The goal of the following exercises is to be able to solve systems of ordinary differential equations without knowledge of the chemical and engineering context.

Exercise 1: gas-phase parallel reactions in a tubular reactor

Here's a problem to solve using Python! We have a reagent A reacting in 3 parallel chemical reactions to form a desired product B and two unwanted products X and Y.

The differential equations to be solved to model this reaction in a tubular reactor are:

$$\frac{dF_A}{dV} = -k_1 C_A - k_2 - 2k_3 C_A^2$$

$$\frac{dF_B}{dV} = k_1 C_A$$

$$\frac{dF_X}{dV} = k_2$$

$$\frac{dF_Y}{dV} = 2k_3 C_A^2$$

$$C_A = F_A/2$$

With constants k1, k2 and k3 of 0.0012, 0.00011 and 0.0041 respectively. The values of F_A, F_B, F_X and F_Y for V=0 are 0.92 mol/s, 0 mol/L, 0 mol/s and 0 mol/s, respectively.

What are V (in liters) and F_B (in mol/s) when F_A is half its initial value (the conversion is 50 %)?

Exercise 2 : fed-batch reaction with a chemical equilibrium

We wish to solve the two differential equations below for t = 5000 s with Python.

$$R = k_1 \cdot C_A C_B - k_2 \cdot C_C C_D$$

$$\frac{dC_A}{dt} = -R - \frac{\dot{V}}{V} \cdot C_A$$

$$\frac{dV}{dt} = \dot{V}$$

$$\frac{dC_B}{dt} = -R + \frac{\dot{V}}{V} \cdot (C_{BF} - C_B)$$

$$\frac{dC_C}{dt} = R - \frac{\dot{V}}{V} \cdot C_C$$

$$\frac{dC_D}{dt} = R - \frac{\dot{V}}{V} \cdot C_D$$

With:

$$k_1 = 9.00 \cdot 10^{-5}, k_2 = 8.33 \cdot 10^{-5}$$

$\dot{V} = 0.05$ for t ≤ 4000 s and $\dot{V} = 0$ otherwise

$C_{BF} = 10.93$ mol/L

The initial conditions are:

$C_{A0} = 7.72$ mol/L

$V_0 = 200$ L

$C_{B0} = 0$ mol/L

$C_{C0} = 0$ mol/L

$C_{D0} = 0$ mol/L

What will be the concentration B when we stop feeding at t = 4000 s ? What will be the concentrations of A, B, C and D after 5000 s ?

Exercise 3: tubular reactor with exothermic reaction

You are asked to solve the problem described by the following ordinary differential equations using the Python programming language:

$\frac{dF_A}{dV} = R_A$ avec $R_A = -r_1 + r_2$ $\qquad r_1 = k \cdot C_A$ $\qquad r_2 = \left(\frac{k}{K}\right) \cdot C_B$

$\frac{dF_B}{dV} = R_B$ avec $R_B = r_1 - r_2$ $\qquad C_A = F_A/Vdot0$ $\qquad C_B = F_B/Vdot0$

$$\frac{dT}{dV} = \frac{(-\Delta H_R)\cdot r_1 - (-\Delta H_R)\cdot r_2 + Ua\cdot(T_j - T)}{F_A\cdot c_{p_A} + F_B\cdot c_{p_B} + F_{I0}\cdot c_{p_I}} \qquad k = 31.12 \cdot \exp\left[\frac{\mathrm{E_a}}{8.314}\left(\frac{1}{360} - \frac{1}{T}\right)\right]$$

$$K = 3.031 \cdot \exp\left[\frac{\Delta H_R}{8.314}\left(\frac{1}{333} - \frac{1}{T}\right)\right]$$

The constant values are

$C_{A0} = 1.86$ kmol/m3, $F_{A0} = 14.67$ kmol/h, $F_{B0} = 0$ kmol/h, $F_{I0} = 1.63$ kmol/h, $E_a = 65700$ J/mol, $T_0 = 305$ K, $T_j = 315$ K, $\Delta H_R = -34500$ kJ/kmol, $c_{p_A} = c_{p_B} = 141$ kJ/kmol/K, $c_{p_I} = 161$ kJ/kmol/K, $Ua = 5000$ kJ/m3/h/K, $Vdot0 = F_{A0}/C_{A0}$ m3/h

The values F_A, F_B and T for $V = 0$ are the constants F_{A0}, F_{B0} et T_0 given above. Draw profiles of F_A, F_B and T as a function of V and find the max value of T in the reactor.