

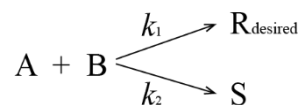
Quiz II

Part I True or False

- F 1. The problem of reactor stability may occur for exothermic reactions in ~~plug flow (or close to plug flow)~~ ^{MFR} reactors.
- F 2. An exothermic ^{放热} reaction may become endothermic ^{吸热} at a different temperature.
- F 3. For reactions in parallel, the concentration level of reactants is the key to proper control of product distribution ^{分配}. A high reactant concentration favors the reaction of lower order, a low concentration favors the reaction of higher order.
- T 4. For irreversible reactions in series the mixing of fluid of different composition is the key to the formation of intermediate ^{中间体的形成}. The maximum possible amount of any and all intermediates is obtained if fluids of different compositions and at different stages of conversion are not allowed to mix.
- T 5. The thermodynamic ^{热力学} equilibrium constant is unaffected by the pressure of the system, by the presence or absence of inerts ^{惰性物质}, or by the kinetics of the reaction, but is affected by the temperature of the system.
- F 6. For an increase in temperature, equilibrium conversion rises for exothermic ^{放热} reactions and drops for endothermic ^{吸热} reactions. } 反了
- F 7. For an increase in pressure in gas reactions, equilibrium conversion rises when the number of moles increases with reaction and drops when the number of moles decreases with reaction.
- T 8. In enzyme fermentation ^{西啤 发西啤}, if a foreign substance and the substance attack the same site on the enzyme and slowdown the enzyme-substrate reaction, then the foreign substance is called competitive inhibitor.

Part II Gap Filling or Multiple Choice

1. Substances A and B in the liquid phase produce R and S by the following mechanism:



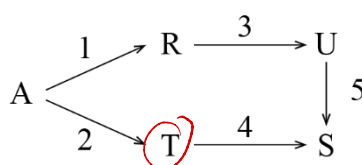
$$r_R = k_1 C_A C_B, r_S = k_2 C_A C_B^{0.5}$$

$$k_1 = k_{10} e^{-\frac{10000}{RT}} \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$$

$$k_2 = k_{20} \mathrm{e}^{-\frac{20000}{RT}} \mathrm{L}^{0.5} \cdot \mathrm{mol}^{-0.5} \cdot \mathrm{s}^{-1}$$

PFR

| | |
|-----|-----|
| 0-1 | 0-9 |
| 0-9 | 0-1 |



$$(E_5 > E_1 > E_2 > E_3 > E_4)$$

$$k_D = \frac{C_A - C_A^*}{C_A} \cdot 0.5$$

$$= \frac{X_A}{(1-X_A)} \cdot 0.5$$
$$= \frac{x_A}{(1-x_A)^{0.5}}$$

Callin

nigh

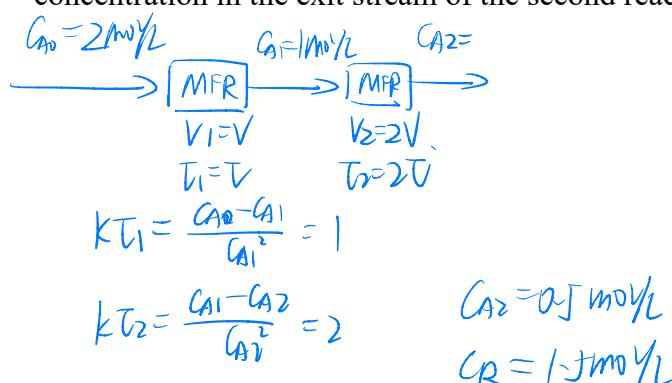
larger

any

PFR

1. Reactant A ($A \rightarrow R$, $-\frac{dC_A}{dt} = kC_A^2$, $C_{A0} = 2\text{mol/liter}$) passes in two mixed flow reactors

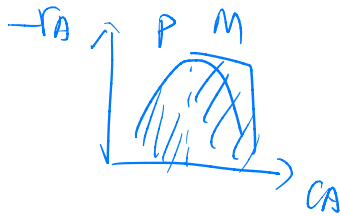
($V_2:V_1=2:1$) in series. If the concentration of A in the first reactor is 1.0 mol/liter, find the



2. Given an autocatalytic reaction with the following rate expression $-r_A = kC_A(C_{A0} - C_A)$,

$$C_{A0} = 2 \text{ mol/L}, k = 1 \text{ L} \cdot \text{mol}^{-1} \cdot \text{min}^{-1}$$

Find the best reactor scheme (without recycle and separation) and the minimum reactor holding time for 90% conversion of pure A.



$$C_{A2} = 0.2$$

~~CMFR~~ to PFR $C_{A1} = 0.1, C_{A0} = 1 \text{ mol/L}$

$$\tau_1 = \frac{C_{A0} - C_{A1}}{k C_{A1} (C_{A0} - C_{A1})} = \frac{2 - 1}{1 \times 1 \times (2 - 1)} = 1 \text{ min}$$

$$\tau_2 = \int_0^{C_{A1}} \frac{dC_A}{k C_A (C_{A0} - C_A)} = \int_0^1 \frac{dC_A}{C_A (2 - C_A)}$$

$$= \int_{0.2}^1 \frac{1}{2} \left(\frac{1}{C_A} - \frac{1}{2 - C_A} \right) dC_A$$

$$= 1.1$$

3. *E.coli* lives and grows on mannitol with the following kinetics

$$r_c = \frac{1.2C_A C_C}{C_A + 2} \quad \phi(C/A) = 0.1$$

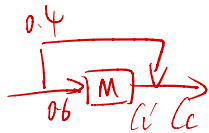
Find the maximum outlet concentration of cells from the reactor when $1 \text{ m}^3 / \text{hr}$ of mannitol solution ($C_{A0} = 6 \text{ gm/m}^3$, $C_{C0} = 0$) is fed directly to a mixed flow reactor of volume 1 m^3 (if necessary, proper bypass may be used).

$$C_m = 2 \quad k = 1.2 \quad v_0 = 1 \text{ m}^3/\text{hr} \quad C_{A0} = 6 \text{ gm/m}^3 \quad C_{C0} = 0 \quad V = 1 \text{ m}^3$$

$$N = \sqrt{1 + \frac{C_{A0}}{C_m}} = \sqrt{1 + \frac{6}{2}} = 2$$

$$k\tau_{\text{opt}} = \frac{N}{N-1} = \frac{2}{2-1} = 2 \quad k = 1.2 \quad \tau_{\text{opt}} = \frac{2}{1.2} \text{ hr}$$

$$v_{\text{opt}} = \frac{V}{\tau_{\text{opt}}} = \frac{1}{\frac{2}{1.2}} = \frac{1.2}{2} \text{ m}^3/\text{hr}$$

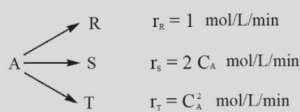


$$C_C' = \frac{\phi(C/A) - C_{A0}N}{N+1} = \frac{0.1 \times 6 \times 2}{3} = 0.4$$

$$C_C = 0.4 \times 0.6 = 0.24$$

1. For reactions in parallel, the concentration level of reactants is the key to proper control of product distribution. A high reactant concentration favors the reaction of (**high**) order, a low concentration favors the reaction of (**low**) order.
2. For irreversible reactions in series the (**mixing**) of fluid of different composition is the key to the formation of intermediate. The maximum possible amount of any and all intermediates is obtained if fluids of different compositions and at different stages of conversion are not allowed to mix.
3. For an increase in pressure in gas reactions, equilibrium conversion rises when the number of moles **decreases** with reaction.

1. Consider the parallel decomposition of A of different orders. S is the desired product and $C_{A0} = 4 \text{ mol/L}$.



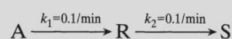
Find the operating condition (x_A , τ and C_S) which maximizes C_S in a mixed flow reactor.

Solution:

$$\phi(S/A) = \frac{2C_A}{C_A^2 + 2C_A + 1} = \frac{2C_A}{(C_A + 1)^2}$$

$$C_S = \phi(S/A) \cdot (C_{A0} - C_A) = \frac{2C_A(4 - C_A)}{(C_A + 1)^2}$$

2. Under appropriate conditions A decomposes as follows



R is to be produced from **1000 L/hr** of feed in which $C_{A0} = 1 \text{ mol/L}$, $C_{R0} = C_{S0} = 0$. What size of mixed flow reactor will maximize the concentration of R, and what is $C_{R\text{max}}$ in the effluent stream from this reactor?

Solution:

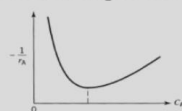
$$\tau_{m,opt} = \frac{1}{\sqrt{k_1 k_2}} = \text{10 min} \quad V_{m,opt} = \tau_{m,opt} \cdot v_0 = 166.67 \text{ L}$$

3. Given an autocatalytic reaction with the following rate expression $-r_A = k C_A (C_{A0} - C_A)$, $C_{A0} = 2 \text{ mol/L}$, $k = 1 \text{ L} \cdot \text{mol}^{-1} \cdot \text{min}^{-1}$

Find the best reactor scheme (without recycle and separation) and the minimum reactor holding time for 90% conversion of pure A.

Solution:

MFR+PFR should be used.



4. In enzyme fermentation, if a foreign substance and the substrate attack the same site on the enzyme and slowdown the enzyme-substrate reaction, then the foreign substance is called (**competitive**) inhibitor.

5. An n th-order reaction takes place in two mixed flow reactors in series, for a given conversion, in order to minimize the size of the two mixed flow reactors, when $0 < n < 1$, (**large**) reactor should come first; when $n > 1$, (**small**) reactor should come first.

6. An enzyme fermentation follows M-M kinetics, $-r_A = k C_A C_{E0} / (C_A + C_M)$. When $C_A \ll C_M$, the better reactor type is (**PFR**) reactor.

$$\frac{dC_S}{dC_A} = \frac{(8 - 4C_A)(C_A + 1) - 4C_A(4 - C_A)}{(C_A + 1)^3} = 0$$

$$C_A = 0.667 \text{ mol/L}$$

$$x_A = 1 - C_A / C_{A0} = 0.833$$

$$C_S = \frac{2C_A(4 - C_A)}{(C_A + 1)^2} = \frac{2 \times 0.667 \times (4 - 0.667)}{(0.667 + 1)^2} = 1.6 \text{ mol/L}$$

$$\tau = \frac{C_{A0} - C_A}{(C_A + 1)^2} = \frac{4 - 0.667}{(0.667 + 1)^2} = 1.2 \text{ min}$$

$$\frac{C_S}{C_A} = \frac{1.6}{0.667} = \frac{8}{3} = \frac{6}{5}$$

$$\tau_{mixed} = \frac{C_{A0} - C_A}{-r_A} \quad (\text{Eq 5.13 on page 95})$$

$$\tau_{mixed} = \frac{2 - 1}{1} = 1 \text{ min}$$

$$\tau_{plug} = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A} \quad (\text{Eq 5.19 on page 102})$$

$$\tau_{plug} = \int_{0.2}^1 \frac{dC_A}{C_A(2 - C_A)} = \frac{1}{2} \ln 9 = 1.1 \text{ min}$$

$$\tau = \tau_{mixed} + \tau_{plug} = 1 + 1.1 = 2.1 \text{ min}$$

4. E. coli lives and grows on mannitol with the following kinetics

$$r_c = \frac{1.2C_A C_C}{C_A + 2}$$

$$\phi(C/A) = 0.1$$

Find the **maximum outlet concentration of cells** from the reactor when 1 m³/hr of mannitol solution ($C_{A0} = 6 \text{ gm/m}^3$, $C_{C0} = 0$) is fed directly to a mixed flow reactor of volume 1.5 m³ (if necessary, proper bypass may be used).

$$\tau_m = \frac{V_m}{v} = \frac{1.5}{1} = 1.5 \text{ hr} \quad k\tau_m = 1.2 \times 1.5 = 1.8 \quad N = \sqrt{1 + \frac{C_{A0}}{C_M}} = \sqrt{1 + \frac{6}{2}} = 2$$

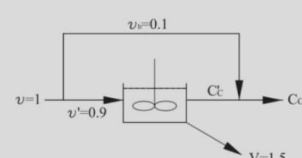
$$k\tau_{washout} = \frac{N^2}{N^2 - 1} = \frac{4}{3} \quad k\tau_{opt} = \frac{N}{(N-1)} = \frac{2}{(2-1)} = 2 \quad k\tau_{opt} > k\tau_m > k\tau_{washout}$$

By-pass is needed to make $k\tau'_m = k\tau_{opt}$

$$\tau'_m = \tau_{opt} = \frac{N}{(N-1)k} = \frac{2}{(2-1) \times 1.2} = \frac{5}{3}$$

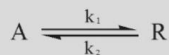
$$v' = v_{opt} = \frac{V}{\tau_{opt}} = \frac{1.5}{5/3} = 0.9$$

$$v_b = v - v' = 1 - 0.9 = 0.1$$

$$C'_C = C_{C,opt} = \frac{\phi(C/A)C_{A0}N}{N+1} = \frac{0.1 \times 6 \times 2}{2+1} = 0.4$$


$C_c = 0.9 \times 0.4 = 0.36$

5. The following reversible first-order liquid reaction



is to be carried out in a plug flow reactor. For operations at 300 K the volume of reactor required is 100 liters for 50% conversion of A when $C_{A0} = 10 \text{ mol/L}$. What should be the volume of the reactor for the same feed rate and conversion but with operations at 350K?

Data:

$$k_1 = 10^3 \exp(-2416 / T) \quad \Delta H_{r,300K} = -8000 \text{ cal/mol}$$

$$\Delta C_P = C_{PR} - C_{PA} = 0 \quad K_{300K} = 10$$

Solution:

(1) at 300K

$$x_{Ae} = \frac{K_{300K}}{K_{300K} + 1} = \frac{10}{10+1} = 0.909$$

$$k_1 \tau = x_{Ae} \ln \left(\frac{x_{Ae}}{x_{Ae} - x_A} \right)$$

$$10^3 \exp(-2416 / 300) \tau = 0.909 \ln \left(\frac{0.909}{0.909 - 0.5} \right)$$

$$\tau_1 = 2.28$$

(2) at 350K

$$\Delta C_P = C_{PR} - C_{PA} = 0, \quad \Delta H_r = \text{constant} = \Delta H_{r,300K} = -8000 \text{ cal/mol}$$

$$\ln \frac{K_2}{K_1} = \frac{-\Delta H_r}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \quad \ln \frac{K_{350K}}{10} = \frac{8000 \times 4.184}{8.314} \left(\frac{1}{350} - \frac{1}{300} \right)$$

$$K_{350K} = 1.47 \quad x_{Ae} = \frac{K_{350K}}{K_{350K} + 1} = \frac{1.47}{1.47 + 1} = 0.595$$

$$10^3 \exp(-2416 / 350) \tau = 0.595 \ln \left(\frac{0.595}{0.595 - 0.5} \right)$$

$$\tau_2 = 1.09$$

$$\frac{v_1}{Q} = \frac{v_2}{Q_2} \quad V_2 = \frac{V_1 \tau_2}{\tau_1} = \frac{100 \times 1.09}{2.28} = 47.8 \text{ L}$$