國立中央大學 110 學年度碩士班考試入學試題

所別： 化學工程與材料工程學系 碩士班 甲組(一般生)

科目： 化工熱力學及化學反應工程

本科考試可使用計算器，廠牌、功能不拘 ＊請在答案卷(卡)內作答

一、單選題(佔 24 分，每題 2 分)

1. A first order gaseous phase reaction is catalyzed by a non-porous solid. The kinetic rate constant and the external mass transfer coefficients are k and k_g respectively. The effective rate constant (k_{eff}) is given by
   A. keff = k + k_g
   B. k_{eff} = (k+ k_g)/2
   C. k_{eff} = (kk_g)1/2
   D. $1/k_{eff} = 1/k + 1/k_g$

2. The half-life period of a first order reaction is given by (where k = rate constant).
   A. 1.5 k
   B. 2.5 k
   C. 0.693/k
   D. 6.93 k

3. The eddy diffusivity for a liquid in plug flow must be
   A. 1
   B. 0
   C. ∞
   D. Between 0 and 1

4. The most suitable reactor for carrying out an auto-thermal reaction is a
   A. Batch reactor
   B. CSTR
   C. Semi-batch reactor
   D. Plug-flow reactor

5. In an ideal tubular-flow reactor
   A. There is no mixing in longitudinal direction.
   B. Mixing takes place in radial direction.
   C. There is a uniform velocity across the radius.
   D. All of the above.

6. A batch reactor is suitable for:
   A. Achieving 100 percent conversion of reactants into products
   B. Large scale gaseous phase reactions
   C. Liquid phase reactions
   D. Obtaining uniform polymerization products in highly exothermic reactions

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7. If Thiele modulus is _____ , then the pore diffusion resistance in a catalyst may be considered as negligible.
   A. 0
   B. ∞
   C. < 0.5
   D. > 0.5
8. Which of the following chemical reactions will be favored by low pressure?
   A. $2HI = H_2 + I_2$
   B. $N_2O_2 = 2NO$
   C. $N_2 + O_2 = 2NO$
   D. None of these

9. In an exothermic chemical reaction, the reactants compared to the products have:
   A. Higher temperature
   B. More energy
   C. Less energy
   D. Same energy

10. In Langmuir treatment of adsorption,
   A. Whole surface of the catalyst does not have the same activity for adsorption and there is attraction between the adsorbed molecule
   B. Whole surface of the catalyst is essentially uniform and the adsorbed molecule has no effect on the rate of adsorption per site
   C. All the adsorption does not take place by the same mechanism
   D. Extent of adsorption is more than one complete monomolecular layer on the surface

11. Conversion increases with increase in temperature in case of a/an _____ reaction.
   A. Autocatalytic
   B. Irreversible
   C. Reversible endothermic
   D. Reversible exothermic

12. Half life period of decomposition of a liquid "A" by irreversible first order reaction is 12 minutes. The time required for 75% conversion of "A"' is _____ minutes.
   A. 18
   B. 24
   C. 6
   D. 12

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二、計算題(佔 76 分)

1. Titanium dioxide is a wide-bandgap semiconductor that is considered as an insulating dielectric in VLSI capacitors and for use in solar applications such as solar cells and photocatalyst. Thin films of TiO_2 can be prepared using chemical vapor deposition from gaseous titanium tetra-isopropoxide (TTIP). The overall reaction is

   $Ti(OC_3H_7)_4 \rightarrow TiO_2 + 4C_3H_6 + 2H_2O$

   The reaction mechanism in a CVD is believed to be

   TTIP (g) + TTIP (g) $\leftrightharpoons$ I (g) + P_1 (g)

   I (g)+ S $\leftrightharpoons$ I·S

   I·S $\rightarrow$ TiO_2 + P_2 (g)

   Where I is an active intermediate, S is an active site, P_1 is one set of reaction products (e.g. H_2O, C_3H_6) and P_2 is another set. Assuming the homogeneous gas-phase reaction for TTIP is in equilibrium, please answer the following question

   (a) (18%) Derive a rate law for the deposition of TiO_2

   (b) (8%) The experimental results show that at 200 °C the reaction is second order at low partial pressure of TTIP and zero order at high partial pressures. While at higher temperature (300 °C) the reaction is second order in TTIP over the entire pressure range. Discuss these results based on the rate law derived above. [Hint: adsorption is exothermic in general]

2. (10%) The intensive state of a *PVT* system containing N chemical species and π phases is in equilibrium. Show that the phase rule is: $F = 2 - \pi + N$, where F is the degree of freedom of the system.

3. For the steady-state, adiabatic, irreversible flow of an incompressible liquid in a horizontal pipe of constant cross-sectional area, show that:

   (a) (5%) The velocity is constant,

   (b) (5%) The temperature increases in the direction of flow, and

   (c) (5%)The pressure decreases in the direction of flow

   (Hint: $dH = C_P dT + (1-\beta T)VdP$ and $dS = C_P(dT/T) - \beta VdP$ where β is defined as the volume expansivity and C_P is the heat capacity at constant pressure).

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4. It is necessary to determine the vapor-liquid equilibrium composition for designing a separation process for a binary mixture of perfluoro-*n*-heptane and *n*-heptane at 25 °C. At this temperature, the vapor pressure of pure perfluoro-*n*-heptane is 0.1101 bar, and the vapor pressure of pure *n*-heptane is 0.0601 bar.
   (a) (6%) Calculate the composition of the vapor in equilibrium with a liquid containing 60 mol % perfluoro-*n*-heptane and 40 mol % of *n*-heptane at 25 °C and 0.6 bar, assuming the solution is ideal.
   (b) (10%) Please derive the expressions of the activity coefficient for both components in a binary mixture, assuming the solution obeys the regular solution theory. The excess Gibbs energy equation of the regular solution theory is as following: $\underline{G}^{ex} = (x_1\underline{V_1} + x_2\underline{V_2})\Phi_1\Phi_2(\delta_1 - \delta_2)^2$, where δ_i is solubility parameter of component i and Φ_i is volume fraction of component i: $\Phi_i = x_i\underline{V_i}/\sum_i x_i\underline{V_i}$
   (c) (6%) Recalculate the composition in part (a), assuming the solution obeys the regular solution theory. The regular solution parameters are

Compound	V^L (cm^3/mol)	δ $(cal/cc)^{1/2}$
perfluoro-*n*-heptane	226	12.3
n-heptane	148	7.4

   (d) (3%) Which model (ideal solution or regular solution) provides better estimation of gas phase compositions? Please give the reason according to the gas phase composition results in (a) and (c).

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