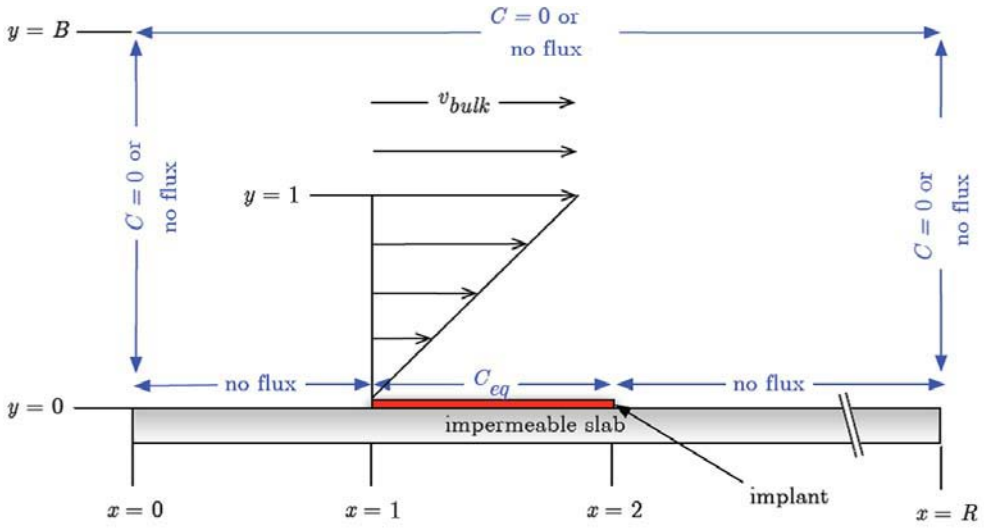
10.34 Numerical Methods Applied to Chemical Engineering Fall 2015

Homework #7: Numerical Simulation of Partial Differential Equations

Problem 1. You will use COMSOL and the finite volume method to solve a problem describing drug release from a medical implant. A simple 2-dimensional model on a rectangle $0 \leq x \leq R$ and $0 \leq y \leq B$ is used to describe the transport of the drug. The implant is resting on an impermeable slab at $y = 0$. We assume that the implant has negligible height in the y direction and covers the slab from $x = 1$ cm to $x = 2$ cm. Above the slab is a fluid bath. The fluid above the slab is flowing in the positive x direction with velocity $v_x(y) = v_o y$ for $y \leq H$. $v_x = 0.5$ cm/s if $y \geq H$ For this problem assume $v_o = 0.5$ /s. Let $H = 1cm$.



The concentration of drug in the fluid immediately above the implant is in equilibrium with the drug implant and can be assumed constant at $C_{eq} = 1$ mol/L. Moreover, because of the flow velocity, the concentration at $x = 0$ is negligible. The diffusion coefficient of the drug in the fluid is 6×10^{-6} $(\text{cm})^2/\text{s}$. The 2-dimensional PDE governing the concentration in the fluid above the implant at steady state is

$$-D\left(\frac{\partial^2 C(x,y)}{\partial x^2} + \frac{\partial^2 C(x,y)}{\partial y^2}\right) + v_x(y)\frac{\partial C(x,y)}{\partial x} = 0 \tag{1}$$

We want to solve for the concentration field $C(x, y)$ in the fluid and calculate the flux of drug from the implant:

$$Flux = -D\int_{1\text{ cm}}^{2\text{ cm}} \left.\frac{\partial C}{\partial y}\right|_{y=0} \frac{dx}{1cm}. \tag{2}$$

This Flux is the average moles of drug released per second per unit area of the patch. This is important for determining how long the implant will last before being depleted of the drug.

Before trying to solve the problem numerically, dimensional analysis and physical insight can be used to predict the form of the solution. The governing equation can be made dimensionless by

defining the characteristic length L and the dimensionless quantities:

$$L^2 = D/v_o \tag{3}$$

$$\hat{C} = C/C_{eq} \tag{4}$$

$$\hat{x} = x/L \tag{5}$$

$$\hat{y} = y/L \tag{6}$$

In terms of these dimensionless quantities, the governing equation becomes:

$$-\left(\frac{\partial^2 \hat{C}(x,y)}{\partial \hat{x}^2} + \frac{\partial^2 \hat{C}(x,y)}{\partial \hat{y}^2}\right) + \hat{y}\frac{\partial \hat{C}(x,y)}{\partial \hat{x}} = 0. \tag{7}$$

The dimensionless group $\mathrm{Pe} = v_o HW/D$ is called the Peclet number. In this problem it can be very large, for example if $H = 1$ cm, $\mathrm{Pe} = (1/12) \times 10^6$. Physically this indicates that advection is much stronger than diffusion. A boundary layer analysis of the type discussed in 10.50 can be used to show that the drug will diffuse a distance $\delta = \mathrm{Pe}^{-1/3}W$ away from the slab in the time it takes the flow field to advect the drug a distance, W. Because the Peclet number is large, this suggests that δ is small, and that the concentration of drug is practically zero when $y \gg \delta$. (Note also that the L used in the scaling is rather small: $L = 0.0035$ cm.) A good numerical solution to this problem will need many points in the y-direction within a distance δ of the slab to resolve this sharp variation in the concentration. Also, we expect to have to use upwind differencing for convection for numerical stability, since we may not able to use a fine enough discretization in the x direction.

1. Describe and justify which combination of boundary conditions you will use.

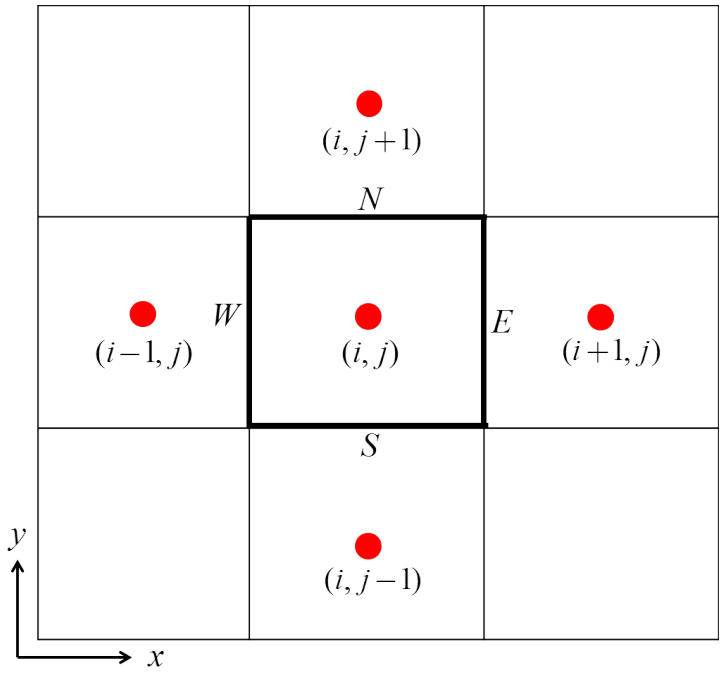
2. One can derive equations for the amount of drug (moles/s) flowing through each of the faces of a rectangular finite volume (i, j) with width and height, Δx and Δy. This is the normal flux through a surface (units of $moles/cm^2 - s$) times the surface area of the face. However, in this 2-d infinite problem everything is done "per Δz " where z is the direction in and out of the plane of the paper, and therefore has extra units of $length^{-1}$. The amount of drug flowing (mole/s per unit depth) through the south, west, and east faces are given by:

$$F^S_{i,j} = -\frac{D}{(\Delta y)}\big(C_{i,j} - C_{i,j-1}\big)\Delta x \tag{8}$$

$$F^W_{i,j} = \left[v(y_{i,j})C_{i-1,j} - \frac{D}{\Delta x}\big(C_{i,j} - C_{i-1,j}\big)\right]\Delta y \tag{9}$$

$$F^E_{i,j} = -\left[v(y_{i,j})C_{i,j} - \frac{D}{\Delta x}\big(C_{i+1,j} - C_{i,j}\big)\right]\Delta y \tag{10}$$

where S, W, E refer to the south, west, and east faces of the finite volume (i, j), $y_{i,j}$ is the y-coordinate at the center of volume (i, j) and $C_{i,j}$ is the average value of $C(x, y)$ in volume i, j. Derive an equation for the moles of drug per second per unit depth flowing through the north face: $F^N_{i,j}$. For reference the finite volume $(i - 1, j)$ sits to the left of (i, j) in the (x, y) plane (see diagram). Although the figure is drawn with a uniform mesh, you also have the option of using a non-uniform mesh.



3. Write a non-dimensional equation for the steady-state material balance of the drug in a finite volume away from any boundary. Also write the equation for a finite volume whose south-edge is coincident with a no-flux boundary, and the equation for a finite volume whose north edge is coincident with a C=0 boundary.

4. Write a MATLAB® program that combines your finite volume derivation with boundary conditions to solve for the steady-state concentration field and compute the flux of drug from the implant once steady-state is achieved. You are free to choose R, B and the width of the finite volumes in the x- and y-directions. Note that your equations are linear in the unknown $C_{i,j}$. Do you need an initial guess for this problem, why or why not? How will you take advantage of the fact that the Jacobian is very sparse?

5. We suggest you start small: use a very small value of $H = B$, with a $C = 0$ boundary condition at $y = H$; physically this corresponds to case where there is an adsorbent wall at that location moving to the right at velocity $v_o y$. This will allow you to use a very small value of δy perhaps even as small as L. Note that imposing this boundary condition should overestimate the computed Flux, with the level of over-estimation decreasing monotonically as H increases. Once you confirm that the simulation is working correctly for small H, increase $H = B$. The flux of drug leaving the patch should converge when H and/or B gets large enough. The real physical situation you are trying to model has $H = 1$ cm and B large.

6. Show that the computed Flux converges as R and B become sufficiently large and Δx, Δy become sufficiently small. Hint: do not try to specify the number of finite volumes in each direction directly. Instead, let the number of volumes in the x-direction be $R/\Delta x$ and the number of nodes in the y-direction be $B/\Delta y$ where these ratios are necessarily integers.

7. Compare your finite volume calculation with a calculation for the same system performed using COMSOL (similar to what we did in class). Make a contour plot of the concentration computed using your MATLAB function, and of the COMSOL solution, and discuss the results.

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