

# Chemical Reaction Engineering

## Practical Session 3

26 November 2021

### 1. Plug flow reactor with heat exchange (uniform, constant $T_{ex}$ ) [from Practical Session 2]

An irreversible and first-order reaction  $A \rightarrow B$  occurs in gaseous phase in a plug flow reactor:

$$r = kC_A \quad k = Ae^{-\frac{E}{RT}} \quad A = 2 \cdot 10^8 \text{ s}^{-1} \quad E = 24000 \text{ cal/mol}$$

The reaction is exothermic, with a reaction heat of  $-5000 \text{ cal/mol}$ . For this reason, the reactor is cooled through a proper fluid, which can be considered at a constant, uniform temperature  $T_e = 300^\circ\text{C}$ . The inlet stream is pure A, with molar flow rate of  $50 \text{ kmol/h}$ , at temperature of  $T_{in} = 300^\circ\text{C}$  and pressure of  $P = 3 \text{ atm}$ . The specific heat of the gaseous mixture can be assumed independent of temperature and composition and equal to  $Cp_{mix} = 30 \frac{\text{cal}}{\text{mol K}}$ . The internal diameter of the reactor is  $8 \text{ cm}$  and its total length is equal to  $150 \text{ m}$ . The global heat exchange coefficient was estimated equal to  $U = 50 \frac{\text{kcal}}{\text{m}^2 \text{ h K}}$ .

- Evaluate the conversion and temperature profile inside the reactor. Calculate the final conversion and the temperature peak.
- If the mixture temperature cannot exceed  $380^\circ\text{C}$ , calculate the minimum value of  $U$  able to respect this constraint. Which would be the corresponding conversion?

### 2. Non-uniform external temperature: co-current configuration

Consider the same reactor studied in Exercise 1. However, now we remove the hypothesis that the external temperature is constant and uniform along the reactor and we imagine that the cooling fluid is fed in a co-current configuration. In particular, we assume that its inlet temperature is  $T_e = 200^\circ\text{C}$ , its constant pressure specific heat  $Cp_e = 30 \frac{\text{cal}}{\text{mol K}}$  and its molar flow rate  $F_e = 30 \frac{\text{kmol}}{\text{h}}$ . The external cross section area is  $A_e = 0.005 \text{ m}^2$ . The global heat exchange coefficient is now  $U = 20 \frac{\text{kcal}}{\text{m}^2 \text{ h K}}$ . By keeping the same data reported in Exercise 1, evaluate the conversion and temperature profile inside the reactor. Calculate the final conversion and the temperature peak.

### 3. Non-uniform external temperature: counter-current configuration

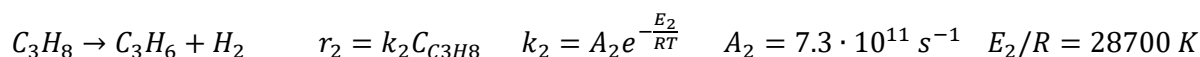
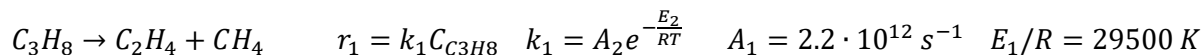
Assuming the same data reported in Exercise 2, repeat the calculations in the case of a counter-current configuration.

## Advanced exercise

### 4. Pyrolysis of propane in a PFR with heat exchange (uniform, constant external temperature)

The pyrolysis of propane is carried out in a PFR, with an internal diameter of  $D = 11 \text{ cm}$ , thickness of  $1 \text{ cm}$  and equivalent length of  $L = 70 \text{ m}$ . The metal conductivity is  $\lambda_w = 15 \frac{\text{kcal}}{\text{mhK}}$ . The inlet feed, made up of  $2000 \frac{\text{kg}}{\text{h}}$  of  $\text{C}_3\text{H}_8$  and  $1000 \frac{\text{kg}}{\text{h}}$  of steam, is at  $T_{in} = 600^\circ\text{C}$  and  $P = 3 \text{ atm}$ .

As a first approximation, the primary reactions of pyrolysis are described through a simplified, first-order model:



Both the reactions are endothermic:  $\Delta H_1 = 18750 \frac{\text{kcal}}{\text{kmol}}$  and  $\Delta H_2 = 30840 \frac{\text{kcal}}{\text{kmol}}$ .

The tubular reactor is inside a furnace, which provides the required heat. As a first simplification, we can assume that the gases inside the furnace, surrounding the reactor, are at  $T_{gas}^f = 1100^\circ\text{C}$ .

- Evaluate propane conversion obtained at the reactor outlet.
- Then, evaluate the reactor performance in terms of profiles of temperature, external temperature of tubes and concentrations of different species.
- Finally, verify that the external temperature of tubes does not exceed  $1000^\circ\text{C}$  to avoid the tubes collapse.

The external heat transfer coefficient was estimated to be uniform and constant and equal to  $h_e = 0.080 \frac{\text{kcal}}{\text{m}^2\text{Ks}}$ . The internal heat transfer coefficient can be estimated using the Dittus-Boelter formula:

$$Nu = 0.023 Re^{0.8} Pr^{1/3}$$

For simplicity we assume that the following properties of the mixture are independent of composition and temperature:  $Cp_{mix} = 0.8 \frac{\text{kcal}}{\text{kg K}}$ ,  $\mu_{mix} = 3.8 \cdot 10^{-5} \frac{\text{kg}}{\text{m s}}$ ,  $\lambda_{mix} = 3.194 \cdot 10^{-5} \frac{\text{kcal}}{\text{mKs}}$ . The pressure drop can be considered negligible.

## Suggested exercises

### 5. Inclusion of pressure drop

Repeat Exercise 2 by including the pressure drop along the reactor. The pressure is described by the following differential equation:

$$\frac{dp}{dz} = -\frac{1}{2} \rho v^2 f a$$

where  $a = p_w/A$  is the ratio between the perimeter and the area of the cross section. The molecular weight of A is  $28 \frac{\text{kg}}{\text{kmol}}$  and the dynamic viscosity of the mixture is  $1.8 \cdot 10^{-5} \frac{\text{kg}}{\text{ms}}$ . The friction factor can be evaluated using the Blasius' correlations:

$$f = 0.079 Re^{-1/4}$$

Compare the solution obtained through the integration of the differential equation governing the evolution of pressure with the approximate analytical solution:

$$\tilde{P} = P_0 \sqrt{1 - \alpha_P A x} \quad \text{where } \alpha_P = \frac{4G^2}{\rho_0 P_0} \frac{f}{DA} \text{ and } G = \rho_{in} v_{in}$$