## 國立成功大學 111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: 0219

節 次:第3節

備 註:可使用計算機

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第1頁,共3頁

※ 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。

## Q1. Answer the following questions (10%):

- (a) What is the physical interpretation of Michaelis-Menten constant in enzyme kinetics?
- (b) Explain why multiple steady states is observed only in a non-isothermal CSTR and is not in a non-isothermal PFR?
- (c) What are the three scenarios occurring in un-steady state operations?
- (d) Explain how the Advanced Reaction System Screening Tool (ARSST) works and what kinetic parameters can be estimated by using this system.
- Q2. A 1<sup>st</sup> order, liquid-phase, exothermic reaction (A  $\longleftrightarrow$  B) is running in a batch reactor. The reactor is well-insulated with no heat loss. To control the temperature, an inert liquid C is added to the reaction. The flow rate of C is adjusted to keep a constant reaction temperature at 150 °F. What is the flow rate of C after 1 h? (25%)

## Additional information

 $T_{C0} = 100 \text{ °F}$  $V_0 = 50 \text{ ft}^3$ 

△H°<sub>RX</sub>=-25000 Btu/lb mol

K forward (150 °F) =  $1.2 \times 10^{-4} \text{ s}^{-1}$ K backward (150 °F) =  $1.5 \times 10^{-4} \text{ s}^{-1}$ Cp, (all components) = 0.5 Btu/lb mol °FCA0 = 1 lb mol/ft<sup>3</sup> 編號: 76

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Q3. For an irreversible reaction carried out in a flow reaction system,  $A \to B$  the relationship between  $\frac{F_{A0}}{-r_A}$  and the conversion X is plotted as below (a Levenspiel plot),

where F<sub>AO</sub> and r<sub>A</sub> are the initial molar flow rate and the reaction rate for the reactant A, respectively. As a chemical engineer, you are asked to produce product B as much as possible. So, finding the most efficient reactors based on the Levenspiel plot is critical. Could you propose a combination of different types of reactors to achieve 80% conversion with the smallest reactor volume in total? Here are the options you can choose: single PFR, single CSTR, multiple PFR in parallel, multiple PFR in series, multiple CSTR in parallel. For reactors in parallel, you can assume the stream is distributed evenly to the parallel reactors. You are free to combine two or more options above

considering the change of  $\frac{F_{A0}}{-r_A}$  at different X. Please state the reasons for your choices.

Answers without justification/reasoning receive no credit. (10%)

Q4. For a gas-phase complex reaction that occurred in a PFR (isothermal and isobaric):

 $7A + 3B \rightarrow 5C + 2D$   $r_{1C} = k_{1C}C_A{}^3C_B{}^2$   $3A + C \rightarrow 4E$   $r_{2E} = k_{2E}C_AC_C{}^2$  $E + 2B + 4D \rightarrow 6F$   $r_{3D} = -k_{3D}C_E{}^2C_BC_D{}^3$ 

The molar flow rates (F) for each reactant and product at different volumes (V) of PFR can be resolved with the above mechanisms and the rate expressions. Ordinary differential equations (ODE) solvers, such as Python, MATLAB, C+, and Polymath, are powerful techniques to resolve kinetic-related problems numerically. A chemical engineer should be familiar with inputting the correct equations/physics to the ODE solvers in order to obtain reasonable results. Please derive and list ALL the necessary differential equations and conditions for the ODE solvers that can be used to resolve the F<sub>i</sub> vs. V (*i* refers to the different reactant/products). Note: you do not have to solve the ODEs by yourself, but your ODE solver will not work if you miss any of the necessary equations. (10%)

Q5. In order to obtain the activation energy of a gas-phase elementary reaction,

$$A \rightarrow 2B + C$$

your RD team conducted two experiments for you:

 Pure A was fed to a 35 L PFR at 290 K with a volumetric flow rate of 5 L/s and the conversion was 80%. 國立成功大學 111 學年度碩士班招生考試試題

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第3頁,共3頁

2. A mixture of 25% A and 75% inert (I) was fed to a 30 L CSTR at 320 K with a volumetric flow rate of 6 L/s and the conversion was 80% as well.

Please calculate the activation energy (J/mol) for the reaction. You can assume the conditions are isothermal and isobaric in each experiment. (15%)

Q6. An enzyme is a high-molecular-weight protein that acts on a substrate (reactant) to transform it chemically at a greatly accelerated rate, usually 10³ to 10¹7 times faster than the uncatalyzed rate. Enzymes provide the alternative pathway for the reaction to occur, thereby requiring a lower activation energy. Moreover, the temperature, pH and substrate concentration affect the kinetic reaction of enzyme. When the analogue of substrate, which called "inhibitor" exists in the reaction, enzyme will be inhibited. There are 3 most common types of reversible inhibition occurring in enzymatic reaction. What are the pathways and rate laws (or equations) for each one by following the Michaelis-Menten equation? (15%)

Q7. The elementary consecutive gas-phase reaction working in a CSTR follows the equation:

$$K_1$$
  $K_2$   $A \longrightarrow B \longrightarrow C$ 

The feed conditions and desired product specifications are known, together with the temperature of the heating medium. The ratio  $C_B/C_C$  in the product is equal to 10% and 50% of A in the feed is converted. The feed is gas-phase and pure A with a molar flow rate of 0.05 lb-mol/s and a volumetric flow rate of 7.85 ft<sup>3</sup>/s. The entering temperature is 400°F at 4 atm in the reactor. The heating medium is saturated high-pressure steam at 350°F and the overall heat-transfer coefficient between the heating medium and the reaction mixture is 400 Btu/(h • ft<sup>2</sup> • °F).

Additional information included:

Rate = Arrhenius constant  $(A_1 \text{ or } A_2) * \exp(-Ea/RT)$ 

Heat capacities: C<sub>PA</sub> =C<sub>PB</sub> =C<sub>PC</sub> = 25 Btu/lb-mol • °F; Gas constant R = 1.986 Btu/lb-mol • °R

Reaction 1:  $A_1 = 2 \times 10^9 \,\text{S}^{-1}$ ;  $E_1 = 31,000 \,\text{Btu/lb-mol}$ ;  $\triangle H_{\text{rxn1}} = 15,000 \,\text{Btu/lb-mol}$  for A

Reaction 2:  $A_2 = 1 \text{ X } 10^{11} \text{ S}^{-1}$ ;  $E_2 = 40,000 \text{ Btu/lb-mol}$ ;  $\triangle H_{rxn2} = 20,000 \text{ Btu/lb-mol}$  for C

Temperature: °R = °F + 460

Calculate:

- (a) The desired operating temperature inside the reactor (5%)
- (b) The volume of the reactor (5%)
- (c) The area of the heating coil (5%)