Model Simulation of Chimney plume using A-D PDE*

A common sight to indicate industrialization and economical activities in a region is the Chimney that spews polluting gases acros the land.

The design of chimney, especially the tower height, was to disperse the polluting gases as far as possible but also hoping to dilute the concentartion of harmful elements through the environment. So the main question is here is what would be the concentration of the element as you move from the centerline of chimney to surrounding. A one dimensional advection-dispersion (or advection-diffusion) partial differential equation (A-D PDE) models this well to find concnetration profiles in one predominant dimension defined by wind flowing usually in one direction.

Here (we keep the details to the Appendix but do go through it*) we would first describe quickly how a PDE is derived, which is important to understand the modeling process, and as well as how it leads to numerical methods to solve them. There are multitude methods to find the solution of PDEs but we just show one practical method here, an implicity first-order difference method. PDEs are considered to be one of the hardest mathematical subject, but our hope is that after going through this section and playing with the program and its solutions you will find it quiet normal to use them in your work. But be warned, that real world problems requiring PDE solutions in three physical dimensions in time dimension may need enormous computing resources, which is its main caveat!

We use an implicit first-order numerical method to find solution of the A-D PDE equation (derived in the appendix below as equation (6)) that models the concentration of plume pollutant in one direction

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - u\frac{\partial c}{\partial x} - \mathrm{kc} \qquad (6)$$

First-order Euler method is simply applying the appropriate finite difference approximations for the above derivatives like where, if "?" is n+1 is the next future time step, then the method is an implicit method (as both LHS and RHS have what are yet to be known concentrations in time n+1, and if "?" is n, then the method is an explicit method as the the RHS has known concentration in time n.

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = D\frac{c_{i+1}^? - 2c_i^? + c_{i-1}^?}{\Delta x^2} - u\frac{c_{i+1}^? - c_{i-1}^?}{2\Delta x} - kc_i^? \qquad (7)$$

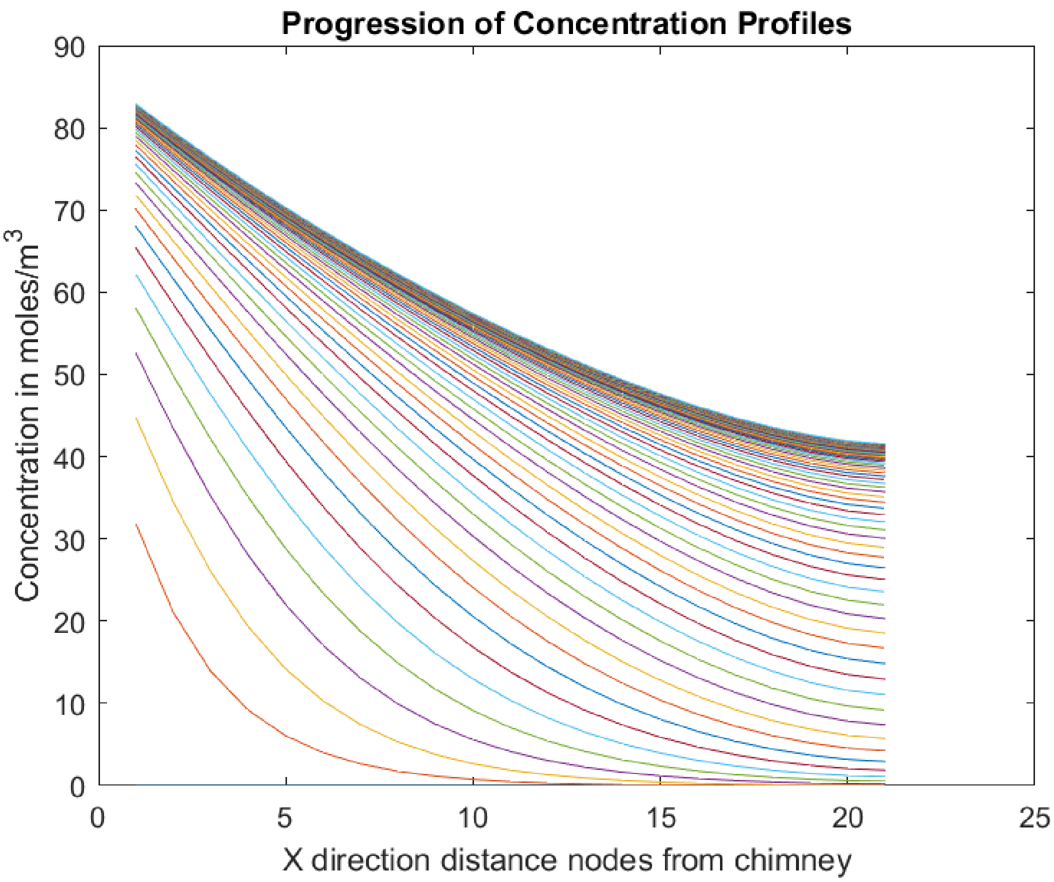
In order to apply the above equation we need to know Initial and Boundary conditions; and then apply the above equation at every node (discretize the entire domain and we apply the continuity equation in finite difference form, equation (7) at each node), more details elsewhere.

```
%Advection-Dispersion-reaction solved with implicit
%finite-difference equation with boundary conditions


clear;
D=5; %Dispersion Coefficient
U=2; %Velocity
k=0.2; %reaction rate coefficient
delx=.5; %should be less than 2*D/U for stability
delt = .2; %should be less than (delx^2)/(2*D+k*delx^2)
L=10; %length of domain
Tfinal=25;
CIN = 100; %input concentration

x=ADPDE1storderEulerImplicit(D,U,k,delx,delt,L,Tfinal,CIN);

plot(x(:,2:end-1)')
%plot(x')
title('Progression of Concentration Profiles')
xlabel('X direction distance nodes from chimney')
ylabel('Concentration in moles/m^3')
```



The concentration profiels must be read from lef to right (for space dimension x) and left bottom corner towards the right hand top corner as time progresses!

Exercises

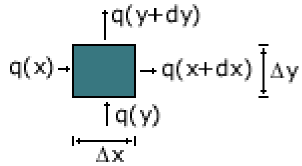
1. Try different D and U (but watch out for bad solutions as you may have to adjust dx and dt as described above for stability).
2. We are assuming constant concentration of 100 on the left hand boundary which indicates economy is booming but what happens to the environment?
3. Height of Chminey is not in our numerical model (then we have to consider the y dimension as well) but taller the chimney the better it is for the local region, but what about the neighbours and the Earth?

Appendix: Derivation of a PDE (only a few minutes needed to understand this section)

** In our last workshop, a famous professor after sitting through this derivation to see how a PDE can be derived, said "You have taken out my fear of PDEs now! Thanks!"*

Let us visualize flow of a pollutant through a small elemental volume in the middle of the plume:

Consider an elemental control volume in two dimenstions here (easy to extend to three dimensions):



Assuming flow along x and y directions at steady-state the flow into the control volume over a unit of time t equals flow out:

$$q(x)\Delta y\Delta z\, t + q(y)\Delta x\Delta z\, t = \quad q(x+\Delta x)\Delta y\Delta z\, t + q(y+\Delta y)\Delta x\Delta z\, t \qquad (1)$$

where q(x) is the flow m3/(m2/second)

Dividing by ΔxΔyΔzΔt and rearranging the Left and Right hand sides of equation (1) we get

$$\frac{q(x) - q(x+\Delta x)}{\Delta x} + \frac{q(y) - q(y+\Delta y)}{\Delta y} = 0 \qquad (2)$$

Taking limits $x \to 0 \text{ and } y \to 0$ we get

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0 \qquad (3)$$

A continuity equation or conservation equation with the variable q changing in both x and y directions and this here is a partial differential equation!

This is still not in terms of concentration of the element but Ficks First Law states:

Flux $q_x = -D_x \dfrac{\partial c}{\partial x}$ (4)

c - is concentration and negative sign is there to show the flow is from higher concentration region to lower concentration region and D is the dispersion coefficient (can be different in each direction).

Substituting equation (4) and (3) and assuming D same in all directions (so gets cancelled) gives the Laplace equation:

$$\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} = 0 \qquad (5)$$

If we have sources and sinks f(x,y) we modify the above to get:

$\dfrac{\partial^2 c}{\partial x^2} + \dfrac{\partial^2 c}{\partial y^2} = f(x,y)$ (Poisson equation)

In the unsteady state, considering just one direction only, where the concentration decreases over time by dispersion with dispersion coefficient D back in, but also has advection (flow due to wind velocity u) and reaction (a sink) with reaction rate k, we get the Advection-Dispersion partial differential equation (A-D PDE)

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - u\frac{\partial c}{\partial x} - \mathrm{kc} \qquad (6)$$

In general cases we only use numerical methods to find solutions of the above equation.

References:

Ponnambalam, K. Interactive Web Notes with automated self-evaluation questionnaires for the Numerical Methods course. see http://epoch.uwaterloo.ca/syde312/welcome2.htm PDE chapter