10.34 – Fall 2006
Homework #8
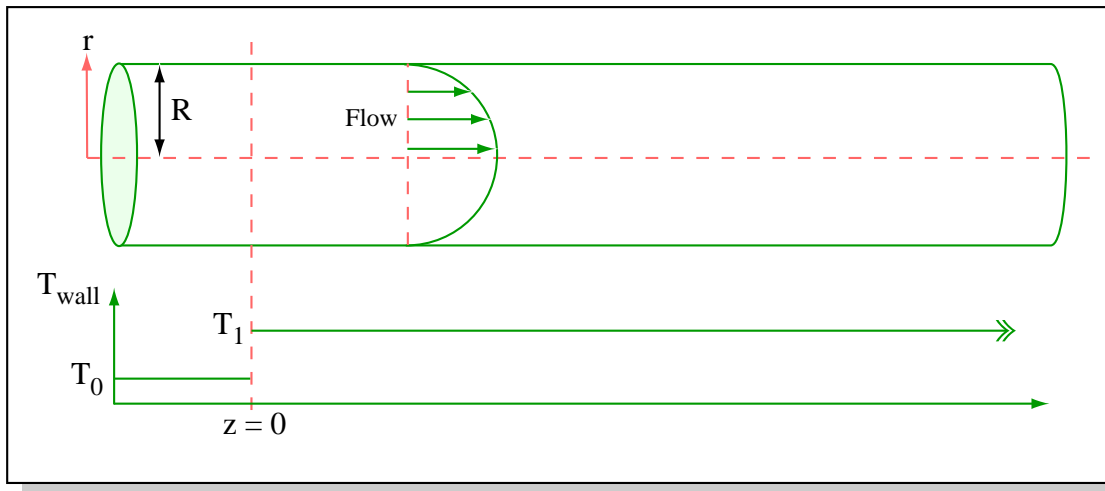**Due Date: Wednesday, November 1ˢᵗ, 2006 – 9 AM**
Problem 1:

Figure by MIT OCW.

Solve 6.B.1 in Beers' (pg. 432) by GMRES, using sparse representation of the large matrix. Note that you may have to restart GMRES after a few iterations, and also things may work better if you pre-condition the matrix. Your Matlab program should take T_0, T_1, lambda, rho, C_P, Re, mu, and R as inputs. Please run your program for the case (you do not need to answer specific questions ask in Beers' book, only the ones asked here):

$T_0 = 300$ K	$T_1 = 400$ K	$\lambda = 0.6$ W/m-K	$\rho = 1$ g/cm^3
$C_P = 4$ J/g-K	Re = 100	$\mu = 0.5$ cP $= 0.5 \times 10^{-3}$ N-s/m^2	R = 5 cm

Generate following plots (over a range that shows all dynamics):
-   A 3-D surface plot and 2-D contour/pcolor plot of the velocity field
-   A plot showing the T(z) for r = 0, 1, 2, 3, 4 cm (all on the same figure)

Hints and notes: The flow in the problem and the ambiguous boundary conditions in the z-direction create a problem: how can we define the axial boundary conditions? This is a place where the scaling analysis you have learned in transport can be important. We know that at -infinity the temperature is T_0, and it is T_1 at +infinity, but what are reasonable approximations to these infinite boundaries. One can define a characteristic time for thermal diffusion/conduction in an analogous way to species diffusion:

$$\tau_{cond} = R^2 / \alpha = \rho C_P R^2 / \lambda$$

This would be an estimate of the time to conduct heat over the radius of the tube. We also can estimate the maximum velocity of the flow based on a given Re. We want to make sure that we have enough length (z-direction) to our mesh so that the heat conduction will have enough time to saturate the flow at the center, and the entire cross-section of the tube will have a temperature of T_1 at the end of this length. As an initial starting point, we recommend that the length be set to allow for 10 characteristic conduction times based upon the centerline velocity in the tube. If you find the to be insufficient to warrant a constant-T boundary condition, then the length may need to be increased further.

Also note that starting at z = 0 and saying T(z=0,r) = T_0 is not valid, since there will be some back-diffusion against the flow (especially near the wall). A good starting point may be to start the grid a length equivalent to 1 or 2 characteristic times upstream (i.e. T(z= -2v$_{centerline}$*t$_{cond}$) = T_0)

Problem 2:

Solve 6.B.2 except ***do not neglect*** external mass transfer resistance. Instead, have your program take the Sherwood number ($Sh_i = 2Rk_{c,i,liq}/D_{i,liq}$) describing the external mass transfer situation as an input. The bulk substrate concentration is 1 M in the main flow, but lower at the surface of the bead. The diffusivity of S in the liquid is 7.0×10^{-6} cm^2/s. You can assume that the partitioning coefficient between the liquid and gel phases is 1.0 (i.e. $S_{liq} = S_{gel}$ @ interface). Please generate a solution for the cases R = 0.5, 1.0, and 5.0 mm (again, you do not need to answer the questions in the original problem).

- Plot the concentration profiles within the bead for each case in a single figure for a Sherwood Number of 10.
- Once you find the concentration profile within the bead, determine the total consumption rate of S (moles/s) in each case.
- Assuming that the enzyme is very expensive, which bead size would you choose to run the reactor?

Problem 3:

Solve 6.C.5 using the method of lines to cope with the stiffness in the y direction. There is a misprint in the problem statement; the correct conditions to assume are:

- $C_A = C_{AB} = 0$ and $C_B = 1$ mole/liter at the top of the slope
- assume mass-transfer in the gas phase is fast, so $p_A = 1 \times 10^{-4}$ atm at the gas-liquid interface.
- Assume the vapor pressures of the solvent, B and AB are negligible (in reality the vapor pressure of the solvent would probably not be negligible).

We suggest you start with a very coarse discretization in the z direction.