Problem 1: fixed bed with surface reaction (1D model, non-isothermal)

An n^{th} order heterogeneous reaction is carried in a tubular reactor. The reaction is described by:

A → P

$$r_A = -k \cdot C_A^n \quad mol \cdot m_{catalyst}^{-2} \cdot s^{-1}$$

The modeling equations are:

$$u\frac{dC^f}{dx} = -k_m a\left(C^f - C^s\right)$$

$$k_m\left(C^f - C^s\right) = k(C^s)^n$$

U is the superficial velocity, k_m the mass transfer coefficient, a the specific area (m^2 of catalyst (external surface) per m^3 reactor) and n the order of the reaction. C^f is the concentration in the fluid phase, C^s the concentration at the surface of the catalyst.

Derive the equations that allow the calculation of the fluid and solid temperature.

Write a model that computes the concentration and temperature profile as function of the reactor length (L). Hint: use the isothermal model derived in class as starting point.

The set of equations is a DAE system (a so-called differential algebraic equation system). The ODE15s solver of Matlab can handle such systems. It uses a Mass matrix to define the system. (see Matlab help files).

Problem 2: Fixed bed model 1D coupled with a catalyst particle model

Write a code that can solve the 1D heterogeneous model as described on slide 24 of the slide package "fixed bed 2 2017". You may limit yourself to the isothermal case, so only solving the mol balances. We consider a n^{th} order reaction A→ P.

You can use a catalyst particle model for a slab. This model should calculate the effectiveness factor at every axial position.

The equation to be solved are:

For the reactor:

$$u\frac{dC^f}{dx} = -k_m a\left(C^f - C^s\right)$$

$$k_m a\left(C^f - C^s\right) = k_v (C^s)^n \eta$$