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Statistical and Numerical Methods
Exercise 8, HS24

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1 Steady State Tubular Reactor (Core)

1. Solve the steady state tubular reactor for 20 different Peclet numbers (between 0.01 and 100) and for a first (n=1) and second (n=2) order reaction. Use a Damköhler number of unity.

$$Pe = \frac{L^2/D}{L/v}, Da = \frac{L/v}{1/(kc_{in}^{n-1})} \tag{1}$$

   - Complete the template rhs.m by implementing the non-linear equations to solve the problem.

2. Plot the conversion at the end of the reactor $1 - c_{out}/c_{in}$ vs. Peclet number Pe for both reaction orders. Also, plot the ratio between the conversions of the first order and second order reaction.
   - What is better for these reactions, a lot of back-mixing (small Pe, CSTR) or ideal plug flow (large Pe, PFR)?
   - What influence does the reaction order have overall and at low or high Peclet numbers?
   - Complete the template TubReact_steady_state.m.

2 Dynamic Tubular Reactor (Core)

1. Solve the dynamic tubular reactor from time 0 to 5 with a MATLAB solver ode23s. Use the rhs.m from assignment 1 and the template TubReact_dynamic.m. Consider only a first order reaction with $Pe = 100$ and $Da = 1$.

2. Plot the dimensionless concentration at the end of the reactor u_N vs. dimensionless time θ
   - At what time does the solution reach a steady state, i.e. how many reactor volumes of solvent will you need?
   - Complete the template TubReact_dynamic.m