ChE 272 Introduction to Chemical Engineering Calculations University of Rhode Island
Professor Greenfield Spring 2007

Project 2
due Monday April 30

In this problem we will work with a simplified model for a drug delivery device. We can think about the device as having two wide dimensions (total area A of 1 cm^2) and one narrow dimension, which we will label as the x direction, with $0 \leq x \leq 0.2$ cm. Initially the device has a uniform concentration of drug molecules, $c_0 = 0.15$ mol/cm^3, and the concentration can be considered to be only a function of x and time t. In other words, we are assuming that the same thing happens at each time at all of the different y and z positions.

The diffusion of drug molecules out of the device is governed by the overall diffusion equation,

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

a partial differential equation for the concentration c as a function of position x and time t. For simplicity we will use the following boundary conditions:

- $c(x,t) = c(x,0) = c_0 = 0.15$ mol/cm^3 for all x at time $t = 0$,
- $c(x,t) = c(0,t) = 0$ at all times t for all positions $x = 0$,
- $c(x,t) = c(L,t) = 0$ at all times t for all positions $x = L$, where $L = 0.2$ cm is the thickness of the device.

Physically, the latter two boundary conditions indicate that the drug is depleted from the device surface at the moment that it is implanted. The first condition indicates that the concentration is equal at all places in the device that aren't the surface. The diffusion coefficient D equals 10^{-9} cm^2/s for the drug in the device in our model.

1. Use the finite difference approach to write a set of finite difference equations for approximating equation 1. In other words, write derivative estimates based on a set of concentrations at various positions and times. Use an explicit or a Crank-Nicholson (implicit) approach (it's your choice).
2. Solve those equations for the concentration profile (i.e. concentration c vs position x) at times of 0 hr, 12 hr, 1 day, and 7 days. Present your results using a plot of c vs x (preferably one graph with multiple data sets). *Hint*: use integration steps that lead to stable results.
3. For each of these times, use numerical integration to solve for the total mass of drug inside the device.

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4. How does the amount of drug released compare with the amount

$$M(t) = 4\left(\sqrt{Dt/\pi}\right) c_0 A \qquad (2)$$

that is calculated from an analytic formula that applies at early times? (This formula assumes release from both sides of the device, i.e. $x = 0$ and $x = L$.) Use a graph to compare your numerical simulation results with the predictions of equation 2.

5. Repeat parts (a)-(d) twice. First, use a smaller spacing Δx. Second, use a smaller time interval Δt. How do the results of the three simulations compare? Use graphs to visualize your comparisons.

Suggestion: you will very likely find it useful to use a computer tool for making the underlying finite difference calculations. You may also find it convenient to write a spreadsheet and/or a small program, which can repeat the calculations as necessary.