考試時間	月 日上午 下午第 節 (星期) 晚間	份數		任課教師	

國立臺灣科技大學 學年度第 學期 Qualify Exam 考試命題用紙 第 一 頁共 二 頁

考試科目：Advanced Chemical Reaction Engineering (高等化工動力學) □研究所 □大學部 □工程在職進修 系班別：

1. There is a solid catalyzed reaction

$$A \underset{}{\overset{\text{solid cat.}}{\rightleftharpoons}} R + S$$

Following are the reaction steps for this reaction

Adsorption: $A + \ell \rightleftharpoons A\ell$

Surface reaction $A\ell + \ell \rightleftharpoons R\ell + S\ell$

Desorption $R\ell \rightleftharpoons R + \ell$

$S\ell \rightleftharpoons S + \ell$

where ℓ represents active site. The overall rate expressions for different controlling steps are shown below:

Adsorption control $$-r_A = \frac{k_A\left(P_A - P_R P_S/K\right)}{1 + \frac{K_A}{K} P_R P_S + K_R P_R + K_S P_S}$$

Surface reaction control $$-r_A = \frac{k_{sr} K_A \left(P_A - P_R P_S/K\right)}{\left(1 + K_A P_A + K_R P_R + K_S P_S\right)^2}$$

R desorption control $$-r_A = \frac{K_R K\left(\frac{P_A}{P_S} - \frac{P_R}{K}\right)}{1 + K_A P_A + K K_R \frac{P_A}{P_S} + K_S P_S}$$

(i) If there is no R or S in the feed of reactor, please write down the rate expressions of the above controlling regimes for $t=0$, i.e. $-r_{A0}$ (initial rate expressions)

(ii) please draw schematic diagrams showing the relationships between $-r_{A0}$ and P_t for different controlling regimes. P_t is the total pressure.

2. An irreversible first-order reaction $A \rightarrow R$ takes place in a spherical porous catalyst pore surface ($R = 0.2$ cm). If there is no film mass transfer resistance and the following data are given:

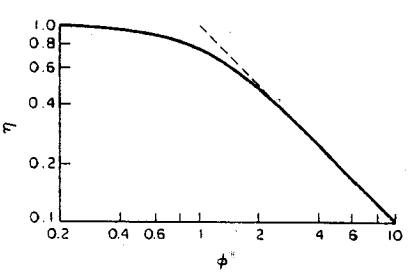
$D_e = 0.015\ cm^2/s$ at 100°C

$k_1 S_a \rho_p = 0.93\ 1/s$ at 100°C

$C_{As} = 3.25 \times 10^{-2}\ mol/L$ at 100°C

$E = 20\ kcal/mol$

please calculate the value of real overall reaction rate, $-r_A$ in mol/L·s.



Sphere $\phi = (R/3)\sqrt{k_1 S_a \rho_p / D_e}$

Cylinder $\phi = (R/2)\sqrt{k_1 S_a \rho_p / D_e}$

Slab $\phi = L\sqrt{k_1 S_a \rho_p / D_e}$

3 A sample of the tracer hytane at 320 k was injected as a pulse to a reactor, and the effluent concentration was measured as a function of time, resulting in the data shown in the following table.

t (min)	0	1	2	3	4	5	6	7	8	9	10	12	14
C (g/m³)	0	1	5	8	10	8	6	4	3.0	2.2	1.5	0.6	0

$\int_0^\infty C(t)dt = 50\ g\cdot min/m^3$

The measurements represent the exact concentrations at the times listed and not average values between the various sampling tests. Construct figures showing $C(t)$ and $E(t)$ as functions of time.

Undergraduate part

4. Titanium dioxide is a wide-band gap semiconductor that is showing promise as an insulating dielectric in VLSI capacitors and for use in solar cells. Thin films of TiO_2 are to be prepared by chemical vapor deposition (CVD) from gaseous titanium tetraisopropoxide (*TTIP*). The overall reaction is

$$Ti(OC_3H_7)_4 \rightarrow TiO_{2(g)} + 4C_3H_6 + 2H_2O$$

The reaction mechanism in a CVD reactor is believed to be

$$TTIP_{(g)} + TTIP_{(g)} \Leftrightarrow I + P_1$$

$$I + S \Leftrightarrow I \cdot S$$

$$I \cdot S \rightarrow TiO_2 + P_2,$$

where I is an active intermediate and 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, derive a rate law for the deposition of TiO_2. The experimental results show that at 200℃ the reaction is second order at low partial pressures of *TTIP* and zero order at high partial pressures, while at 300℃ the reaction is second order in *TTIP* over the entire pressure range. Discuss these results in light of the rate law you derived. (20%)

5. The reaction $A \rightarrow B$ is to be carried out isothermally in a continuous-flow reactor. Calculate both the CSTR and PFR reactor volumes necessary to consume 99% of A (i.e., C_A = 0.01 C_{A0}) when the entering molar flow rate is 5 *mol/h*, assuming the reaction rate $-r_A$ is :

(a) $-r_A = k$ with $k = 0.05\frac{mol}{h \cdot dm^3}$

(b) $-r_A = kC_A$ with $k = 0.0001 s^{-1}$

(c) $-r_A = kC_A^2$ with $k = 3\frac{dm^3}{mol \cdot h}$

The entering volumetric flow rate is 10 dm^3/h. (15%)