Homework 7, due Dec. 10.

1. Consider the following boundary value problem that models diffusion-limited regime in a catalyst particle with Michaelis-Menten (MM) kinetics:

$$D\frac{d^2C}{dx^2} - V\frac{C}{K+C} = 0,\ C(x=0) = C_{0,}\ C(\infty) = 0$$

   a) Define the set of transformations that puts the problem into the following dimensionless form: $\dfrac{d^2u}{dz^2} - \dfrac{u}{b+u} = 0,\ u(0) = 1, u(\infty) = 0$.

   b) Use this problem to calculate the dimensionless flux into the particle: $\left.\dfrac{du}{dz}\right|_{z=0}$.

   c) Plot your answer as a function of b. What is the approximate behavior of this function for small values of b?

   d) When $K = C_0$ ($b = 1$), the MM reaction term can be approximated by the zeroth-order kinetics: $\dfrac{u}{b+u} \approx F_0(u) \equiv 1$. Evaluate the flux into the particle within the framework of this approximation. How does it compare with the one obtained from the original problem?

   e) The $F_0(u)$ approximation overestimates the reaction term. We can use a better approximation, which is linear below a threshold concentration and constant above it: $\dfrac{u}{b+u} \approx F_1(u) \equiv \begin{cases} \dfrac{u}{b},\ u \le b \\ 1, u > b \end{cases}$. Explain the basis for this approximation. Calculate the flux into particle for this approximation.

   f) Plot your answer as a function of b. How does the b-dependence predicted by this approximation compare with the exact solution, especially for small values of b? Is the overall quality of this approximation better than the one predicted by the $F_0(u)$ function?

   g) Derive the analytical expressions for the concentration profile predicted by the $F_0(u)$ approximation.

   h) Formulate the initial value problem that can be used to find the concentration profile for the original problem. Hint: the idea here is similar to the one used in the shooting method, except that you do not have to guess the second initial condition, which can be found analytically.

   i) Solve this problem numerically for $b = 0.1$ and compare the result with the concentration profile obtained with the $F_0(u)$ approximation. What are the quantitative and qualitative differences between the two solutions?

2. Consider the following boundary value problem that models a first order exothermic reaction, diffusion, and heat conduction in a catalyst pellet with negligible external heat and mass transfer resistance:

$$DC_{xx} - k_0 e^{-\frac{E_A}{R_g T}} C = 0$$

$$k_{eff} T_{xx} + k_0 e^{-\frac{E_A}{R_g T}} (-\Delta H_R) C = 0$$

$$C(0) = C_f, C_x(L) = 0, T(0) = T_f, T_x(L) = 0$$

where C_f and T_f are the concentration and temperature of the surrounding fluid; k_{eff} is thermal conductivity (that does not depend on temperature); $-\Delta H_R$ is the heat of the reaction, k_0 and E_A are the pre-exponential and activation energy, respectively; R_g is the gas constant.

a) Nondimensionalize the problem using the following set of transformations: $z \equiv x/L, u \equiv C/C_f, v \equiv T/T_f$. The resulting problem should have the following dimensionless groups:
$\varphi_0^2 \equiv \dfrac{L^2 k(T_f)}{D}$, $\gamma \equiv \dfrac{E_A}{R_g T_f}$, $\beta \equiv \dfrac{(-\Delta H_R) C_f D}{k_{eff} T_f}$, where $k(T_f) = k_0 e^{-\frac{E_A}{R_g T_f}}$
Interpret the physical meaning of these parameters.

b) Derive the algebraic expression that relates dimensionless temperature and concentration. Hint: use the same approach that was used to analyze the adiabatic CSTR problem.

c) What is the maximal temperature within the pellet?

d) What is the maximal value of reaction rate constant within the pellet?

e) Use this expression to reduce the two-variable problem to a single boundary value problem for the dimensionless concentration:
$$u_{zz} - \varphi_0^2 u \exp\left(\frac{\gamma\beta(1-u)}{1+\beta(1-u)} \right) = 0, \; u(1) = 1, \; u_z(0) = 0$$

f) Write a Matlab code to solve this problem numerically by shooting. Submit your code.

g) Use this code to solve the problem for the following set of parameters: $\beta = 0.1, \gamma = 15$ and φ_0^2 =0.1, 0.5, 1.5, and 2.0. For each of these parameter sets, plot the profiles of dimensionless concentration and temperature and calculate the effectiveness factor.