7. Exercise Optimization in Engineering Summer Term 2025

Constrained optimization

Recall the **isothermal tubular reactor from the 4th exercise** (unconstrained multidimensional optimization): Component A reacts to a target component B, which further breaks down into components C and D (the model equations are once again given on the following page). The optimization variables T (reactor temperature) and L (reactor length) are to be specified to maximize the profit.

However, in this exercise **additional constraints** to the process are considered:

1. Component B crystallizes at concentrations above thSe saturation concentration. This must be avoided! The saturation concentration depends on the temperature and can be described by:

$$c_{B,sat}(T) = \exp(-3.75 + 1.42 \cdot 10^{-2} \cdot T)$$

2. Due to technical reasons, a reactor length of more than 20 m is not applicable.

3. The component C is highly flammable. Therefore, the maximum reactor temperature is strictly limited. To enable safe operation, the maximum partial pressure of component C should not exceed 120 mbar. The vapor pressure of this substance C is determined by the following Antoine-relation:

$$p_C = \exp\left(8 - \frac{1730}{208 + (T/°C)}\right) \; [mbar]$$

   This equation can be used to calculate the reactor temperature limit.

4. Obviously, no negative values can be chosen for both the reactor temperature and reactor length.

Tasks:

Adjust the formulated optimization problem to the given constraints and find the optimal reactor length and reactor temperature.

a) Formulate the complete optimization problem (objective function, constraints, dimensions of variables). Give the mathematical formulation!

b) Re-use the program from exercise 4 and extend it by penalty functions to consider the constraints. Solve the optimization problem using initial values of $x_0 = [15\text{m} \quad 300\text{K}]$ with weighting factors of $\sigma = 0.1$ and $\sigma = 10$. In MATLAB, apply `fminsearch` and in Python apply `scipy.optimize.minimize(fun, x0, method='Nelder-Mead')`. Prove that the constraints have been met sufficiently!

c) Furthermore, solve the optimization problem using the MATLAB solver `fmincon` / the Python solver `scipy.optimize.minimize` for constrained optimization problems. Choose a suitable algorithm / method by yourself. Prove that the constraints have been met sufficiently!

As a reminder: In steady state the reactor can be described by the following ODE system:

$$\frac{dc_A}{dx} = \frac{A_0}{q}\left[-k_{10}exp\left(\frac{-E_{A_1}}{RT}\right)c_A^{n_1}\right],$$

$$\frac{dc_B}{dx} = \frac{A_0}{q}\left[+k_{10}exp\left(\frac{-E_{A_1}}{RT}\right)c_A^{n_1} - k_{20}exp\left(\frac{-E_{A_2}}{RT}\right)c_B^{n_2} - k_{30}exp\left(\frac{-E_{A_3}}{RT}\right)c_B^{n_3}\right],$$

$$\frac{dc_C}{dx} = \frac{A_0}{q}\left[+k_{20}exp\left(\frac{-E_{A_2}}{RT}\right)c_B^{n_2}\right],$$

$$\frac{dc_D}{dx} = \frac{A_0}{q}\left[+k_{30}exp\left(\frac{-E_{A_3}}{RT}\right)c_B^{n_3}\right].$$

With:

$c_{A,\mathrm{In}} = 12\ \mathrm{mol/m^3}$	$c_{B,\mathrm{In}} = c_{C,\mathrm{In}} = c_{D,\mathrm{In}} = 0\ \mathrm{mol/m^3}$
$k_{10} = 5.4 \cdot 10^{10}\ \mathrm{s^{-1}}$	$E_{A,1} = 7.5 \cdot 10^4\ \mathrm{J/mol}$
$k_{20} = 4.6 \cdot 10^{17}\ \mathrm{s^{-1}}$	$E_{A,2} = 1.2 \cdot 10^5\ \mathrm{J/mol}$
$k_{30} = 5.0 \cdot 10^{7}\ \mathrm{s^{-1}}$	$E_{A,3} = 5.5 \cdot 10^4\ \mathrm{J/mol}$
$n_1 = 1.1$	$n_2 = n_3 = 1$
$R = 8.3145\ \mathrm{J/mol/K}$	
$A_0 = 0.1\ \mathrm{m^2}$	$q = 0.12\ \mathrm{m^3/s}$
$p_A = 2\,€/mol$	$p_B = 7\,€/\mathrm{mol}$
$p_T = 0.06\,€/m^3\,K$	

The revenue (E) of the process can be calculated as follows:

$$E = q\left(p_A\left(c_{A.out} - c_{A,in}\right) + p_B\left(c_{B,out} - c_{B,in}\right) - p_T|T - 298K|\right)$$

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