

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 $k = 0.01 \text{ s}^{-1}$. 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:

$$A + B \rightarrow C \quad r = kC_A C_B$$
$$k = 0.05 \frac{\text{l}}{\text{mol s}} \quad C_A^{\text{in}} = 3 \frac{\text{mol}}{\text{l}} \quad C_B^{\text{in}} = 4 \frac{\text{mol}}{\text{l}}$$

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:

$$r = r_f - r_b = k_f C_A - k_b C_B$$
$$k_f = 0.5 \text{ min}^{-1} \quad k_b = 0.1 \text{ min}^{-1}$$

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.

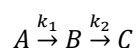
5. Find the residence time required to ensure a conversion of species A equal to 95% in a isothermal CSTR, where the following irreversible, 2nd order reaction occurs (ideal gas, isobaric reactor):

$$A \rightarrow 3B$$
$$r = kC_A^2 \quad k = 0.5 \frac{\text{l}}{\text{mol min}}$$

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:



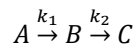
The reactor works at a temperature of 750 °C, a pressure of 3 bar and is fed by a molar flow of A ($MW = 25 \text{ kg/kmol}$) equal to 20 kmol/h. Both the reaction rates are of order 1:

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

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:



The kinetic constants k_1 and k_2 are respectively:

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

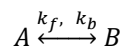
The reactor works at a temperature of 500 K with a liquid mixture. Its volume is 0.5 m³, and at the beginning of each cycle 20 kmol of A are introduced.

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:



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/m³.

The reaction heat, measured at the reference temperature of 300 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 and compare it to the volume of a CSTR working in the same conditions.