Final Examination Solutions
May 6, 2019

1. A System of Non-Linear Parabolic PDEs

Consider a plug flow reactor. (This is a pipe with a reaction taking place in the fluid flowing inside it.) Consider the irreversible dimerization reaction 2A → B taking place in a non-reactive solvent. The molar balance for each component, A and B, is given by

$$\frac{\partial C_i}{\partial t} = -v_z \frac{dC_i}{dz} + D_i \frac{d^2 C_i}{dz^2} + \nu_i r$$

where *z* is the spatial dimension in the axial direction, *t* is time, C_i is the molar concentration of species i, v_z is the axial velocity, D_i is the diffusion coefficient of species i, ν_i is the stochiometric for species i, (namely -2 for A +1 for B) and *r* is the reaction rate. The reaction rate is given by

$$r = kC_A^2$$

where k is the rate constant. Assume the reactor is operated isothermally so we have no need for an energy balance. The circular pipe is 10 m long with a diameter of 0.1 m. The axial velocity is 0.15 m/s. The diffusivities are all 2.0x10^{-9} m^2/s. The rate constant is $k = 1.0x10^{-5} \frac{m^3}{mol \cdot s}$. Initially, the pipe contains nothing but solvent. At the inlet, the reactants, A is fed in at a concentration of 1200.0 mol/m^3 respectively. No B is present in the feed stream. At the outlet, assume the concentrations no longer change (i.e. a no flux boundary condition).

(a) Solve the problem. Estimate how long it takes this reactor to get to steady state.
(b) Show the steady state profile.
(c) What is the fractional consumption of A at steady state? Reminder: $Y_A = \frac{C_{A,in} - C_{A,out}}{C_{A,in}}$.
(d) What can be done to the axial velocity to increase the fractional consumption? How does this impact the amount of product, B, made per hour, i.e. the through-put? Reminder: $Q_B = v_z A_x C_{B,out}$ where A_x is the cross-sectional area of the pipe.

2. Multivariate Nonlinear Optimization

Download the data located at
http://utkstair.org/clausius/docs/mse510/data/mse510_xm02_p02.txt
The first column corresponds to wavelength, x. The second column corresponds to signal intensity, y.

Perform a multivariate nonlinear optimization in order to fit this data to **two** weighted Gaussian curves. The equation for a normalized Gaussian is

$$f_G(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

where μ is the mean and σ is the standard deviation. Your model should take the form

$$y_{model} = w_1 f_G(x;\mu_1,\sigma_1) + w_2 f_G(x;\mu_2,\sigma_2)$$

where w is the weighting constant for each Gaussian.

Determine the optimal values of the weighting constant, the mean and the standard deviation for each Gaussian.