Mohammad Homanloo
Homanloom@gmail.com | GitHub | Website

Access the source code here

1D Advection-Diffusion numerical analysis with Python

Introduction

When transfer phenomena, including momentum, mass, and energy transfer within a medium, occur due to diffusion and convection, one can predict the behavior of the system employing the advection-diffusion equation, as defined in Equation (1).

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

where u (m/s), D (m²/s), and c (mol/m³) are respectively celerity of flow, diffusion coefficient, and concentration. Moreover, the initial can be determined by Equation (2):

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

Solution

Finite Difference Method (FDM) is a numerical method to solve differential equations. This method calculates the desired property of the system in each of the nodes regarding to the neighbor nodes in the mesh grid. This is done by converting differential equations to algebraic form as in Equations (3) to (5). By defining Δx and Δt, which are distance and time steps respectively, differential equations are transformed as below:

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

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

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

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

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

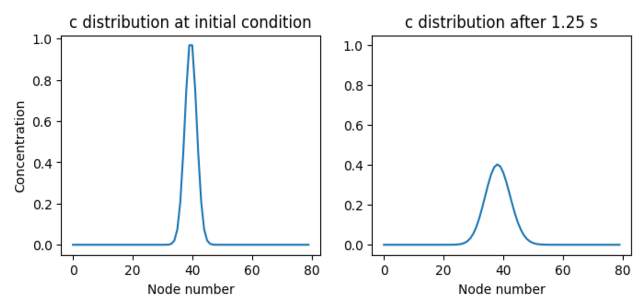
Finally, after adapting the finite difference terms of the derivatives in Equation (1) and applying appropriate boundary conditions, an explicit solution is obtained [1], as shown in Equation (6):

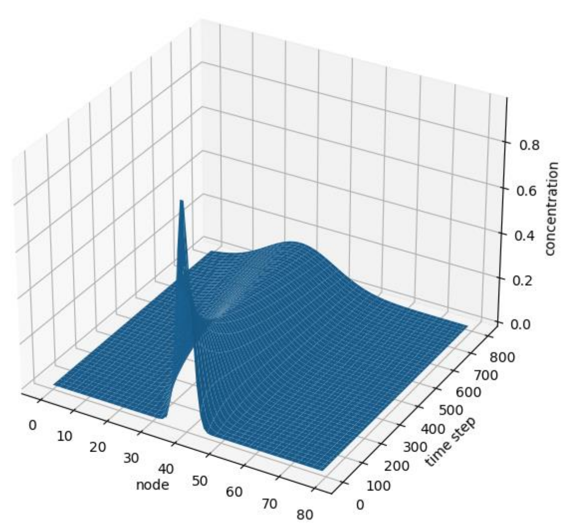
$$c(i,n+1) = \begin{bmatrix} \left(\frac{Cr}{Pe} - \theta\frac{Cr}{Pe}\right)c(i-1,n) \\ +\left(1 + \frac{Cr}{2} - 2\frac{Cr}{Pe} + \theta\frac{Cr}{Pe}\right)c(i,n) \\ +\left(\frac{Cr}{Pe} - \frac{Cr}{2}\right)c(i+1,n) \\ +\left(\frac{Cr}{2} + \theta\frac{Cr}{Pe}\right)c(i-1,n+1) \end{bmatrix} \times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

In Equation (6), 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, the initial concentration is dispersed through the x axes in both directions and the maximum local concentration decreases over time.
After sufficient amount of time, all the concentration will be removed and the concentration distribution line in the graph will be flatten.





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