

Derivation of Convection Dispersion Equation for Porous Media

Mike Sukop, Florida International University

The fundamental mass balance equation is

$$\sum I + \sum P - \sum O - \sum L = \sum A \quad (1)$$

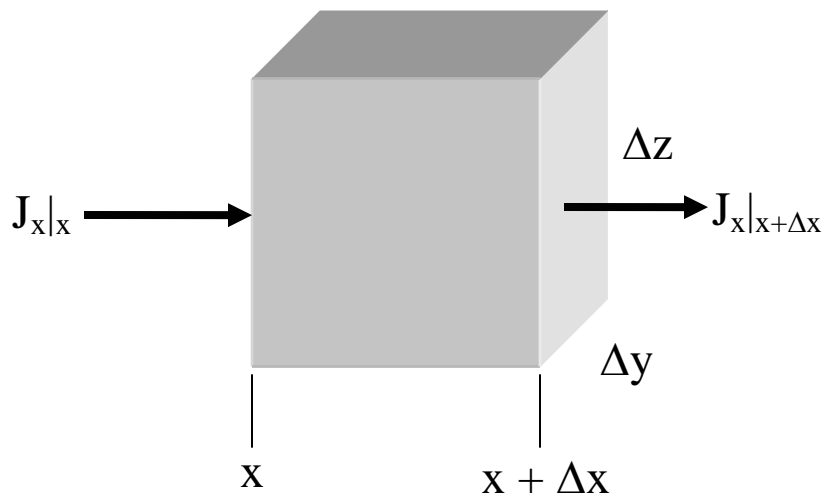
where:

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

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

$$\sum I - \sum O = \sum A \quad (2)$$

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

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

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.

The flux J_x has two components; there is an advective component J_c and a dispersive component J_d . The flux of solute due to convection is $J_c = v\theta C$. Dispersion mimics diffusion in the sense that the dispersive flux appears to be driven by concentration gradients (e.g., $\partial C/\partial x = 0.001 \text{ mg/cm}^4$), and can be expressed using the same mathematical form as Fick's law for diffusive flux:

$$J_d = -D^* \frac{\partial C}{\partial x} \quad (4)$$

where J_c and J_d are areal fluxes ($\text{ML}^{-2}\text{T}^{-1}$) and D^* is the dispersion coefficient (L^2T^{-1}).

Incorporating the two flux components into equation (3), we have

$$\left(v\theta C \Big|_x - D^* \frac{\partial C}{\partial x} \Big|_x - v\theta C \Big|_{x+\Delta x} + D^* \frac{\partial C}{\partial x} \Big|_{x+\Delta x} \right) \Delta y \Delta z = \frac{\partial C}{\partial t} \theta \Delta x \Delta y \Delta z \quad (5)$$

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

$$\frac{\left(vC \Big|_x - \frac{D^*}{\theta} \frac{\partial C}{\partial x} \Big|_x - vC \Big|_{x+\Delta x} + \frac{D^*}{\theta} \frac{\partial C}{\partial x} \Big|_{x+\Delta x} \right)}{\Delta x} = \frac{\partial C}{\partial t} \quad (6)$$

Or, collecting terms containing v and D^* and assuming that v , θ , and D^* are constant in space, we have

$$v \frac{(C \Big|_x - C \Big|_{x+\Delta x})}{\Delta x} + \frac{D^*}{\theta} \frac{\left(-\frac{\partial C}{\partial x} \Big|_x + \frac{\partial C}{\partial x} \Big|_{x+\Delta x} \right)}{\Delta x} = \frac{\partial C}{\partial t} \quad (7)$$

Shrinking Δx to differential size, the first term is simply $-v \partial C/\partial x$. In the second term, we are obviously just taking the gradient of the gradients, and if we shrink Δx to differential size we have

$$-v \frac{\partial C}{\partial x} + \frac{D^*}{\theta} \frac{\partial \left(\frac{\partial C}{\partial x} \right)}{\partial x} = \frac{\partial C}{\partial t} \quad (8)$$

or equivalently,

$$-v \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t} \quad (9)$$

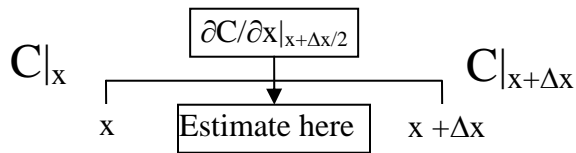
It is customary to replace D^*/θ with D . This is the 1-D version of the CDE.

Finite Difference Expression of the CDE

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 $x + \Delta x$.



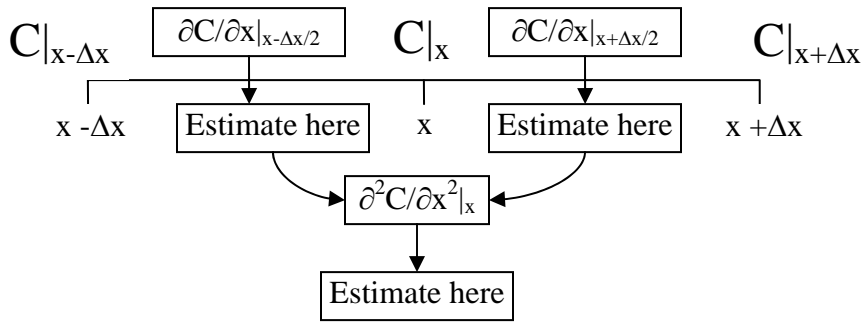
The gradient of C in the x direction at $x + \Delta x/2$ (i.e., $\partial h/\partial x|_{x+\Delta x/2}$) would be linearly approximated by

$$\frac{\partial C}{\partial x} \Big|_{x+\Delta x/2} \cong \frac{C|_{x+\Delta x} - C|_x}{x + \Delta x - x} = \frac{C|_{x+\Delta x} - C|_x}{\Delta x} \quad (10)$$

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 $x - \Delta x/2$:

$$\frac{\partial C}{\partial x} \Big|_{x-\Delta x/2} \cong \frac{C|_x - C|_{x-\Delta x}}{x - (x - \Delta x)} = \frac{C|_x - C|_{x-\Delta x}}{\Delta x} \quad (11)$$



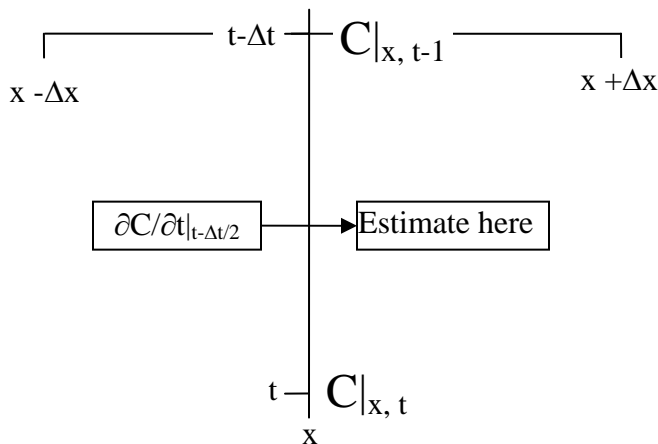
Then, taking the gradient between $\partial C/\partial x|_{x+\Delta x/2}$ and $\partial C/\partial x|_{x-\Delta x/2}$ gives

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

$$\cong \frac{\frac{C|_{x+\Delta x} - C|_x}{\Delta x} - \frac{C|_x - C|_{x-\Delta x}}{\Delta x}}{\Delta x} \tag{12}$$

$$\cong \frac{C|_{x+\Delta x} - 2C|_x + C|_{x-\Delta x}}{\Delta x^2}$$

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

$$\frac{\partial C}{\partial t} \cong \frac{\Delta C}{\Delta t} = \frac{C_{x,t} - C_{x,t-\Delta t}}{\Delta t} \quad (13)$$

Finally, we need an expression for the space derivative. Previously we found

$$\left. \frac{\partial C}{\partial x} \right|_{x+\Delta x/2} \cong \frac{C|_{x+\Delta x} - C|_x}{\Delta x} \quad (14)$$

and used it to develop an expression for $\partial^2 C / \partial t^2$. This worked well because the result was centered at x . The first order derivative itself though was at $x + \Delta x/2$. For a derivative centered at x , we can use

$$\left. \frac{\partial C}{\partial x} \right|_x \cong \frac{C|_{x+\Delta x} - C|_{x-\Delta x}}{2\Delta x} \quad (15)$$

Putting it all together

The CDE is:

$$-v \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t} \quad (16)$$

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

$$-v \frac{C|_{x+\Delta x,t-\Delta t} - C|_{x-\Delta x,t-\Delta t}}{2\Delta x} + D \frac{C|_{x+\Delta x,t-\Delta t} - 2C|_{x,t-\Delta t} + C|_{x-\Delta x,t-\Delta t}}{\Delta x^2} = \frac{C_{x,t} - C_{x,t-\Delta t}}{\Delta t} \quad (17)$$

Written this way, nearly all of the concentrations (those with the $t - \Delta t$ 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 $C_{x,t}$:

$$C_{x,t} = C_{x,t-\Delta t} + \frac{D\Delta t}{\Delta x^2} (C|_{x+\Delta x,t-\Delta t} - 2C|_{x,t-\Delta t} + C|_{x-\Delta x,t-\Delta t}) - \frac{v\Delta t}{2\Delta x} (C|_{x+\Delta x,t-\Delta t} - C|_{x-\Delta x,t-\Delta t}) \quad (18)$$

This is the 'fully explicit' finite difference approximation for the CDE. It is 'explicit' because it works with the known concentrations from the previous time step. While this is relatively simple, it is prone to numerical instabilities depending on the values of the factors $D\Delta t/\Delta x^2$ and $v\Delta t/2\Delta x$. This can be a serious limitation. There are other approaches that avoid these stability restrictions.

Initial and Boundary Conditions

Initial and boundary conditions must be specified when differential equations like the CDE 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

The fixed concentration boundary concept is simple and we'll use it in for the inlet condition in our numerical model.

The chemical flux boundary is slightly more difficult. We go back to the flux

$$J = vC\theta - D \frac{\partial C}{\partial x} \quad (19)$$

and notice that if $\partial C/\partial x = 0$, then there is no dispersive flux but there can still be a convective flux. This would apply at the end of a soil column for example; the water carrying the chemical still flows out of the column but there is no more dispersion. One of the finite difference expressions we developed for $\partial C/\partial x$ is

$$\frac{\partial C}{\partial x} \Big|_{x+\Delta x/2} \cong \frac{C|_{x+\Delta x} - C|_x}{\Delta x} \quad (20)$$

Setting this to 0 is equivalent to

$$C|_{x+\Delta x} = C|_x \quad (21)$$

So, if x is the last point inside the problem domain, we could put some 'ghost' points outside the domain at $x + \Delta x$. Then, if we make the concentration at the ghost points equal to the concentration inside the domain, there will be no dispersive flux. The 'real' end of the domain is between the grid points at $x + \Delta x/2$.

Note that a better inlet boundary condition also uses the flux as in (19). In fact, it is this boundary condition that corresponds to the analytical solution below. See Toride et al (1995) for more information.

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

Analytical Solution

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

- Initial condition: $C(x,0) = 0$
- Left boundary condition: $C(0,t) = C_0$
- Right boundary condition: $\partial C/\partial x (\infty,t) = 0$

Note that the right boundary is at infinite distance.

The solution is

$$\frac{C}{C_0} = \frac{1}{2} \operatorname{erfc} \left[\frac{Rx - vt}{2(DRt)^{1/2}} \right] + \frac{1}{2} \exp \left(\frac{vx}{D} \right) \operatorname{erfc} \left[\frac{Rx + vt}{2(DRt)^{1/2}} \right] \quad (22)$$

R is the retardation factor given by $R = 1 + \rho_b K_D / \theta$ where ρ_b is the soil bulk density and K_D is the soil/water distribution coefficient. In essence, R tells how 'retarded' the movement of a chemical is relative to that of the water ($R = v_{\text{water}}/v_{\text{chemical}}$). When $K_D = 0$, $R = 1$.

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

Summary

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

Our development of the finite difference expression for the CDE equation was essentially the same process in reverse; we considered how to express the derivatives in terms of discrete concentrations in space and time and eventually derived a simple algebraic equation that could be used to solve the CDE equation numerically.

Reference

Toride N, Leij FJ and van Genuchten M Th (1995) The CXTFIT Code for estimating transport parameters from laboratory or field tracer experiments. Research Report No. 137, U.S. Salinity Laboratory, USDA-ARS, Riverside, CA.
<http://www.ussl.ars.usda.gov/models/cxtfit.HTM>