# 元智大學 九十七 學年度研究所 **碩士班** 招生試題卷

系(所)別：化學工程與材料科學學系碩士班　組別：不分組　科目：化工動力學　用紙第 / 頁共 / 頁

●可以使用電子計算機

1. The reversible gas-phase decomposition of nitrogen tetroxide $N_2O_4$ to nitrogen dioxide $NO_2$ : $N_2O_4 \rightleftarrows 2NO_2$ is carried out at constant temperature. The feed consists of pure $N_2O_4$ at 340 K and 202.6 kPa (2 atm). The concentration equilibrium constant $K_c$ at 340 K is 0.1mol/dm$^3$. (40%)

(i) calculate the equilibrium conversion of $N_2O_4$ in a constant volume batch reactor. (10%)

(ii) Calculate the equilibrium conversion of $N_2O_4$ in a flow reactor. (10%)

(iii) Assuming the reaction is elementary, express the rate of reaction solely as a function of conversion for a flow system (the rate constant is $k_A$). (10%)

(iv) Determine the CSTR volume necessary to achieve 80% of the equilibrium conversion. (10%

2. The elementary gas-phase reaction $(CH_3)_3COOC(CH_3)_3 \rightarrow C_2H_6 + 2CH_3COCH_3$ is carried out isothermally in a flow reactor with no pressure drop. The specific reaction rate at 50°C is $10^{-4}$ min$^{-1}$ and the activation energy is 85 kJ/mol. Pure di-tert-butyl peroxide enters the reactor at 10 atm and 127°C and a molar flow rate of 2.5 mol/min.

(i) Calculate the reactor volume to achieve 90% conversion in a plug flow reactor (use 4 intervals Trapezoidal or Simpson rule for the integration if it is necessary). (20%)

(ii) Calculate the reactor volume to achieve 90% conversion in a CSTR. (20%).

3. Normal butane is to be isomerized to isobutane in a CSTR reactor: n-$C_4H_{10} \rightleftarrows$ i- $C_4H_{10}$. The reaction is to be carried out adiabatically in the liquid phase under constant pressure. The specific reaction rate is 30 h$^{-1}$ at 360K. The inlet includes 90 mol % of normal butane and 10 mol % isopentane, where isopentane is just an inert which do not participate chemical reaction. Calculate the volume necessary to achieve 40% conversion. (20%)

Additional information:

$\triangle H_{Rx}$(heat of reaction)= -6900 J/(mol butane), activation energy=65kJ/mol, $K_c$ (equilibrium constant)= 3.0 at 60°C, $C_{A0}$(inlet reactant concentration)=10 kmol/dm$^3$. Heat capacity of normal butane or isobutane = 140 J/(mol K), heat capacity of isopentane=160 J/(mol K). $F_{T0}$(inlet total molar flow rate)=160 kmol/h. $T_0$ (inlet temperature)=330K.

*Ideal Gas Constant*

$$R = \frac{0.73\ \text{ft}^3 \cdot \text{atm}}{\text{lb mol} \cdot {}^\circ\text{R}} \qquad R = \frac{1.987\ \text{Btu}}{\text{lb-mol} \cdot {}^\circ\text{R}}$$

$$R = \frac{8.314\ \text{kPa} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}} \qquad R = \frac{8.3144\ \text{J}}{\text{mol} \cdot \text{K}}$$

$$R = 0.082\ \frac{\text{dm}^3 \cdot \text{atm}}{\text{mol} \cdot \text{K}} = \frac{0.082\ \text{m}^3 \cdot \text{atm}}{\text{kmol} \cdot \text{K}} \qquad R = \frac{1.987\text{cal}}{\text{mol} \cdot \text{K}}$$

*Pressure*

| | |
|---|---|
| 1 torr (1 mmHg) | = 0.13333 kPa |
| 1 in. $H_2O$ | = 0.24886 kPa |
| 1 in. Hg | = 3.3843 kPa |
| 1 atm | = 101.33 kPa |
| 1 psi | = 6.8943 kPa |
| 1 megadyne/cm$^2$ | = 100 kPa |

*Temperature*

| | |
|---|---|
| °F | = 1.8 × °C + 32 |
| R | = °F + 459.69 |
| K | = °C + 273.16 |
| °R | = 1.8 × K |
| °Réamur | = 1.25 × °C |

*Length*

| | |
|---|---|
| 1 Å | = $10^{-8}$ cm |
| 1 dm | = 10 cm |
| 1 μm | = $10^{-4}$ cm |
| 1 in. | = 2.54 cm |
| 1 ft | = 30.48 cm |
| 1 m | = 100 cm |

*Energy (Work)*

| | |
|---|---|
| 1 kg·m$^2$/s$^2$ | = 1 J |
| 1 Btu | = 1055.06 J |
| 1 cal | = 4.1868 J |
| 1 L·atm | = 101.34 J |
| 1 hp·h | = 2.6806 × $10^6$ J |
| 1 kWh | = 3.6 × $10^6$ J |

(命題請用黑色鋼筆、原子筆繕寫或電腦打字；試題字體務求清晰，並一律以正面單頁書寫，背面請勿書寫。)