Advection-Diffusion Modeling with the Finite Difference Method

Earlier in the course we looked at transient diffusion modeling for both groundwater flow and thermal modeling. Here we will look at a similar governing partial differential equation, but now we will expand it to include an *advection* term. By advection, we mean the transport of a quantity by the bulk motion of matter. For example, the thermal diffusion equation can be augmented with an advection term, giving:

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} = \kappa \frac{\partial^2 T}{\partial x^2}. \tag{1}$$

Here $u\frac{\partial T}{\partial x}$ is the new advection term, where u is the velocity (along the x direction). Notice how the advection term includes the first-order spatial derivative of temperature. The above equation could be used to model (in 1D) convection of thermal structure including both diffusive and advective transport. For example, this equation would apply for temperature variations in a slow moving stream, where the temperature cools laterally by diffusion (as we looked at previously in the cooling dike problem), but also by the bulk motion of the water in the down stream direction.

The advection diffusion equation can also be applied to chemical concentrations using the partial differential equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \kappa_c \frac{\partial^2 C}{\partial x^2} \tag{2}$$

where C is the concentration of a chemical species (i.e., its mass per unit volume) and κ_c is its chemical diffusivity in the medium. This equation could be used to track how a chemical concentration changes over time due to diffusion and advection. For example, it could be used to simulate the concentration of a toxic spill in a river over time as the river water flows downstream. Another example would be to model the diffusion and advection of a certain chemical species due to a current u on the surface of the ocean or as a gas in atmospheric winds.

Figure 1 shows example solutions to this equation for diffusion-only (i.e., when $u = 0$), advection-only (i.e., when $\kappa_c = 0$) and advection-diffusion (both u and κ_c are non-zero).

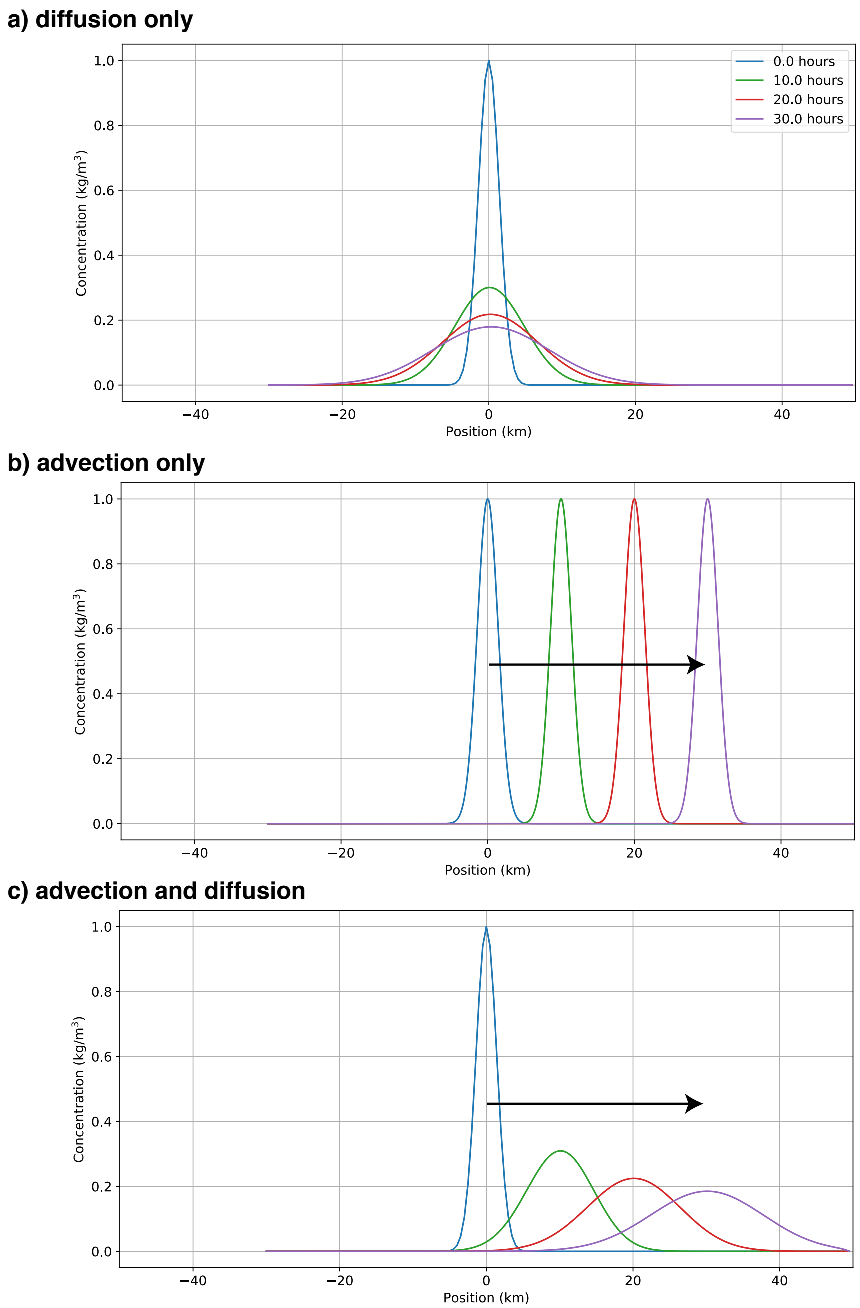

Figure 1: Examples of (a) diffusion ($u = 0$, $\kappa_c = 1$), (b) advection ($u = 1$, $\kappa_c = 0$) and (c) advection and diffusion(with, for example, $u = 1$, $\kappa_c = 1$).

For diffusion, the peak of high concentration lowers and spreads out symmetrically from its initial location, whereas for advection the peak maintains the same shape but moves laterally with velocity $u = 1$. The advection-diffusion solution in (c) is the combination of both of these effects.

The two dimensional (2D) version of the advection diffusion equation has the form

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} = \kappa\frac{\partial^2 T}{\partial x^2} + \kappa\frac{\partial^2 T}{\partial y^2} \tag{3}$$

where v is the velocity in the y direction. Thus is it only slightly more complicated than the 1D version. As you might guess, the 3D version of the advection diffusion equation is similar to the above but adds on terms for the z derivatives:

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} + w\frac{\partial T}{\partial z} = \kappa\frac{\partial^2 T}{\partial x^2} + \kappa\frac{\partial^2 T}{\partial y^2} + \kappa\frac{\partial^2 T}{\partial z^2} \tag{4}$$

where w is the velocity in the z direction. If you are familiar with vector calculus, the above equation can be written in shorter form as:

$$\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T = \kappa \nabla^2 T \tag{5}$$

where $\vec{v}$ is the velocity vector (i.e. it has both magnitude and direction).

Here we will only consider simple applications of the advection-diffusion equation where velocity is constant in both time and space, but you should know that there are significantly more complicated versions of these equations that govern fluid dynamics, such as the Navier-Stokes equations. In more complicated scenarios, the velocity may vary dynamically (in time and space) as the temperature T changes and thus the viscosity and buoyancy of a material changes. In such a scenario, another partial differential equation is introduced to govern the velocity as a function of time and space. This is commonly done for geodynamic models of convective flow in Earth's mantle. Non-constant and spatially varying velocity is also required for modeling complicated ocean currents and atmospheric winds.

Advection-Diffusion with the FTCS Finite-Difference Method

Here we will consider the one-dimension (1D) chemical concentration advection diffusion equation and will assume a uniform medium with chemical diffusivity κ_c:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \kappa_c\frac{\partial^2 C}{\partial x^2} \tag{6}$$

We will use the forward-in-time, center-in-space (FTCS) finite difference method that we have previously used for the diffusion equation.

We define time and spatial sampling grids and again will use superscripts to denote time indices and subscripts to denote spatial node indices. The various terms in the above equation have FTCS approximations at position x_i and time t_k:

$$\frac{\partial C}{\partial t} \approx \frac{C_i^{k+1} - C_i^k}{\Delta t}, \tag{7}$$

$$u\frac{\partial C}{\partial x} \approx u\frac{C_{i+1}^k - C_{i-1}^k}{2\Delta x}, \tag{8}$$

$$\kappa_c\frac{\partial^2 C}{\partial x^2} \approx \kappa_c\frac{C_{i-1}^k - 2C_i^k + C_{i+1}^k}{\Delta x^2} \tag{9}$$

You have already seen the first and third expressions above, while equation 8 is a center-in-space approximation of the first order spatial derivative at x_i. Notice how it uses the values at positions x_{i-1} and x_{i+1} to approximate the spatial derivative at x_i. Thus it uses the neighboring values but not the value at x_i itself.

Inserting these expressions into the equation 6 gives:

$$\frac{C_i^{k+1} - C_i^k}{\Delta t} + u\frac{C_{i+1}^k - C_{i-1}^k}{2\Delta x} = \kappa_c\frac{C_{i-1}^k - 2C_i^k + C_{i+1}^k}{\Delta x^2} \tag{10}$$

which we rearrange as

$$\frac{C_i^{k+1} - C_i^k}{\Delta t} = \kappa_c\frac{C_{i-1}^k - 2C_i^k + C_{i+1}^k}{\Delta x^2} - u\frac{C_{i+1}^k - C_{i-1}^k}{2\Delta x} \tag{11}$$

and then we isolate the only "next time" term C_i^{k+1} so that it's on the left-hand side of the equation, giving us our 1D FTCS solution to the advection diffusion equation:

$$C_i^{k+1} = C_i^k + \frac{\kappa_c\Delta t}{\Delta x^2}\left(C_{i-1}^k - 2C_i^k + C_{i+1}^k\right) - \frac{u\Delta t}{2\Delta x}\left(C_{i+1}^k - C_{i-1}^k\right) \tag{12}$$

Using the substitutions:

$$a = 1 - 2\frac{\kappa_c\Delta t}{\Delta x^2} = 1 - 2b \tag{13}$$

$$b = \frac{\kappa_c\Delta t}{\Delta x^2} \tag{14}$$

$$c = -\frac{u\Delta t}{2\Delta x} \tag{15}$$

We can write the FTCS expression even more compactly as:

$$C_i^{k+1} = aC_i^k + b\left(C_{i-1}^k + C_{i+1}^k\right) + c\left(C_{i+1}^k - C_{i-1}^k\right). \tag{16}$$

This is the equation you will use to solve the homework assignment.

Stability of the FTCS Method for Advection-Diffusion

Earlier in this course when considering the transient diffusion problem we saw that the time step Δt had to be limited to achieve a stable solution with the FTCS method. Likewise, the advection-diffusion method needs a suitably small time step to be stable in the presence of both diffusion and advection. We don't have time to derive the stability criteria in this course, so below we will just state them and discuss their significance.

Grid spacing Δx stability limit

The ratio of the diffusion coefficient over the velocity limits the maximum grid spacing Δx to be:

$$\Delta x \leq \frac{2\kappa_c}{u}. \tag{17}$$

This is the maximum the grid spacing can be to obtain a numerical stable solution with the FTCS method. As velocity increases or the diffusion coefficient decreases, a finer grid spacing is needed. Often the grid is made even smaller than the value above in order to represent narrow features in the initial conditions for the values of C (or T if thermal modeling) at $t = 0$.

You can also see from the above that if $\kappa_c = 0$, the grid spacing apparently must also be zero (i.e., $\Delta x = 0$)! This is because the FTCS method is *unconditionally unstable* for modeling purely advective systems. In unstable solutions, errors in the finite difference approximation grow at each time step and compound, resulting in an unusable solution (often they will blow up to large numerical values within a few time steps). Unstable solutions can also result in numerical diffusion of the solution, even when the physical diffusion is set to zero ($\kappa_c = 0$). Thus when modeling advection with the FTCS method, we will always make κ_c a small but non-zero value so that the solution remains stable. More complicated and stable finite difference solutions for modeling pure advection have been derived, such as the upwind scheme, the Lax-Wendroff method, and the Crank-Nicolson method.

Note that as you decrease κ_c, the grid spacing decreases and thus there are more points over which to compute the solution. So as you make κ_c smaller and correspondingly decrease Δx using the limit above, the run-time of your FTCS solver will increase.

Time spacing Δt stability limit

Given the grid spacing limit defined above, the time step must satisfy the inequality:

$$\Delta t \leq \frac{\Delta x^2}{2\kappa_c}, \tag{18}$$

which is the diffusion time step stability limit that we saw previously in this course. We can gain some insight by inserting the maximum grid spacing Δx at the stability limit as defined above:

$$\Delta t \leq \frac{\Delta x^2}{2\kappa_c} = \frac{2\kappa_c}{u^2} = \frac{\Delta x}{u} \tag{19}$$

The expression $\frac{2\kappa_c}{u^2}$ arises from the advection terms and shows that the time step should decrease in inverse proportion to the square of the velocity. Since velocity u is equivalent to distance over time, the expression $\frac{\Delta x}{u}$ shows that the time step Δt should be small enough that material does move further than the grid spacing in a given time step.

2D Advection Diffusion

In two dimensions (x, y), the FTCS solution to the advection diffusion equation starts with:

$$\frac{C_{i,j}^{k+1} - C_{i,j}^{k}}{\Delta t} + u\frac{C_{i+1,j}^{k} - C_{i-1,j}^{k}}{2\Delta x} + v\frac{C_{i,j+1}^{k} - C_{i,j-1}^{k}}{2\Delta y} = \tag{20}$$

$$+\kappa_c\frac{C_{i-1,j}^{k} - 2C_{i,j}^{k} + C_{i+1,j}^{k}}{\Delta x^2} + \kappa_c\frac{C_{i,j-1}^{k} - 2C_{i,j}^{k} + C_{i,j+1}^{k}}{\Delta y^2} \tag{21}$$

Assuming an equal grid spacing $\Delta x = \Delta y$ and rearranging terms to isolate $C_{i,j}^{k+1}$ on the left side yields the 2D FTCS update equation:

$$C_{i,j}^{k+1} = a\,C_{i,j}^{k} + b\left(C_{i-1,j}^{k} + C_{i+1,j}^{k} + C_{i,j-1}^{k} + C_{i,j+1}^{k}\right) \tag{22}$$

$$+c\left(C_{i+1,j}^{k} - C_{i-1,j}^{k}\right) + d\left(C_{i,j+1}^{k} - C_{i,j-1}^{k}\right) \tag{23}$$

where

$$a = 1 - 4\frac{\kappa_c\Delta t}{\Delta x^2} = 1 - 4b \tag{24}$$

$$b = \frac{\kappa_c\Delta t}{\Delta x^2} \tag{25}$$

$$c = -u\frac{\Delta t}{2\Delta x} \tag{26}$$

$$d = -v\frac{\Delta t}{2\Delta x} \tag{27}$$

The i subscript refers to the 2D grid's x index and the j subscript refers to the grid's y index.

In 2D, the time step must satisfy the inequality:

$$\Delta t \leq \frac{\Delta x^2}{4\kappa_c}. \tag{28}$$