Quiz Ⅰ

Part Ⅰ True or False

T 1. A batch reactor has neither inflow nor outflow of reactants or products while the reaction is carried out. 正在反应

位置依赖性

T 2. It is usually considered that there is no position dependence of the concentration, the temperature, or the reaction rate inside the mixed flow reactor.

F 3. The flow reactor has the disadvantage of high labor costs and the difficult of large-scale production.

F 4. Ideal reactors include two types, that is plug flow reactors and batch reactors.

F 5. The mixed flow reactor volume is less than the volume of plug flow reactor to achieve the same conversion of a first-order reaction. MFR: $\tau = \frac{C_{A0}-C_A}{-r_A} = \frac{C_{A0}-C_A}{kC_A}$ PFR: $\tau = \int_{C_A}^{C_{A0}} \frac{dC_A}{r_A} = \frac{\ln\frac{C_{A0}}{C_A}}{k}$

T 6. Whether you place two plug-flow reactors in series or have one plug-flow reactor, the total reactor volume required to achieve the same conversion is identical. 同样的

F 7. The space-velocity, s, is obtained by dividing reactor volume by the volumetric flow rate entering the reactor. $\tau = \frac{V}{v_0} = \frac{1}{s}$

T 8. For most liquid-phase reactions, the density change with reaction is usually small and can be neglected.

Part Ⅱ Gap Filling or Multiple Choice

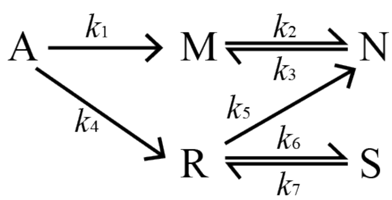
1. A reaction with stoichiometric equation A + 2B → 4R + 2S has the following rate expression

$$-r_A = 2C_A^{0.5}C_B$$

What is the rate expression of the other three reaction components B, R and S for the reacion?

$-r_B =$ $4C_A^{0.5}C_B$; $r_R =$ $8C_A^{0.5}C_B$; $r_S =$ $4C_A^{0.5}C_B$

2. The following isothermal reactions have first-order kinetics in a constant volume batch reactor. Find the rate expression for these reactions in terms of reactant concentrations.



$-\frac{dC_A}{dt} = \underline{k_1C_A + k_4C_A}$; $\frac{dC_M}{dt} = \underline{k_1C_A + k_3C_N - k_2C_M}$; $\frac{dC_N}{dt} = \underline{k_2C_N + k_5C_R - k_3C_N}$;

$\frac{dC_R}{dt} = \underline{k_4C_A + k_7C_S}$ $- k_5C_R - k_6C_R$; $\frac{dC_S}{dt} = \underline{k_6C_R - k_7C_S}$;

3. For a liquid reaction with rate equation $-r_A = kC_A^2$, the conversion of A is 70% when C_{A0} is 1.5 mol / L and reaction time is *t*. Find the time needed to reach the same conversion when C_{A0} equals 3.0 mol / L.

$t = \int_{C_{Af}}^{C_{A0}} \frac{dC_A}{kC_A^2} = \frac{1}{k}\left(\frac{1}{C_{Af}} - \frac{1}{C_{A0}}\right) = \frac{C_{A0}-C_{Af}}{kC_{Af}C_{A0}} = \frac{X_A}{kC_{Af}} \propto \frac{1}{C_{Af}} \propto \frac{1}{C_{A0}}$

$t' = \frac{t}{2}$

(*t*/2, *t*, 2*t*, 4*t*)

4. For a irreversible reaction(A→R) with rate constant $k = 1\,\text{mol}/(\text{L}\cdot\text{s})$, the conversion of A is 90% when C_{A0} is ~~1.5~~ 1.0 mol / L and reaction time is *t*. Find the time needed to reach the same conversion when C_{A0} equals 3.0 mol / L.

$n=0$.

$t' = \int_{C_{Af}}^{C_{A0}} \frac{dC_A}{k} = \frac{C_{A0}-C_{Af}}{k} = \frac{C_{A0}X_A}{k} = 3t$

(*t*/9, *t*/3, *t*, 3*t*)

5. For a liquid reaction with rate equation $-r_A = kC_A$, the half-life $t_{1/2}$ is 5 minutes when C_{A0} is 10 mol / L. Find the half-life $t_{1/2}$ when when C_{A0} is less than 10 mol / L. __=__ 5 minutes

$n=1$

$t = \int_{C_{Af}}^{C_{A0}} \frac{dC_A}{-r_A} = \frac{\ln\frac{C_{A0}}{C_A}}{k}$.

(< , > , = , unsure)

6. A liquid first-order irreversible reaction takes place in a plug flow reactor. The volume of reactor needed for 80% conversion of pure A to product is 1 m^3. Find the volume of reactor for 80% conversion when the reaction takes place in a mixed flow reactor? __>__ 1 m^3

PFR: $k\tau_p = -\ln(1-X_A) = \ln 5$

MFR: $k\tau_m = \frac{X_A}{1-X_A} = 4$

$\tau_m > \tau_p$

(< , > , = , unsure)

7. For an isothermal gas-phase reaction (A→4R), when starting with pure reactant A, ε_A is __3__, when with 50% inerts present at the start, ε_A is __1.5__.

$\varepsilon_A = \frac{2+0.5-1}{1} = 1.5$

$\varepsilon_A = \frac{4-1}{1} = 3$

8. A liquid reaction(A→R) with rate equation $-r_A = kC_A^n$ takes place in a plug flow reactor, if the conversion increases with the increse of C_{A0}, then we could conclude that n__>1__.

(=0, >0, <0, =1, >1, <1)

Part Ⅲ Calculation

1. 1L/min of A (1 mol/L) • B (0.2 mol/L) mixture enters a mixed flow reactor (2 liters) and reacts and the kinetic eauations and stoichiometric equations are unknown. The concentrations of A, B and C in the exit stream are 0.2 mol/L, 0.4 mol/L, 0.8 mol/L reapectively. Find the reaction rate of the three components in the reactor.

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$C_{A0}=1\,mol/L$　$C_{B0}=0.2\,mol/L$　$v_0=1\,L/min$ → $V=2L$ MFR → $C_A=0.2\,mol/L$　$C_B=0.4\,mol/L$　$C_C=0.8\,mol/L$

$4A \rightarrow B+4C$

$\tau=\frac{V}{v_0}=2\,min$

$-r_A=\frac{-\Delta C_A}{\tau}=\frac{0.8}{2}=0.4\,mol/L\cdot min$

$-r_B=0.1\,mol/L\cdot min$

$-r_C=0.4\,mol/L\cdot min$

2. A plug flow reactor (2 m^3) processes an aqueous leed (100 liter/min) containing reactant A ($C_{A0}=100$mmol/liter). The reaction is reversible and represented by

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$$A \leftrightarrow R \qquad -r_A=0.04C_A-0.01C_R \quad \text{(mol/liter/min)}$$

What is the equilibrium conversion and the actual conversion in the reactor?

$K=\frac{k_1}{k_2}=\frac{0.04}{0.01}=4$　$-r_A=0.04C_A-0.01C_R=0$　$C_A=\frac{1}{4}C_R$　$C_A=20\,mmol/L$　$X_{Ae}=0.8$

PFR: $k_1\tau=X_{Ae}\ln\left(\frac{X_{Ae}}{X_{Ae}-X_A}\right)$　$X_A=0.5027$

3. For a gas reaction at 800K in a constant-volume batch reactor the rate is expressed as

$$-\frac{dP_A}{dt}=10P_A^2\text{(atm • h-1)}$$

What is the value of the rate constant k for this reaction if the rate equation is expressed as

$$-r_A=-\frac{1}{V}\frac{dn_A}{dt}=kC_A^2\,(\mathrm{mol\cdot L^{-1}\cdot}h^{-1})$$

Note:1atm = 101325Pa

$-\frac{dP_A}{dt}=10P_A^2\,(atm\cdot h^{-1})$　$k_p=10\,atm^{-1}\cdot h^{-1}$

$PV=nRT$

$R=\frac{PV}{nT}$

$-\frac{dP_A}{dt}=-\frac{d(C_ART)}{dt}=366[C_ART]^2$

$-\frac{dC_A}{dt}=10(atm^{-1}h^{-1})RT\,C_A^2\ (mol\cdot L^{-1}h^{-1})$

$k'=10\frac{1}{atm\cdot h}\cdot\frac{1atm\cdot 22.4L}{1mol\cdot 273K}\cdot 800K$

$=656\ L/mol\cdot h$

1. 1 L/min of A (1mol/L)-B (0.2mol/L) mixture enters a mixed flow reactor (2 liters) and reacts and the kinetic equations and stoichiometric equations are unknown. The concentrations of A, B and C in the exit stream are 0.2 mol/L, 0.4 mol/L, 0.8 mol/L respectively. Find the rate of three components.

Solution:

$$\frac{V}{F_{A0}} = \frac{\Delta x_A}{-r_A} \qquad \frac{V}{v_0} = \frac{C_{A0}-C_A}{-r_A}$$

$$-r_A = \frac{C_{A0}-C_A}{V/v_0} = \frac{C_{A0}-C_A}{2} = \frac{1-0.2}{2} = 0.4 mol/L\cdot\min$$

$$-r_B = \frac{C_{B0}-C_B}{V/v_0} = \frac{C_{B0}-C_B}{2} = \frac{0.2-0.4}{2} = -0.1 \qquad r_B = 0.1 mol/L\cdot\min$$

$$-r_C = \frac{C_{C0}-C_C}{V/v_0} = \frac{C_{C0}-C_C}{2} = \frac{0-0.8}{2} = -0.4$$

2. In a homogeneous isothermal liquid polymerization, 20% of the monomer disappears in 34 minutes for initial monomer concentration of 0.04 mol/liter and also for 0.8 mol/liter. What rate equation represents the disappearance of the monomer?

Solution:

Since the conversion is independent of initial concentration, it is a first-order reaction

聚合反应 ⇒ batch

$$kt = \ln\frac{1}{1-x_A} \qquad k\times 34 = \ln\frac{1}{1-0.2}$$

$$k = 6.56\times10^{-3}\ \min^{-1}$$

$-r_A = kC_A = 6.56\times10^{-3} C_A$ mol/L·min

3. A plug flow reactor (2 m³) processes an aqueous feed (100 liter/min) containing reactant A (C_{A0} = 100 mmol/liter). The reaction is reversible and represented by

$$A \longleftrightarrow R \qquad -r_A = 0.04C_A - 0.01C_R$$

What is the equilibrium conversion and the actual conversion in the reactor?

$$-r_A = 0.04C_{Ae} - 0.01C_{Re} = 0$$

$$C_{Ae} = C_{A0}(1-x_{Ae}) \qquad C_{Re} = C_{A0}x_{Ae}$$

$$0.04C_{A0}(1-x_{Ae}) - 0.01C_{A0}x_{Ae} = 0 \qquad x_{Ae} = 0.8$$

Table 5.1 (page 111) or Eq.3.54

$$k_1\tau = \left(1-\frac{C_{Ae}}{C_{A0}}\right)\ln\left(\frac{C_{A0}-C_{Ae}}{C_A-C_{Ae}}\right) = x_{Ae}\ln\left(\frac{x_{Ae}}{x_{Ae}-x_A}\right)$$

$$0.04*\frac{2000}{100} = 0.8*\ln\left(\frac{0.8}{0.8-x_A}\right)$$

$X_{Ae} = 0.5057$

4. A stream of pure gaseous reactant A (C_{A0} = 660 mmol/liter) enters a plug flow reactor at a flow rate of F_{A0} = 540 mmol/min and polymerizes there as follows

$$3A \to R, \qquad -r_A = 54\ \frac{\text{mmol}}{\text{liter}\cdot\text{min}}$$

How large a reactor is needed to lower the cocentration of A in the exit stream to C_{Af} = 330 mmol/liter?

According to Eq.5.20 on page 103

$$k\tau = \frac{kC_{A0}V}{F_{A0}} = C_{A0}x_A \qquad x_A \neq 1-\frac{C_A}{C_{A0}}$$

$$x_A = \frac{C_{A0}-C_A}{C_{A0}+\varepsilon_A C_A} \qquad (Eq.4.5 \text{ on page } 87)$$

$$\varepsilon_A = \frac{1/3-1}{1} = -2/3$$

$$\tau = \frac{C_{A0}X_A}{k}$$

$$x_A = \frac{660-330}{660+(-\frac{2}{3})\times330} = 0.75$$

$$V = v_0\tau = \frac{v_0 C_{A0} X_A}{k} = \frac{F_{A0}X_A}{k} = \frac{540\times0.75}{54} = 7.5L$$

5. At present conversion is 2/3 for our elementary liquid reaction 2A→2R when operating in an isothermal plug flow reactor with a recycle ratio of 1. What will be the conversion if the recycle stream is shut off?

Solution:

It's a second-order reaction

$$\frac{k\tau C_{A0}}{R+1} = \frac{C_{A0}(C_{A0}-C_{Af})}{C_{Af}(C_{A0}+RC_{Af})}$$

$$\frac{k\tau C_{A0}}{1+1} = \frac{C_{A0}(C_{A0}-\frac{1}{3}C_{A0})}{\frac{1}{3}C_{A0}(C_{A0}+\frac{1}{3}C_{Af})} = \frac{\frac{2}{3}}{\frac{4}{9}} = \frac{3}{2}$$

$$k\tau C_{A0} = \frac{X_A}{1-X_A} = 3 \qquad X_A = \frac{3}{4}$$

5. At present conversion is 2/3 for our elementary liquid reaction 2A→2R when operating in an isothermal plug flow reactor with a recycle ratio of 1. What will be the conversion if the recycle stream is shut off?

Solution:

It's a second-order reaction

$$\frac{k\tau C_{A0}}{R+1} = \frac{C_{A0}(C_{A0}-C_{Af})}{C_{Af}(C_{A0}+RC_{Af})} \qquad \frac{k\tau C_{A0}}{1+1} = \frac{C_{A0}(C_{A0}-\frac{1}{3}C_{A0})}{\frac{1}{3}C_{A0}(C_{A0}+\frac{1}{3}C_{A0})} = 1.5$$

$$k\tau C_{A0} = 3 \qquad k\tau C_{A0} = \frac{x_A}{1-x_A} = 3$$

6. For a gas reaction at 800K in a constant-volume batch reactor the rate is expressed as

$$-\frac{dP_A}{dt} = 10P_A^{\ 2}(atm \cdot h^{-1})$$

What is the value of the rate constant k for this reaction if the rate equation is expressed as

$$-r_A = -\frac{1}{V}\frac{dn_A}{dt} = kC_A^{\ 2}(mol \cdot L^{-1} \cdot h^{-1})$$

Solution:

$$P_A = \frac{n_A RT}{V} = C_A RT \qquad -\frac{dP_A}{dt} = -RT\frac{dn_A}{Vdt} = 10(\frac{n_A RT}{V})^2 = 10(C_A RT)^2$$

$$-\frac{dn_A}{Vdt} = 10RTC_A^{\ 2}$$

Attention:

$$-\frac{dp_A}{dt} = 10p_A^{\ 2} \quad atm/hr = 10p_A^{\ 2}\frac{101325p_a}{3600s}$$

$$-r_A = 10p_A^{\ 2} = kC_A^2 = k(\frac{p_A}{RT})^2 \Rightarrow k = 10R^2T^2$$

$$-r_A = -\frac{1}{V}\frac{dN_A}{dt} = -\frac{1}{V}\frac{d\left(\frac{p_A V}{RT}\right)}{dt} = -\frac{1}{RT}\frac{dp_A}{dt} = \frac{1}{RT}10p_A^2 = kC_A^{\ 2} \Rightarrow k = 10/RT$$

6. For a gas reaction at 800K in a constant-volume batch reactor the rate is expressed as

$$-\frac{dP_A}{dt} = 10P_A^{\ 2}(atm \cdot h^{-1})$$

What is the value of the rate constant k for this reaction if the rate equation is expressed as

$$-r_A = -\frac{1}{V}\frac{dn_A}{dt} = kC_A^{\ 2}(mol \cdot L^{-1} \cdot h^{-1})$$

Solution:

$$P_A = \frac{n_A RT}{V} = C_A RT \qquad -\frac{dP_A}{dt} = -RT\frac{dn_A}{Vdt} = 10(\frac{n_A RT}{V})^2 = 10(C_A RT)^2$$

$$-\frac{dn_A}{Vdt} = 10RTC_A^{\ 2}$$

$$k = 10RT = 10(\frac{1}{atm \cdot h}) \times 0.08206(\frac{atm \cdot L}{mol \cdot K}) \times 800(K) = 656(\frac{L}{mol \cdot h})$$