TU Clausthal
Clausthal University of Technology
Institute of Chemical and Electrochemical Process Engineering

# 2. Exercise Optimization in Engineering Summer Term 2025
## (Solving an ODE System)

The following reaction takes place in a continuously operated ideal tubular reactor:

$$A \overset{r_1}{\rightarrow} B \overset{r_2}{\rightarrow} C$$

Here, B represents the desired target product, and C is a worthless by-product. Furthermore, the target product also decomposes into the worthless component D:

$$B \overset{r_3}{\rightarrow} D$$

The reactor is operated in steady state, so that the following balance equations can be formulated:

$$\frac{dc_A}{dx} = \frac{A_o}{q}\left[-k_{10}exp\left(\frac{-E_{A_1}}{RT}\right)c_A^{n_1}\right],$$

$$\frac{dc_B}{dx} = \frac{A_o}{q}\left[+k_{10}exp\left(\frac{-E_{A_1}}{RT}\right)c_A^{n_1} - k_{20}exp\left(\frac{-E_{A_2}}{RT}\right)c_B^{n_2} - k_{30}exp\left(\frac{-E_{A_3}}{RT}\right)c_B^{n_3}\right],$$

$$\frac{dc_C}{dx} = \frac{A_o}{q}\left[k_{20}exp\left(\frac{-E_{A_2}}{RT}\right)c_B^{n_2}\right],$$

$$\frac{dc_D}{dx} = \frac{A_o}{q}\left[k_{30}exp\left(\frac{-E_{A_3}}{RT}\right)c_B^{n_3}\right].$$

Calculate the steady-state axial concentration profile that occurs in the reactor given the following parameter values.

Given:

| | |
|---|---|
| $c_{A,In} = 12 \text{ mol/m}^3$ | $c_{B,In} = c_{C,In} = c_{D,In} = 0 \text{ mol/m}^3$ |
| $k_{10} = 5.4 \cdot 10^{10} \text{ s}^{-1}$ | $E_{A,1} = 7.5 \cdot 10^4 \text{ J/mol}$ |
| $k_{20} = 4.6 \cdot 10^{17} \text{ s}^{-1}$ | $E_{A,2} = 1.2 \cdot 10^5 \text{ J/mol}$ |
| $k_{30} = 5.0 \cdot 10^7 \text{ s}^{-1}$ | $E_{A,3} = 5.5 \cdot 10^4 \text{ J/mol}$ |
| $n_1 = 1.1$ | $n_2 = n_3 = 1$ |
| $R = 8.3145 \text{ J/mol/K}$ | $T = 340 \text{ K}$ |
| $A_o = 0.1\, m^2$ | $q = 0.12 \text{ m}^3/\text{s}$ |

Tasks:

a) Define a structure (in MATLAB) / class (in Python) "p" for all constant parameters.

b) Implement the given differential equation system as a function. The output of the function should be a column vector containing the concentration gradients of all species.

c) Solve the given differential equation system using the ODE solver "ode45" (in MATLAB) / "RK45" (in Python) for a reactor length of 50 meters and plot the concentration profiles in one figure!

d) At which length is the concentration of B maximized. How can you determine this length as accurately as possible using MATLAB/Python (don't use in-build functions)?

e) How would you formulate a suitable optimization problem, and how can you classify it (present a proper mathematical formulation of the optimization problem as discussed in the lecture and specify the dimensions of your functions and variables)?

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Submission per .zip file on Stud.IP
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