國立成功大學
114學年度碩士班招生考試試題

編　號：58

系　所：化學工程學系

科　目：化學反應工程

日　期：0210

節　次：第 3 節

注　意：1.可使用計算機
2.請於答案卷(卡)作答，於試題上作答，不予計分。

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1. (簡答題) A zero-order homogeneous gas reaction, $A \rightarrow 5\ R$, takes place isothermally in a constant volume bomb reactor at 27 °C. The reactor initially contains 80 mol% of A and 20 mol% of inert, and the reactor pressure is increased from 1 to 1.8 atm in 2 min of reaction. Assuming the ideal gas law is followed.

   a、 Find the value of the reaction rate constant, k, in units of gmol/(L·min) **(10%)**

   b、 After reaction for 5 min, what is the total pressure in the reactor, and what is the partial pressure of A? **(7%)**

   [Note: gas constant $\boldsymbol{R} = 0.082$ (atm·L)/(gmol·K)]

2. (簡答題) The hydrolysis of acetic anhydride is a 1st order reaction with respect to acetic anhydride:

   i.e., $-r_A = 0.158\ C_A$, (gmol)/(cm^3·min) at 25 °C, C_A in gmol/cm^3.

   The hydrolysis takes place in five CSTRs operated in series at 25 °C, with each CSTR having a volume of 1800 cm^3. The feed rate to the first reactor was 582 cm^3/min.

   a、 Calculate the conversion of hydrolysis accomplished in the 5 reactors. **(10%)**

   b、 To reach a conversion identical to that in (a) using a single CRTR, what is the volume needed for the single reactor operated at the same temperature and feed rate? **(6%)**

3. (簡答題) The following mechanism has been proposed for the thermal decomposition of AB:

$$AB \overset{k_1}{\rightarrow} A^* + B^*$$
$$A^* + AB \overset{k_2}{\rightarrow} X + AB^*$$
$$AB^* \overset{k_3}{\rightarrow} Y + A^*$$
$$A^* + A^* \overset{k_4}{\rightarrow} Z$$

   Note that $k_4 >> k_2$ and k_4, $k_3 >> k_1$. A*, B*, and AB* are reactive fragments; X, Y, and Z are stable compounds.

   a、 Derive an expression of the concentration of Z along the reaction time based on the pseudo-steady state treatment. Given that the initial concentration of AB is $C_{AB,0}$. **(10%)**

   b、 If Z is the desired product of this reaction. Derive the selectivity of Z to Y. **(5%)**

   c、 To maximize the yield of Z in an isothermal and continuous process, is a CSTR or PFR more recommended? A suitable reason should be provided to support your answer to get full credit for this question. **(5%)**

4. (簡答題) A vigorously mixed slurry tank conducts a catalytic reaction of $A \rightarrow B$. The system is in the internal diffusion control with the effectiveness factor: $\varepsilon = \frac{6}{d_p}\sqrt{\frac{2D_e}{(n+1)\,k\,C_A^{n-1}}}$ where d_p is the diameter of the spherical catalyst (4 mm), D_e is the effective diffusivity inside the porous catalyst (3×10^{-8} m^2 s^{-1}), n is the reaction order (a 2nd order irreversible reaction of A), k is the heterogeneous reaction rate constant, and C_A is the concentration of A. The feed of this continuous reactor is 1 mol m^{-3} of A at a molar rate of 10 mol s^{-1}. The information about the catalyst: the catalyst density is 4 kg m^{-3}, and the rate constant based on the catalyst weight is 10 m^6 mol^{-1} kg^{-1} s^{-1}.

   a、 Find the total catalyst required in the tank to achieve a conversion of 50%. **(8%)**

   b、 If the mass transport inside the catalyst is improved and the reaction is conducted under reaction control, what will be the total catalyst required in the tank to achieve a conversion of 50%? **(6%)**

5. (選擇題) In non-isothermal reactors, it is crucial to distinguish between the heat generated by the reactions, denoted *G(T)*, and the heat removed from the system, denoted *R(T)*. Where these two curves intersect, we find steady states (S.S.). However, not all of these S.S. are necessarily stable operating points.

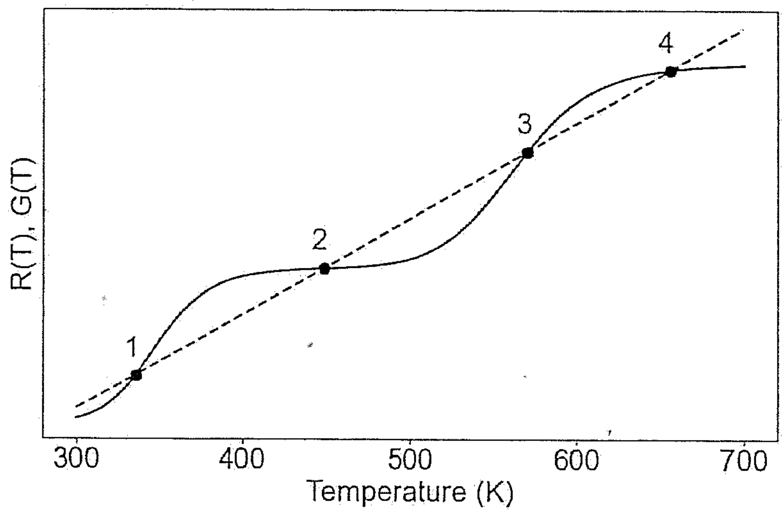
a、The figure below shows the plots of *G(T)* and *R(T)* versus temperature for a system with four observed S.S., labeled 1, 2, 3, and 4. Now consider small variations in temperature around each of the four S.S., what happens? Which of these four steady states are stable, and which are unstable? Select all correct statements from the options below. Note that the correct answer may include multiple choices, and only those who select the fully correct set will receive the points. You can assume constant flow rate and feed temperature, negligible changes in physical properties with temperature, and fixed cooling conditions. **(6%)**

(A) Upper point 4 is stable. (B) Upper point 4 is unstable. (C) Not enough information for upper point 4.

(D) Middle point 3 is stable. (E) Middle point 3 is unstable. (F) Not enough information for middle point 3.

(G) Middle point 2 is stable. (H) Middle point 2 is unstable. (I) Not enough information for middle point 2.

(J) Lower point 1 is stable. (K) Lower point 1 is unstable. (L) Not enough information for lower point 1.



b、Multiple S.S. can sometimes lead to problems due to unstable S.S., which may cause thermal runaway or make it difficult to maintain a stable temperature. Consider endothermic and irreversible reactions in a CSTR, where initially there is only one S.S. Under the following conditions, which changes might lead to the formation of multiple S.S.? Select all possible options. Points will only be awarded for selecting the fully correct set of answers. You can assume the reactor includes adequate external heating/cooling and the overall heat-transfer capacity is sufficiently large. **(7%)**

(A) Increase the heat-transfer coefficient *U* of the cooling system. (B) Raise the coolant temperature T_a.

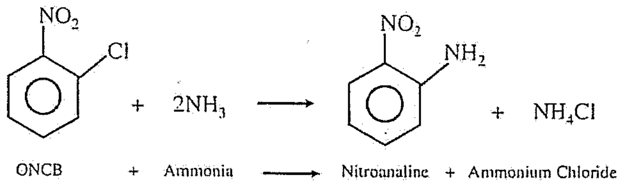
(C) Lower the inlet temperature T_{in}. (D) Increase the feed concentration C_{A0}. (E) Decrease the residence time τ

(F) Increase the activation energy E_a. (G) Increase the coolant flow rate. (H) Increase the feed flow rate.

(I) None of the above will result in multiple S.S.

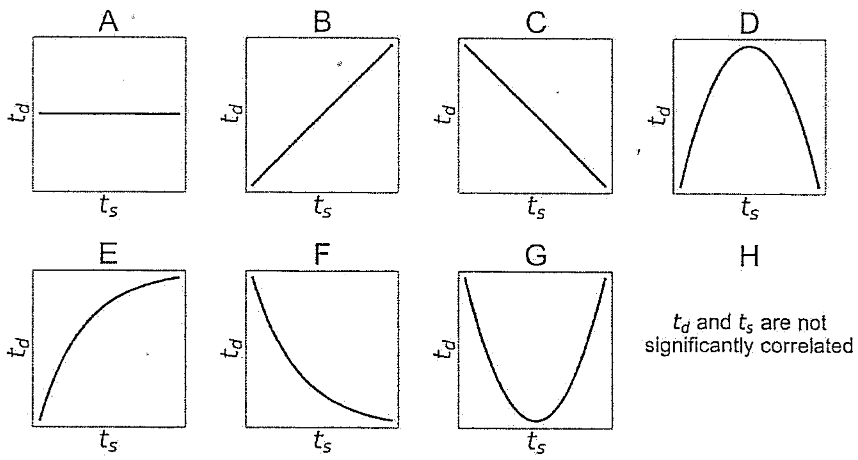
c、Building on question b, now consider an exothermic and reversible reaction in a CSTR. Which of the conditions might lead to the formation of multiple S.S.? The options remain the same as in question b. **(7%)**

6. (選擇題) At 12:18 AM on August 8, 1969, a serious accident occurred at a Monsanto plant in Sauget, Illinois, involving a batch reactor used to produce nitroaniline from ammonia and o-nitrochlorobenzene (ONCB). The reaction rate depended solely on the concentration of ONCB. Normally, the process was conducted isothermally at 175°C, with temperature controlled by coolant water at 25°C. On the day of the incident, the reactor was charged with 9.044 kmol of ONCB, 33.0 kmol of ammonia, and 103.7 kmol of water—nearly triple the usual 3.17 kmol of ONCB. During the reaction, the cooling system failed for 10 minutes, 45 minutes after the isothermal process began. Such a brief interruption had not previously caused issues under standard conditions. However, this time, 88 minutes after cooling was restored, a massive explosion occurred, strong enough to wake people 10 miles away.



This combination of increased reactant charge and cooling interruption pushed the reactor into a state of thermal runaway, a dangerous escalation in temperature caused by the exothermic nature of the reaction outpacing heat removal. Once the reaction exceeded a critical threshold, or point of no return, the temperature and pressure rose uncontrollably. The inability to halt the rapid escalation ultimately led to an explosion.

a、Which of the following figures or statements illustrates the relationship between the downtime of the cooling system (t_d) and the time from startup to failure of cooling (t_s), for which the reactor would not explode? Please select all applicable options from choices A to H. (6%)



b、Which of the following conditions may efficiently prevent the explosion? Select all applicable options. Points will only be awarded for identifying the complete and correct set of answers. Assume no side reactions. (7%)

(A) The cooling system fails at 150 minutes instead of 45 minutes, with operations remaining isothermal up until the failure.

(B) Lower the initial isothermal operating temperature to 165°C.

(C) Add inert species to the reactor, which do not participate in the reaction.

(D) Decrease the input amount of NH_3 to 25 kmol.

(E) Decrease the downtime to 5 mins.

(F) Introduce the 9.044 kmol of ONCB into the reactor through a semi-batch operation, dividing the addition into three intervals during the 175°C isothermal process (the first 45 mins).