國立成功大學
112學年度碩士班招生考試試題

編　號：76

系　所：化學工程學系

科　目：化學反應工程

日　期：0206

節　次：第 3 節

備　註：可使用計算機

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※ 考生請注意：本試題可使用計算機。 請於答案卷(卡)作答，於本試題紙上作答者，不予計分。

1. The conversion of buckeyelene (B) to wulfrene (W) and carbon dioxide,

$$2B \rightarrow W + CO_2$$

follows an elementary rate law over fresh catalyst. This gas-phase reaction is carried out in a 1-dm^3 batch reactor filled with 1 kg of fresh catalyst. The catalyst follows a zero-order decay law with a decay constant k_d equal to 0.05 min^{-1}. If the reaction rate constant is 0.01 dm^6/(kg cat·mol·min) and 10 mol of B is introduced into the batch reactor, what is the conversion after 40 min? **(15%)**

2. On the basis of following simplified mechanisms with chlorofluorocarbons (CFCs) and their derivative chlorine radicals (R ∗), please derive the rate law for:
   a、 the decomposition of ozone. **(5%)**
   b、 the generation of molecular oxygen **(5%)**

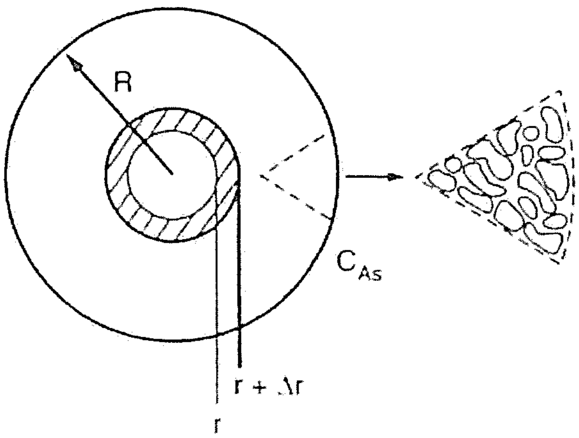
$$\text{CFCs} \xrightarrow{hv,\ k_I} \text{R}*$$

$$\text{O}_3 + \text{R}* \xrightarrow{k_1} \text{O}_2 + O + \text{R}*$$

$$\text{O}_3 + \text{O} \xrightarrow{k_2} 2\,\text{O}_2$$

$$\text{R}* + \text{R}* \xrightarrow{k_D} \text{CFCs (inactive)}$$

3. Please define the Thiele modulus (ϕ_n^2) and derive the Thiele modulus from the diffusion and reaction of reactant A in the pellet. **(15%)**



B.C.1	C_A is finite	at r = 0
B.C.2	$C_A = C_{As}$	at r = R

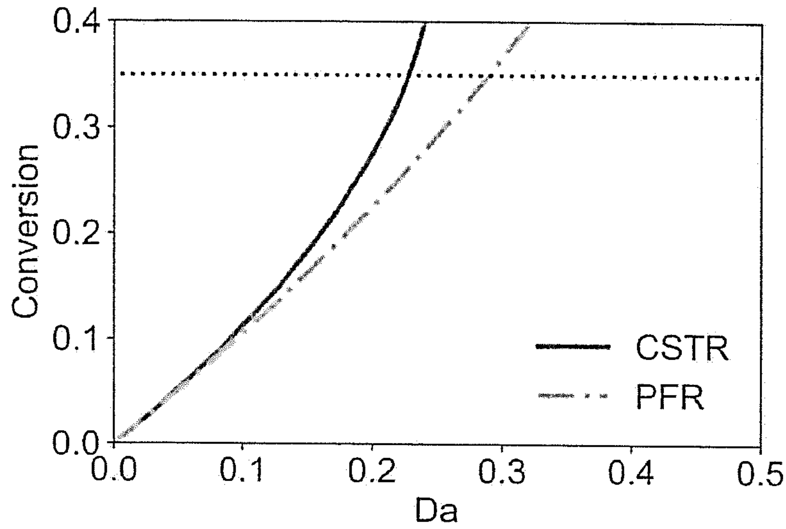
B.C.: boundary condition

Figure. Shell balance on a catalyst pellet.

4. Below is a plot of the Conversion vs. Damköhler number (Da) for a liquid-phase reaction $A \rightarrow B$. However, the reaction rate expression and the reaction order are unknown. Upon checking the figure, it looks like the Plug Flow Reactor (PFR) has a larger Da than the Continuous Stirred-Tank Reactor (CSTR) at the same conversion (0.35). You can assume it is under isothermal conditions, and the feed concentration is the same for the two reactors.

　a、 Could you propose a possible **rate expression** and explain why it has such a difference? **(10%)**

　b、 Could you draw a **Levenspiel plot** based on the rate expression that you proposed? **(10%)**



5. For multiple reactions of C ← A ⇄ B in a mixed flow fluidized bed reactor filled with 100 kg of solid catalyst and with a heating jacket (heat transfer constant: UA = 1600 J/min-K, heating temperature: T_a = 500 K), please respond the following question:

　a、 What are the final outlet concentrations of A, B, and C in a sequence arranged from largest to smallest? **(10%)**

　b、 To promote the final outlet concentration of B, it is suggested to increase or decrease the temperature of reactor? **(5%)**

Additional information about this non-isothermal reaction are provided:

Inlet concentration: $C_{T0} = 2$ mol/dm^3, where $C_{A0} = C_{B0} = 1$ mol/dm^3

Molar flow rate: $F_{T0} = 2$ mol/min

Heat capacity: $C_{pA} = C_{pB} = C_{pC} = 100$ J/mol-K

Rate constant: $k_{A\rightarrow B} = k_1 = 0.5\exp(2 - 640/T)$ dm^3/kg of cat.-min

$k_{A\rightarrow C} = k_3 = 0.005\exp[4.6(1 - 460/T)]$ dm^3/kg of cat.-min

Equilibrium constant: $K_c = k_{A\rightarrow B} / k_{B\rightarrow A} = k_1 / k_2 = 10\exp[4.8(430/T - 1.5)]$

Reaction heat: $\Delta H_{R1} = -1800$ J/mol of A, $\Delta H_{R3} = -1100$ J/mol of A

Inlet: $T_0 = 330$ K, outlet: $T_f = 400$ K

6. For a gas-phase complex reaction occurs in an isothermal PFR:

   $2A + 3B \rightarrow 3C + 2D$　　$r_{1D} = k_{1D}C_A^3C_B$

   $5A + C \rightarrow 2F + E$　　$r_{2C} = -k_{2C}C_AC_C^2$

   $2E + 7B \rightarrow 3F + C$　　$r_{3F} = k_{3F}C_E^4C_B^2$

   In such gas-phase conditions, it is essential to know how the concentration of species changes with residence time or reactor volume. Assume all the gaseous species are ideal gases and the inlet stream includes 100 moles of A and 60 moles of B per second. As the number of molecules changes when reactions occur, will the **total concentration** and **pressure** change? If yes, please calculate them when the conversion of A is 0.3. If no, please state your reasons. Answers without reason receive no credits. **(15%)**

7. For a gaseous, reversible, and exothermic reaction of $A_{(g)} \rightleftarrows B_{(g)} + C_{(g)}$ with an equilibrium constant K_c, what is the relationship between the equilibrium concentration (C_{Ae}) and the final outlet temperature (T_f) in an adiabatic flow reactor? Please describe C_{Ae} in terms of K_c, T_f, inlet temperature (T_0), reaction heat ($\Delta H_R(T_R)$) at a reference temperature T_R, and the respective heat capacity: C_{pA}, C_{pB}, and C_{pC}. Assume that all of the heat capacities are independent from temperature spanning the range of T_R, T_0, and T_f. **(10%)**