# Øving 11

The elementary first order gas phase reaction

$$A = B + C$$

Is first performed adiabatically in reactors packed with a particulate catalyst material. The feed consists of pure A with a feed rate of 20 dm$^3$/s, at 10 bar pressure and a temperature of 450 K. Assume ΔP=0.

1. Use python to draw the curves for the conversion and temperature against catalyst amount up to 80% conversion in a PFR.

Given:
The heat capacities are regarded constant within the temperature inte

$C_{PA}$ = 40 J/mol·K, $C_{PB}$ = 25 J/mol·K , $C_{PC}$ = 15 J/mol·K

The formation enthalpy at 273 K:

$H^0_A$ = -70 kJ/mol, $H^0_B$ = -50 kJ/mol , $H^0_C$ = -40 kJ/mol

The reaction rate coefficient: $k = 0.133 \exp\frac{E}{R}\left(\frac{1}{450} - \frac{1}{T}\right)$ dm$^3$/s·kg c

The activation energy, E = 31.4 kJ/mol

The gas constant: R = 8.314 J/mol·K = 0.082 dm$^3$·bar/mol·K

Answers: 2) 39.4 kg 3) 660 kg

$\delta = 1+1-1 = 1$, $\varepsilon = \delta y_{A0} = 1 \cdot 1 = 1$

For PFR: $-r_A = F_{A0}\frac{dX}{dW}$

1st order rx: $-r_A = kC_A = k\frac{F_A}{V} = k\frac{F_{A0}(1-X)}{V_0(1+\varepsilon X)\frac{P}{P_0}\frac{T}{T_0}} \overset{P_0,\ \Delta P=0}{=} k\frac{F_{A0}(1-X)}{V_0(1+X)\frac{T}{T_0}}$

$\Rightarrow F_{A0}\frac{dX}{dW} = k\frac{F_{A0}(1-X)}{V_0(1+X)\frac{T}{T_0}}$

$dW = \frac{V_0}{T_0}\cdot\frac{k}{T}\cdot\frac{1+X}{1-X}dX$

$W = \frac{V_0}{T_0}\int\frac{T}{k}\cdot\frac{1+X}{1-X}dX$ (1)

Given: $k = 0{,}133\cdot\exp\left(\frac{31.4\cdot10^3}{8{,}314}\left(\frac{1}{450} - T\right)\right)$ (2)

Energy balance

Steady state $\Rightarrow \frac{dE}{dt} = 0$

No heat added $\Rightarrow \dot{Q} = 0$

Adiabatic $\Rightarrow W_s$ is negligible

$\Rightarrow$ Generated heat = Heating the flow

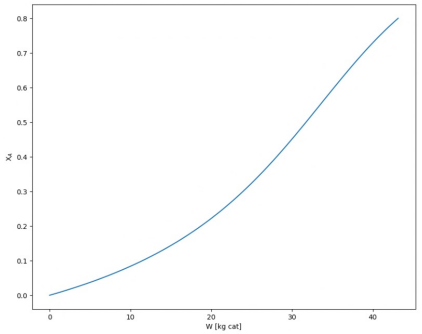
$F_{A0}X(-\Delta H_{rx}) = F_{A0}C_{PA}(T-T_0)$

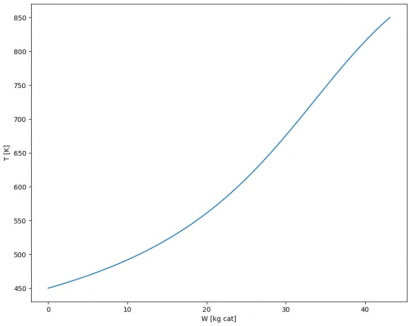
$\Delta H_{rx} = H^\circ_B + H^\circ_C - H^\circ_A = -50 - 40 + 70 = -20$ kJ/mol

$$\Rightarrow T = \frac{20\,000\ J/mol}{40\ J/mol \cdot K} X + T_0$$

$$T = T_0 + 500\,X \quad (3)$$

Equation 1-3 are used in python, the plots are:




2. How much catalyst material does it take to reach 80% conversion in an adiabatic CSTR?

CSTR is not a differential reactor

$\Rightarrow$ Same as in 1), but without integral sign, $dX \rightarrow X$

$$\Rightarrow W = \frac{V_0}{T_0} \cdot \frac{I}{k} \cdot \frac{1+x}{1-x} \cdot x$$

Done in python

$\Rightarrow$ W = 39,4 kg cat

The two reactors will no be equipped with cooling mantels. The flowing cooling liquid holds an approximately constant temperature of 50°C. The heat exchangers are characterized by:

U = total heat transfer number, J/s·m²·K
a = contact area pr. volume for the PFR heat exchanger, m²/m³
A = contact area for the CSTR heat exchanger, m²
$\rho_B$= density of the catalyst material, kg/m³

3. Determine the amount of catalyst in the CSTR when UA = 500 J/s·K

We get a new energy balance:

Added heat Generated heat = Heating of the flow

$$Q + F_{A0} X(-\Delta H_{rx}) = F_{A0} C_{pA} (T-T_0)$$

$$UA(T_a - T) + F_{A0} X(-\Delta H_{rx}) = F_{A0} C_{pA} (T-T_0)$$

$$UA T_a + F_{A0} X(-\Delta H_{rx}) + F_{A0} C_{pA} T_0 = F_{A0} C_{pA} T + UAT$$

$$T = \frac{F_{A0}(-\Delta H_{rx})}{F_{A0} C_{pA} + UA} + \frac{UAT_a + F_{A0} C_{pA} T_0}{F_{A0} C_{pA} + UA} = 151{,}23X + 361{,}41$$

Where $F_{A0}$ was found from the ideal gas law

$$F_{A0} = \frac{P_0 \cdot V_0}{R T_0} = \frac{10 \cdot 20}{0{,}082 \cdot 450} = 5{,}42 \text{ mol/s}$$

Inserting new expression for T into python:

$$\Rightarrow \underline{W = 660{,}6 \text{ kg cat}}$$

4. Formulate the differential equations that describe the evolution of temperature and conversion in the PFR when $Ua/\rho_B = 0.8$ J/s·K·kg catalyst. Use python to plot the conversion and temperature in the catalyst bed.

The added heat changes along the length/volume of the reactor

$$\Rightarrow \dot{Q} = \int_0^V U_a(T_a - T)\,dV$$

New energy balance

$$\int_0^V U_a(T_a - T)\,dV + F_{A0} X(-\Delta H_{rx}) = F_{A0} C_{pA} (T-T_0)$$

Differentiating

$$U_a(T_a - T) + F_{A0}(-\Delta H_{rx})\frac{dX}{dV} = F_{A0}\,C_{PA}\frac{dT}{dV}\text{, har at}$$

$$\frac{dT}{dV} = \frac{U_a(T_a - T) + (-\Delta H_{rx})\cdot F_{A0}\frac{dX}{dV}}{F_{A0}C_{PA}} \qquad / \cdot \frac{1}{\rho_b}$$

$$\frac{dT}{d(V\cdot\rho_b)} = \frac{\frac{U_a}{\rho_b}(T_a - T) + (-\Delta H_{rx})\cdot F_{A0}\frac{dX}{d(V\rho_b)}}{F_{A0}C_{PA}}$$

$$\frac{dT}{dW} = \frac{\frac{U_a}{\rho_b}(T_a - T) + (-\Delta H_{rx})\cdot F_{A0}\frac{dX}{dW}}{F_{A0}\,C_{PA}}$$

From 1), $F_{A0}\frac{dX}{dW}$ was found to be $-r_A$

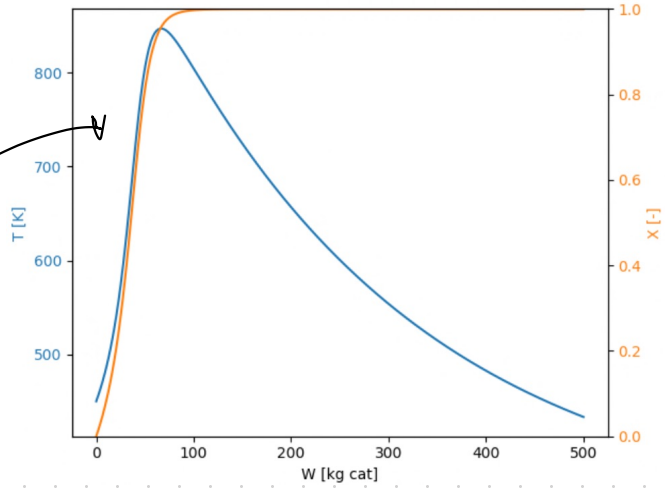
$$\frac{dT}{dW} = \frac{\frac{U_a}{\rho_b}(T_a - T) + (-\Delta H_{rx})\cdot(-r_A)}{F_{A0}\,C_{PA}}$$

$$\frac{dT}{dW} = \frac{\frac{U_a}{\rho_b}(T_a - T) + (-\Delta H_{rx})\cdot\frac{k\cdot F_{A0}(1-X)}{V_0(1+X)\frac{T}{T_0}}}{F_{A0}\,C_{PA}} \qquad (1)$$

And:

$$\frac{dX_A}{dW} = \frac{-r_A}{F_{A0}} = \frac{k(1-X)}{V_0(1+X)\frac{T}{T_0}} \qquad (2)$$

Inserted the two equations into python




I'm not sure if this makes sense, but I am not able to ~~get~~ anything better either, I think it is because $\frac{U_A}{\rho_b}$ is very low.