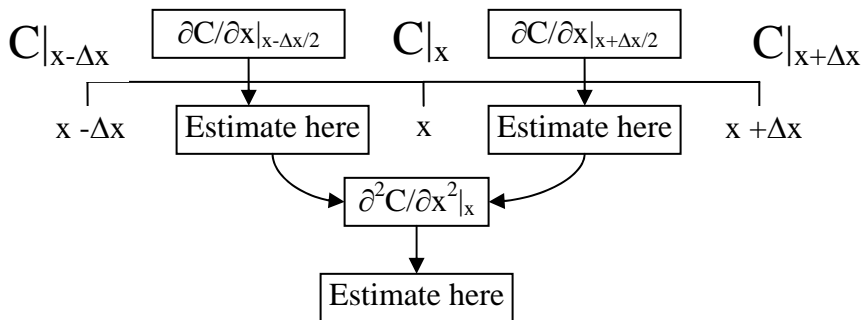

The gradient of C in the x direction at x + Δx/2 (i.e., $\partial h/\partial x|_{x+\Delta x/2}$) would be linearly approximated by

$$\left.\frac{\partial C}{\partial x}\right|_{x+\Delta x/2} \cong \frac{C\big|_{x+\Delta x} - C\big|_x}{x + \Delta x - x} = \frac{C\big|_{x+\Delta x} - C\big|_x}{\Delta x} \qquad (9)$$

This should be a reasonable approximation when Δx is small enough.

What about second order derivatives like $\partial^2 C/\partial x^2$? Remember from Calculus that $\partial^2 C/\partial x^2$ can be written as $\partial[\partial C/\partial x]/\partial x$. So, basically we need a gradient of gradients for the second order derivative. We have already estimated the gradient $\partial C/\partial x|_{x+\Delta x/2}$. We could look the other direction and compute a gradient at x - Δx/2:

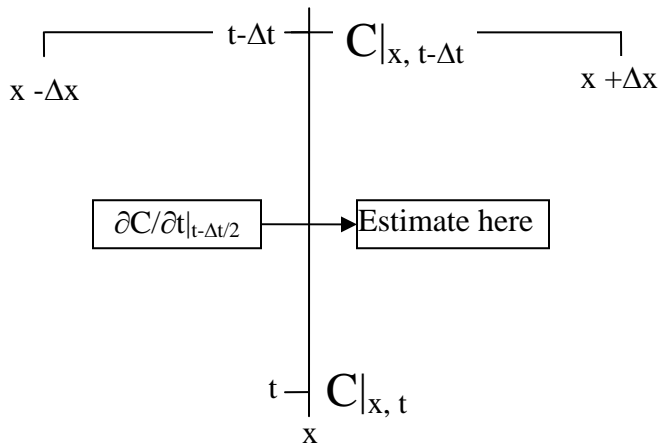$$\left.\frac{\partial C}{\partial x}\right|_{x-\Delta x/2} \cong \frac{C\big|_x - C\big|_{x-\Delta x}}{x - (x - \Delta x)} = \frac{C\big|_x - C\big|_{x-\Delta x}}{\Delta x} \qquad (10)$$

Then, taking the gradient between $\partial C/\partial x|_{x+\Delta x/2}$ and $\partial C/\partial x|_{x+\Delta x/2}$ gives

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{\left.\frac{\partial C}{\partial x}\right|_{x+\Delta x/2} - \left.\frac{\partial C}{\partial x}\right|_{x-\Delta x/2}}{\Delta x}$$

$$\cong \frac{\dfrac{\left.C\right|_{x+\Delta x} - \left.C\right|_{x}}{\Delta x} - \dfrac{\left.C\right|_{x} - \left.C\right|_{x-\Delta x}}{\Delta x}}{\Delta x} \qquad (11)$$

$$\cong \frac{\left.C\right|_{x+\Delta x} - 2\left.C\right|_{x} + \left.C\right|_{x-\Delta x}}{\Delta x^2}$$

We need a finite difference estimate for $\partial C/\partial t$ too. This is a little more complicated because now we have to include time.

The simplest approach is to use the 'known' concentration from the previous time step. At the start of any numerical solution, the Initial Condition will be the time 0 concentration. So, we can approximate the derivative $\partial C/\partial t$ by $\Delta C/\Delta t$ or

$$\frac{\partial C}{\partial t} \cong \frac{\Delta C}{\Delta t} = \frac{C_{x,t} - C_{x,t-\Delta t}}{\Delta t} \qquad (12)$$

Putting it all together

The heat equation is:

$$D\frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t} \qquad (13)$$

Let's replace the derivative terms with their finite difference approximations.

$$\mathrm{D}\frac{C|_{x+\Delta x,t-\Delta t} - 2C|_{x,t-\Delta t} + C|_{x-\Delta x,t-\Delta t}}{\Delta x^2} = \frac{C_{x,t} - C_{x,t-\Delta t}}{\Delta t} \qquad (14)$$

Written this way, nearly all of the concentrations (all of those with the t – Δt subscript) are known from the previous time step or from the initial condition. $C_{x,t}$ is the only exception and it is what we are trying to determine.

Let's rearrange to solve for $C_{x,t}$:

$$C_{x,t} = C_{x,t-\Delta t} + \frac{\mathrm{D}\Delta t}{\Delta x^2}\left(C|_{x+\Delta x,t-\Delta t} - 2C|_{x,t-\Delta t} + C|_{x-\Delta x,t-\Delta t}\right) \qquad (15)$$

This is the 'fully explicit' finite difference approximation for the Heat equation. It is 'explicit' because it works with the known concentrations from the previous time step. While this is relatively simple, it is only stable when the factor $\mathrm{D}\Delta t/\Delta x^2$ is less or equal to ½. This can be a serious limitation. Say we want to simulate a diffusion coefficient of 10^{-2} cm^{2}s^{-1} (gas in soil). That means $\Delta t/\Delta x^2$ has to be less than 0.02 s cm^{-2}. If we wanted to simulate the process with one second time steps, we'd need space steps of 0.02 cm. Simulating a 2 m soil profile would require calculations at 10,000 space nodes!

There are other approaches for the time derivative that avoid this stability restriction.

Initial and Boundary Conditions

Initial and boundary conditions must be specified when differential equations like the heat equation are to be solved. Initial conditions simply specify the concentrations throughout the problem domain at time zero.

Boundary conditions specify either
   1. The concentrations at the boundaries, or
   2. The chemical flux at the boundaries (usually zero)

The fixed concentration boundary concept is simple. The chemical flux boundary is slightly more difficult. We go back to Fick's law

$$J = -D\frac{\partial C}{\partial x} \qquad (16)$$

and notice that if $\partial C/\partial x = 0$, then there is no flux. The finite difference expression we developed for $\partial C/\partial x$ is

$$\left.\frac{\partial C}{\partial x}\right|_{x+\Delta x/2} \cong \frac{C|_{x+\Delta x} - C|_x}{\Delta x} \qquad (17)$$

Setting this to 0 is equivalent to

$$C\big|_{x+\Delta x} = C\big|_{x} \qquad \textbf{(18)}$$

So, if x is the last point inside the problem domain, we could put some 'ghost' points outside the domain at x + Δx. Then, if we make the concentration at the ghost points equal to the concentration inside the domain, there will be no flux.

Often the boundary conditions are constant in time, but they need not be.

Analytical Solution

A number of analytical solutions for the heat equation are available. Here we present one for the following conditions:

- Initial condition: C(x,0) = 0
- Left boundary condition: C(0,t) = 1
- Right boundary condition: C(∞,t) = 0

Note that the right boundary is at infinite distance.

The solution is

$$C = erfc\left[\frac{x}{\sqrt{4Dt}}\right] \qquad \textbf{(19)}$$

Analytical solutions can be used to check the results of finite difference computer programs when the boundary conditions are equivalent.

Summary

Hopefully, you have the idea that we've come full circle in our derivation of the Heat equation and its finite difference approximation. We began with a macroscopic consideration of fluxes and chemical mass changes in time and incorporated concentration gradients via Fick's law. Then we showed how this led to a second order partial differential equation, the Heat equation.

Our development of the finite difference expression for the Heat equation was essentially the same process in reverse; we considered how to express the derivatives in terms of the concentration and eventually derived a simple algebraic equation that can be used to solve the Heat equation numerically.