Problem 1: First order reaction with diffusion in a catalyst particle (slab)

In this exercise we will discuss and develop models that describe chemical kinetics and transport phenomena inside catalyst particles. The chemical reactions under consideration take place on the surface of the pore walls of the catalyst. We first consider the simplest case of a first order reaction (A→P), equimolar counter diffusion, and isothermal conditions. Next to pore diffusion, we will also take mass transfer resistance from the bulk to the catalyst particle into account. Also, the simplest geometry of a slap of catalyst will be used. Mathematically this model is described by:

$$D_e \frac{d^2 C_a}{dz^2} - k_v C_a = 0$$

$$\left(D_e \frac{dC_a}{dz} \right)\Bigg|_{z=L} = k_m (C_{a,b} - C_a)$$

$$\left. \frac{dC_a}{dz} \right|_{z=0} = 0$$

Where

D_e ($m_f^3/(m_p.s)$) (m^2/s) is the effective diffusion coefficient

C_a (mol/m_f^3) is the concentration of A

$C_{a,b}$ (mol/m_f^3) is the concentration of A in the bulk

k_v ($m_f^3/(m_p^3.s)$) is the reaction rate constant based on the catalyst's volume

k_m ($m_f^3/(m_p^2.s)$) (m/s) is the external mass transfer coefficient

L (m) is half the "thickness" of the slab

The subscripts f and p stand for fluid (gas) and particle respectively.

A) Make the differential equation and the boundary conditions dimensionless by introducing the following dimensionless numbers:

$$\overline{C} = \frac{C_a}{C_{a,b}},\ \theta = \frac{z}{L},\ \Lambda = L\sqrt{\frac{k_v}{D_e}},\ Bi_m = \frac{k_m L}{D_e}$$

Z = 0 is the symmetry axis, L is the surface of the particle.

If the diffusion rate of reactant A is slow compared to the rate of the chemical reaction, a concentration profile of A will exist in the catalyst. Consequently, the reaction rate inside catalyst is lower than at the surface / in the bulk. To relate the volume average reaction rate of

the catalyst particle (r_{obs}) to the reaction rate at bulk conditions (r_b), Thiele introduced the effectiveness factor (η) and Thiele modulus (Λ) concept:

$$r_{obs} = \eta(\Lambda) r_b$$

$$\eta = \int \frac{r(C_a) dV_p}{V_p r(C_{a,b})} = \int \frac{r(C_a) dV_p}{V_p r_b}$$

In this equation, r (mol/(m_p^3.s)) is the reaction rate based on the particle's volume, and V_p (m^3) is the particle's volume. For a first order reaction these equations can be solved by elementary mathematics. The concentration gradient is:

$$\bar{C} = \frac{\cosh(\Lambda\theta)}{\cosh(\Lambda) + \frac{\Lambda}{Bi}\sinh(\Lambda)}$$

The effectiveness factor becomes then:

$$\eta = \frac{\frac{\tanh(\Lambda)}{\Lambda}}{1 + \frac{\Lambda}{\mathrm{Bi_m}}\tanh(\Lambda)}$$

B) Write a code that solves these equations. For this you can use the solver BVP4c. Compare your numerical solutions with the analytical ones.

Problem 2: n^{th} order reaction with diffusion in a spherical catalyst particle

Idem to problem 1, only now the reaction is of order n and we consider a sphere. For this you can also use the bvp4c solver. However we now to include a singularity matrix (S). In this way the solver can handle the following system:

$$\frac{dy_i}{dx} = \sum_j S_{i,j} \frac{y_i}{x} + f(y, x)$$

More info can be found in the Matlab help files.