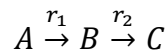


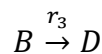


2. Exercise Optimization in Engineering Summer Term 2025 (Solving an ODE System)

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



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:



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

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

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

Given:

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



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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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