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Access the source code here

1D Advection-Diffusion numerical analysis with Python

Introduction

Advection Diffusion equation is the result of combining the advective and diffusive mass transfer through mediums such as porous medias.
The equation is as below:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \qquad (1)$$

Where u is celerity of flow (m/s), D is diffusion coefficient (m^2/s), and c is concentration. Moreover, boundary conditions are determined by known functions g(t) and h(t) and the initial condition formulations is as follows:

$$c(x,0) = \exp\left(-\frac{(x-1)^2}{D}\right) \qquad (2)$$

Solution

One approach to solve differential equations numerically is **Finite Difference Method (FDM)** which calculates the desired property of the system using a weighted average or other relations regarding to the neighbor nodes in the mesh grid.

By defining Δx and Δt which are node and time steps respectively, differential terms can be simplified into algebraic forms:

$$\frac{\partial c}{\partial t} = \frac{c(i,n+1) - c(i,n)}{\Delta t} \qquad (3)$$

The notation $c(i,n)$ refers to the concentration of node i in the time step n.

$$\frac{\partial c}{\partial x} = \left(\frac{1}{2\Delta x}\right)\begin{pmatrix} c(i,n+1) \\ -c(i-1,n+1) \\ +c(i+1,n) - c(i,n) \end{pmatrix} \qquad (4)$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{\theta}{(\Delta x)^2}\begin{bmatrix} c(i-1,n+1) - c(i,n+1) \\ +c(i+1,n) - c(i,n) \end{bmatrix} + \frac{1-\theta}{(\Delta x)^2}\begin{bmatrix} c(i-1,n) - 2c(i,n) \\ +c(i+1,n) \end{bmatrix} \qquad (5)$$

Where θ is the weighting factor and its value varies between 0 and 1.

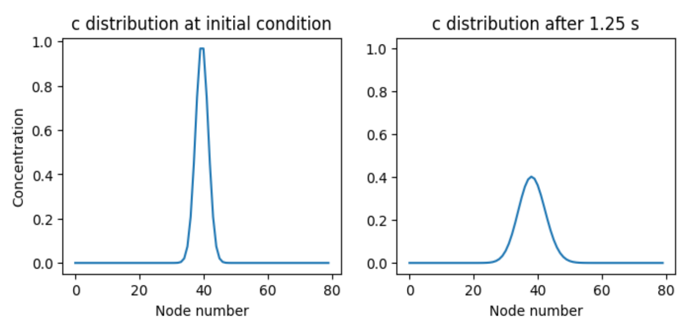
Finally, after using the finite difference terms of the derivatives in the equation and applying the boundary conditions, an explicit solution is obtained [1]:

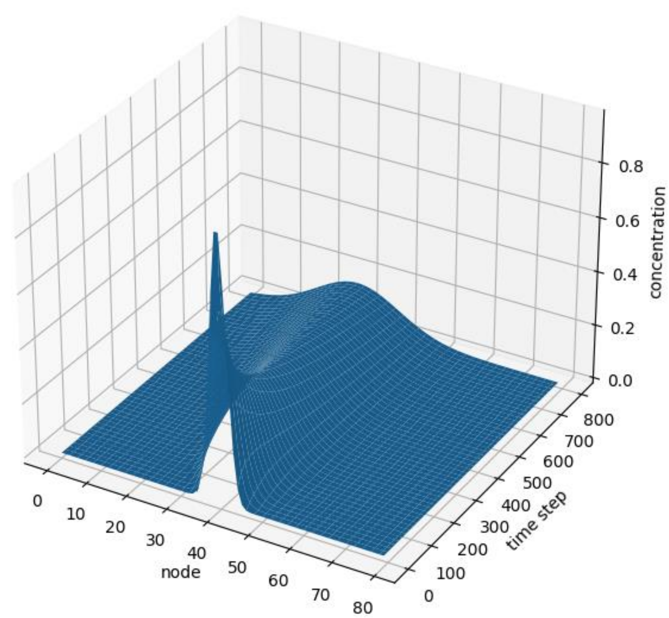
$$c(i,n+1) = \begin{bmatrix} \left(\frac{Cr}{Pe} - \theta\frac{Cr}{Pe}\right)c(i-1,n) \\ +\left(1 + \frac{Cr}{2} - 2\frac{Cr}{Pe} + \theta\frac{Cr}{Pe}\right)c(i,n) \\ +\left(\frac{Cr}{Pe} - \frac{Cr}{2}\right)c(i+1,n) \\ +\left(\frac{Cr}{2} + \theta\frac{Cr}{Pe}\right)c(i-1,n+1) \end{bmatrix} \times \begin{bmatrix} 1 \\ +\frac{Cr}{2} \\ +\theta\frac{Cr}{Pe} \end{bmatrix}^{-1} \qquad (6)$$

In the equation above, the Courant number is defined as $Cr = u\Delta t/\Delta x$ and Peclet number is $Pe = u\Delta x/D$.

Results

Regarding the graphs below, it is evident that the initial concentration is dispersed through the x axes in both directions and the maximum local concentration decreases over time.





[1] F. Sanjaya, S. Mungkasi, "A simple but accurate explicit finite difference method for the advection-diffusion equation", 2017