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:

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

   - Define the set of transformations that puts the problem into the following dimensionless form: $\dfrac{d^2u}{dz^2} - \dfrac{u}{b+u} = 0,\ u(0) = 1, u(\infty) = 0$.
   - Use this problem to calculate the dimensionless flux into the particle: $\left.\dfrac{du}{dz}\right|_{z=0}$.
   - Plot your answer as a function of b. What is the approximate behavior of this function for small values of b?
   - 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?
   - 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.
   - 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?
   - Derive the analytical expressions for the concentration profile predicted by the $F_0(u)$ approximation.
   - 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.
   - 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.

- 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:

  $$\varphi_0^2 \equiv \frac{L^2 k(T_f)}{D},\ \gamma \equiv \frac{E_A}{R_g T_f},\ \beta \equiv \frac{(-\Delta H_R) C_f D}{k_{eff} T_f}, \text{ where } k(T_f) = k_0 e^{-\frac{E_A}{R_g T_f}}$$

  Interpret the physical meaning of these parameters.
- Derive the algebraic expression that relates dimensionless temperature and concentration. Hint: use the same approach that was used to analyze the adiabatic CSTR problem.
- What is the maximal temperature within the pellet?
- What is the maximal value of reaction rate constant within the pellet?
- Use this expression to reduce the two-variable problem to a single boundary value problem for the dimensionless concentration:

  $$u_{zz} - \varphi_0^2 u \exp\left(\frac{\gamma\beta(1-u)}{1+\beta(1-u)} \right) = 0,\ \ u(1) = 1,\ u_z(0) = 0$$

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