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

3. Exercise Optimization in Engineering Summer Term 2025
One-dimensional Optimization
Search Methods

The continuously and stationary operated ideal tubular reactor from the last exercise should now be optimized regarding the reactor temperature. As a reminder: The following reactions occur in the reactor:

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

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

Following the reactor section, the components A, B, C and D are completely separated from each other. The separation costs are negligible. The reactant A must be purchased for a price of 2 €/mol (pA = 2 €/mol), while the product B can be sold for a price of 7 €/mol (pB = 7 €/mol). Components C and D are worthless by-products. The revenue E (E in €/s) of the process is to be maximized. The costs for the temperature control of the reactor (fixed length of L = 30 m) can be calculated as follows:

$$\boldsymbol{E_T = -q p_T |T - 298K|},$$

with $p_T = 0.06$ €/m³/K

Tasks:

a) Define the objective function F and give a mathematical formulation of the optimization problem.

b) Write a function that returns the value of the objective function F for a given reactor temperature! Check your implementation using the given control solution.

   Control: F (T = 340 K) = 3.03 €/s, $c_{A,out}$ = 0.182 mol/m³, $c_{B,out}$ = 0.134 mol/m³

c) Perform an equidistance search in the interval of T = [300 K ... 380 K]. Divide the interval into 25 equal sections and plot the course of the objective function.

d) Carry out another equidistant search in the remaining uncertainty interval. Also divide this interval into 25 equal sections. What accuracy can be expected? How many function calls would be required to achieve the same accuracy if only a single equidistant search is performed?

Bonus Task (highly recommended):

e) Write a function in which the simultaneous search based on the golden section method is implemented and solve the given optimization problem for the interval T = [300 K … 380 K]. Determine the optimal reactor temperature so that the remaining uncertainty interval is smaller than the one of task d)! Compare the number of function calls to task d).

As a reminder: In steady state the reactor can be described by the following balance equations:

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

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

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

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

With:

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

Lecturer
Lukas Gottheil, M.Sc.
gottheil@icvt.tu-clausthal.de

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