Chemical Reaction Engineering

Practical Session 2

22 November 2019

Plug Flow Reactors with heat exchange

1. ***Uniform, constant external temperature***

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

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

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

   a. Evaluate the conversion and temperature profile inside the reactor. Calculate the final conversion and the temperature peak.
   b. If the mixture temperature cannot exceed 380 °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 $T_e = 200°C$, its constant pressure specific heat $Cp_e = 30 \frac{cal}{mol\, K}$ and its molar flow rate $F_e = 30 \frac{kmol}{h}$. The global heat exchange coefficient is now $U = 20 \frac{kcal}{m^2\, h\, K}$. 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.

4. ***Inclusion of pressure drop***

Repeat Exercise 3 by including the pressure drop along the reactor. The molecular weight of *A* is $28 \frac{kg}{kmol}$ and the dynamic viscosity of the mixture is equal to $1.8 \cdot 10^{-5} \frac{kg}{ms}$. The friction factor can be evaluated using the Blasius' correlations:

$$f = \frac{0.079}{Re^{1/4}}$$

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

$$\tilde{P} = P_0\sqrt{1 - \alpha_P A x}$$

$$\alpha_P = \frac{4G^2}{\rho_0 P_0}\frac{f}{DA}$$