

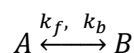
# Chemical Reaction Engineering

## Practical Session 2

18 November 2021

### 1. Design of an adiabatic PFR for isomerization reaction

Species A is to be isomerized to species B in a plug-flow reactor, according to the following elementary reversible reaction:



where  $k_f$  and  $k_b$  are the kinetic constants of forward and backward constants, respectively. The forward kinetic constant is equal to  $31.1 \text{ h}^{-1}$  at  $360 \text{ K}$ , and its activation energy is  $65700 \text{ J/mol}$ . The equilibrium constant  $K_{eq}$  is equal to 3.03 at  $60^\circ\text{C}$ .

The inlet mixture is fed at  $330 \text{ K}$ , with a volumetric flow rate of  $163 \text{ kmol/h}$ . Its molar composition is equal to 90% of species A and 10% of inert species (I). The inlet concentration of A is  $9.30 \text{ kmol/m}^3$ .

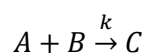
The reaction heat, measured at the reference temperature of  $300 \text{ K}$ , is  $-6900 \frac{\text{J}}{\text{mol}}$ . The constant-pressure specific heats of species are independent of temperature:  $C_p^A = 131$ ,  $C_p^B = 171$ ,  $C_p^I = 161 \frac{\text{J}}{\text{mol K}}$ .

Calculate the PFR volume necessary to convert 60% of species A.

### 2. Production of propylene glycol in adiabatic CSTR

Propylene glycol (C) is produced from the hydrolysis of propylene oxide (A) in a steady-state, perfectly stirred reactor. To this purpose, a reactor with a volume of  $1135 \text{ l}$  is used. The reactants are fed to the reactor through two streams: the first is made up of propylene oxide (A) and methanol (M), in equi-volumetric quantities, each of  $1320 \text{ l/h}$ . The second is made up of water (B) and is equal to  $6600 \text{ l/h}$ . The corresponding molar flows of propylene oxide, methanol and water are equal to  $19.50 \text{ kmol/h}$ ,  $32.6 \text{ kmol/h}$  and  $364 \text{ kmol/h}$ . The temperature of the two streams is  $14^\circ\text{C}$ , but after their mixing (before entering the reactor) and increment of  $10^\circ\text{C}$  is observed.

The reaction can be considered as irreversible and first-order with respect to propylene oxide (A), and of order zero with respect to water (B):



$$r = kC_A \quad k = Ae^{-\frac{E}{RT}} \quad A = 16.96 \cdot 10^{12} \text{ h}^{-1} \quad E = 72000 \text{ J/mol}$$

The reactor, working in adiabatic conditions, must operate at a temperature not higher than  $53^\circ\text{C}$ , in order to be sufficiently far away from the boiling point of propylene oxide.

Is then possible using the reactor with this constraint on temperature? Which would be the corresponding propylene oxide conversion?

Constant-pressure specific heats are indicated in the table below, as well as the enthalpy of formation of the different compounds. The variation of density of the liquid (which is experimentally known as ~3%) can be ignored.

Specific heat in $J/mol/K$	
$Cp_A$	146
$Cp_B$	75
$Cp_C$	192
$Cp_M$	82

Formation enthalpy in $J/mol$	
$H_A(20^\circ C)$	-148918
$H_B(20^\circ C)$	-275000
$H_C(20^\circ C)$	-505360

### 3. Plug flow reactor with heat exchange (uniform, constant external temperature)

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  $T_e = 300^\circ C$ . The inlet stream is pure A, with molar flow rate of  $50 \text{ kmol/h}$ , at temperature of  $T_{in} = 300^\circ C$  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  $380^\circ C$ , calculate the minimum value of  $U$  able to respect this constraint. Which would be the corresponding conversion?

## Suggested exercises

### 4. Isothermal CSTR with parallel reactions

The two following parallel reactions (liquid phase) occur in an isothermal CSTR at  $T = 80^\circ C$ :

$$A \rightarrow B \quad r_1 = k_1 C_A \quad k_1 = A_1 e^{-\frac{E_1}{RT}} \quad A_1 = 3 \cdot 10^{14} \text{ s}^{-1} \quad E_1 = 20000 \frac{\text{cal}}{\text{mol}}$$

$$A \rightarrow C \quad r_2 = k_2 C_A \quad k_2 = A_2 e^{-\frac{E_2}{RT}} \quad A_2 = 2 \cdot 10^{13} \text{ s}^{-1} \quad E_2 = 18000 \frac{\text{cal}}{\text{mol}}$$

The reactor is fed with pure A at concentration  $C_A^0 = 55 \frac{\text{kmol}}{\text{m}^3}$ . The total residence time is  $\tau = 1 \text{ min}$ .

Evaluate numerically the outlet concentrations of species A, B and C and compare them with the analytical solution.

**5. Adiabatic CSTR with parallel reactions**

The same reactor described in Exercise 4 is now working in adiabatic conditions. In particular, the inlet temperature is  $T_{in} = 20\text{ }^{\circ}\text{C}$ . Evaluate numerically the outlet temperature and the concentrations of species A, B, and C. Additional data are here provided.

Species	$H_f^0(T_0 = 20\text{ }^{\circ}\text{C})$ [kcal/kmol]	$C_p$ [kcal/kmol/K]
A	6000	5
B	5802	6
C	5620	4