Homework 3 : Mathematical Modelling of Bioprocesses and system.

Aim:
Run simulation of mass diffusion in 1D-system.

Methodology:

1. Run based on Finite Difference method with spatial discretization.

   Internodal Algorithm:

   $$C^{t+\Delta t}_i = C^t_i + D\Delta t\,(C^t_{i+1} - 2C^t_i + C^t_{i-1})/\Delta x^2$$

   Boundary nodal Algorithm:

   First node.

   $$C^{t+\Delta t}_1 = C^t_1 + 2D\Delta t\,(C^t_2 - C^t_1)/\Delta x^2$$

   Last Node.

   $$C^{t+\Delta t}_N = C^t_N - 2D\Delta t\,(C^t_N - C^t_{N-1})/\Delta x^2$$

2. Define Simulation Conditions.

   Simulation-1:
   Diffusion Constant [D]: 2 (A)^2/sec
   Time step [H]: 0.1sec
   Total time [T]: 10sec
   System size [X]: 10A
   System step increment [x]: 1A

   Simulation-2:
   Diffusion Constant [D]: 0.268 (A)^2/sec
   Time step [H]: 0.1sec
   Total time [T]: 10sec
   System size [X]: 10A
   System step increment [x]: 1A

   Simulation-3:
   Diffusion Constant [D]: 0.268 (A)^2/sec
   Time step [H]: 0.1sec
   Total time [T]: 5sec
   System size [X]: 10A
   System step increment [x]: 1A

   Initial Concentration is given as 100 particles per cubic amstrong.

3. Check Stability Condition.

Von Neumann Stability Condition.

$$(2D\Delta t) / (\Delta x^2) \;<=\; 1$$

4. Run Simulation as per the given condition and plot the graph as Concentration vs Distance/Position.

Result:

1. Simulation codes were attached as "1D Diffusion Equation.pdf"
2. Von Neumann Stability condition is satisfied for all three simulation.
3. Plots for all three simulations are compiled into a time resolved animated plot and attached as both line plot and colour map plots.

Observation:

1. Diffusion algorithm exibits the distribution of unequal arrangement of mass concentration in system while it attains comparatively equilibrium system with concentration.
2. Difference in total time of simulation exibits the distribution of mass concentration attains its equilibrium along the longer time of simulation.
3. Higher the Diffusion contant faster the diffusion.