10.34 Quiz 2
November 15, 2006

An isomerase (an enzyme that catalyzes an isomerization reaction) is used to convert a cheap unpalatable substrate S into its isomer, a delicious high-value product P called fructose (used to make soft drinks and candy).

The enzyme reaction is expected to follow the Michaelis-Menton rate law:

$$R = n_E V_m \left(\frac{[S] - \frac{[P]}{K_{eq}}}{K_m + [S]} \right) \quad [=] \quad \frac{moles\ S \rightarrow P}{\sec} \qquad \text{Eq.(1)}$$

where V_m and K_m depend on the enzyme, and K_{eq} is for the equilibrium S=P, and n_E is the moles of enzyme in the reactor.

Note that throughout the isomerization process [S]+[P] = constant. We therefore suggest you use the dimensionless concentration C = [Substrate]/[Substrate]$_o$ rather than tracking S and P separately.

1) Simulate the batch conversion of S into P by writing a couple of short Matlab functions. Your Matlab functions should take $[S]_o$, n_E, V, Km, and Keq as inputs. Feel free to call any built-in Matlab functions.

A microreactor for accomplishing this process continuously is constructed this way: a coating of the isomerase is chemically bonded to two flat plates. The coating density is 10^{-11} moles enzyme/cm^2. The two plates are then bonded to a thin spacer, to create a very thin channel (gap between the plates Y=0.01 cm (0.005 cm from the centerline to the wall), length X=5 cm, width of channel Z=2 cm), see figure. Inside the channel, flow can be accurately modeled as being laminar and two-dimensional, i.e. we only need to be concerned about gradients in x and y directions, not z, don't worry about what happens close to z=0 or z=Z. The enzyme's substrate, initial concentration $[S]_o$ is flowed at a rate of 0.1 ml/second through the channel from x=0, and the output stream (hopefully rich in product P) exits at x=X.

2) Write the finite difference equations that can be solved to compute $C_i = C(x_i,y_i)$ at a set of N_x*N_y mesh points (x_i,y_i) inside the channel when the system is running in steady state, in the limit where the enzyme reaction is so fast that the Substrate and Product are in equilibrium at the walls. That is, at the inlet C=1, and along the walls $C = (1+K_{eq})^{-1}$. At the outlet assume von Neumann boundary conditions. What is the boundary condition along the centerline of the channel Y=0 cm? Write the special equations that apply for the mesh points at or near the boundaries (the centerline is one of the boundaries).

3) Is the system of equations you wrote in part 2 linear or nonlinear in the unknowns? What Matlab function would you use to solve this system of equations?

4) It would be interesting to compute values of X,Y,Z which would maximize the yield, i.e. the moles of P made per second, subject of course to a couple of practical constraints:

a) safety: the total pressure drop cannot exceed some maximum set by our pump and the materials used to construct the microreactor.
b) product specifications: the [P] in the output stream must be at least $[P]_{min}$

Explain whether or not one should expect this maximum productivity to occur at the point where:

$$\partial(\text{yield})/\partial X = 0 \quad \text{and} \quad \partial(\text{yield})/\partial Y = 0 \quad \text{and} \quad \partial(\text{yield})/\partial Z = 0$$

Note no computations are required, just a sentence or two.

5) In reality, the enzymatic reaction will not be fast enough to achieve perfect equilibrium at the walls. Instead, the rate of conversion per unit area at the walls will be (with n_E now being in moles Enzyme/cm^2)

$$(\text{moles converted /second/ } cm^2) = R \qquad \text{Eq.(3)}$$

Write the new boundary condition at the walls that replaces $C=(1+K_{eq})^{-1}$ and the corresponding finite difference equation for a point (x_n,y_n) near the wall.

6) If you were solving the BVP problem using non-uniform grid points, where would you want to make the density of grid points the largest? Explain with a sentence or to why that is the case.