Chemical Reaction Engineering

Practical Session 1

11 November 2019

Design of isothermal Batch reactors

1. The irreversible, first-order reaction $A \rightarrow B$ has a kinetic constant $k = 0.01\ s^{-1}$. If the initial concentration of A is $2\ mol/l$, what is the time required to obtain a 90% conversion in a constant-volume batch reactor? And what if the desired conversion is 99.9%?
2. Considering the same reaction of Exercise 1 with a generic order n different from 1, how would be the concentration profiles of A over time? Which would be the required time to obtain a 90% conversion with $n = 0.5$ and $n = 2$?

Design of isothermal CSTRs

3. Calculate the conversion of a species A as a function of the residence time for a bimolecular reaction in a constant-density CSTR:

$$A + B \rightarrow C \qquad r = kC_AC_B$$

$$k = 0.05\ \frac{l}{mol\ s} \qquad C_A^{in} = 3\ \frac{mol}{l} \qquad C_B^{in} = 4\ \frac{mol}{l}$$

   How much time would be required to get a conversion of A = 95%?

4. Consider the reversible reaction $A \leftrightarrow B$ whose reaction rate is:

$$r = r_f - r_b = k_fC_A - k_bC_B$$

$$k_f = 0.5\ min^{-1} \qquad k_b = 0.1\ min^{-1}$$

   Find the time required to obtain a conversion of species A equal to 50%, knowing that the inlet concentration of A is $1\ mol/l$, while B is not fed. The density can be considered constant.

5. Find the residence time required to ensure a conversion of species A equal to 95% in a isothermal CSTR, where the following irreversible, 2nd order reaction occurs (ideal gas, isobaric reactor):

$$A \rightarrow 3B$$

$$r = kC_A^2 \qquad k = 0.5\ \frac{l}{mol\ min}$$

   Assume the initial concentration of A is equal to $3\ mol/l$, and no feeding of B. The inlet molar flow of A is equal to $0.2\ mol/s$.

Simulation of a PFR

6. Build up the numerical model of a plug flow reactor, with an internal diameter of $8\ cm$ and a length of $100\ m$. The following reactions occur within the PFR:

$$A \overset{k_1}{\rightarrow} B \overset{k_2}{\rightarrow} C$$

The reactor works at a temperature of $750\ °C$, a pressure of $3\ bar$ and is fed by a molar flow of A ($MW = 25\ kg/kmol$) equal to $20\ kmol/h$. Both the reaction rates are of order 1:

$$\begin{cases} r_1 = k_1 C_A \\ r_2 = k_2 C_B \end{cases} \qquad \begin{cases} k_1 = A_1 e^{-\frac{E_1}{RT}} & A_1 = 1.2 \cdot 10^8\ s^{-1} & E_1 = 37000\ cal/mol \\ k_2 = A_2 e^{-\frac{E_2}{RT}} & A_2 = 4 \cdot 10^8\ s^{-1} & E_2 = 39000\ cal/mol \end{cases}$$

Evaluate the concentration profiles of A, B, and C throughout the reactor. What would be the PFR length that maximizes the production of B?

Design/Simulation of a batch reactor

7. Starting from species A, the species B must be produced in an isothermal batch reactor:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

The kinetic constants k_1 and k_1 are respectively:

$$\begin{cases} k_1 = A_1 e^{-\frac{E_1}{RT}} & A_1 = 1.5 \cdot 10^4\ h^{-1} & E_1 = 9000\ cal/mol \\ k_2 = A_2 e^{-\frac{E_2}{RT}} & A_2 = 6 \cdot 10^6\ h^{-1} & E_2 = 19000\ cal/mol \end{cases}$$

The reactor works at a temperature of $500\ K$ with a liquid mixture. Its volume is $0.5\ m^3$, and at the beginning of each cycle $20\ kmol$ of A are introduced.

Knowing that the total time required for reactor loading, unloading, and cleaning is $1\ h$:

i. Evaluate the reaction time to maximize the yield of B.
ii. Define the optimal conditions to maximize the daily production of B. In detail, evaluate:
   - cycle length (sum of reaction and downtimes)
   - conversion of A per cycle
   - number of cycles per day
   - daily production of B

Design of flow reactors for isomerization

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

$$A \xleftrightarrow{k_f,\ k_b} B$$

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

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

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

Calculate the PFR volume necessary to convert 60% of species A and compare it to the volume of a CSTR working in the same conditions.