Ph.D. Qualify Exam for Advanced Chemical Reaction Engineering

(Department of Chemical Engineering, National Taiwan U of Science and Technology)

December, 2007

Part I.

1. (25%)

An elementary gas-phase reaction

$$A \rightarrow B + C$$

is carried out isothermally at 127°C in a flow reactor with no pressure drop. The specific reaction rate at 127°C is 0.044 min^{-1}. Pure A enters the reactor at 10 atm and 127°C and a molar flow rate of 2.5 mol/min. Calculate the reactor volume and space time to achieve 90% conversion in:

(a) a continuous-stirred tank reactor (CSTR) (10%)

(b) a plug-flow tubular reactor (PFR) (10%).

(c) Assume that the reaction is reversible with $K_C = 0.11$ mol/dm^3, calculate the equilibrium conversion, X_e. (5%)

Hint: Useful formula for this problem

(1) $\int_0^x \frac{1+\varepsilon x}{1-x} dx = (1+\varepsilon)\ln\frac{1}{1-x} - \varepsilon x$

(2) The five-point quadrature formula for the integration $\int_{x0}^{x4} f(x)dx = h/3(f_0+4f_1+2f_2+4f_3+f_4)$,

where f_i is the function value at x_i, and $h = (x_4-x_0)/4$

(3) For $ax^2 + bx + c = 0$, the roots, p and q, are $\frac{-b \pm \sqrt{b^2-4ac}}{2a}$

Show All Your Work.

2. (15%)

Pharmacokinetics concerns the ingestion, distribution, reaction, and elimination reaction of drugs in the body. Consider the application of pharmacokinetics to one of the major problems in Taiwan, drinking and driving. Here, we shall model how long one must wait to drive after having a tall martini. In Taiwan, the legal intoxication limit is 0.53 g of ethanol per liter of body fluid. (In the United States, it is 0.8 g/L, in Sweden it is 0.5 g/L, and in Eastern Europe and Russia it is any value above 0.0 g/L.) The ingestion of ethanol into the bloodstream and subsequent elimination can be modeled as a series reaction. The rate of absorption from the gastrointestinal tract into the bloodstream and body is a first-order reaction with a specific reaction rate constant of 10 h^{-1}. The rate at which ethanol is broken down in the bloodstream is limited by regeneration of a coenzyme. Consequently, the process may be modeled as a zero-order reaction with a specific reaction rate of 0.192 g/h·L of body fluid.

(a) How long would a person have to wait to drive in Taiwan if they drank two tall martinis immediately after arriving at a party? (10%)

(b) Suppose that one went to a party, had one and a half tall martinis right away, and then received a phone call saying an emergency had come up and the person needed to drive home immediately. How many minutes would the individual have to reach home before he/she became legally intoxicated, assuming that the person had nothing further to drink? (5%)

(Hint: Base all ethanol concentrations on the volume of body fluid. Calculate and plot the concentration of ethanol in the blood as a function of time.)

Additional information:

Ethanol in a tall martini: 40 g

Volume of body fluid: 40 L

Show All Your Work.

3. (10%)

The elementary irreversible organic liquid-phase reaction

$$A + B \rightarrow C$$

is carried out adiabatically in a flow reactor. An equal molar feed in A and B enters at 27°C, and the volumetric flow rate is 2 dm^3/s.

Calculate the PFR and CSTR volumes necessary to achieve 85% conversion.

Additional information:

$H_A^0(273) = -20$ kcal/mol

$H_B^0(273) = -15$ kcal/mol

$H_C^0(273) = -41$ kcal/mol

$C_{A0} = 0.1$ kmol/m^3

$C_{PA} = C_{PB} = 15$ cal/mol.K $\qquad C_{PC} = 30$ cal/mol.K

$k = 0.01$ dm^3/mol.s at 300K $\qquad E = 10{,}000$ cal/mol

Show All Your Work.

Part II

4. (20%) The following data have been reported for the hydrogenation of ethylene, $C_2H_2 + H_2 \rightleftharpoons C_2H_6$, (or $A + B \rightleftharpoons C$)

$-r_A$ (mmol/g-cat h)	P_A (atm)	P_B (atm)
8.8	0.60	0.40
11.7	0.39	0.61
14.4	0.22	0.78
19.6	0.09	0.91
20.1	0.05	0.95

(a) Show that the rate equation

$$-r_A = \frac{P_A P_B}{a + bP_A}$$

is consistent with the data and then determine the parameters, *a* and *b*. (10%)

(b) Propose a reaction mechanism that can lead to the rate equation. (10%)

5. (30%) A vapor phase catalytic reaction, $A + B \rightleftharpoons C$, was studied at 136 atm using a packed bed reactor, and obtained the following rate equation:

$$-r_A = \frac{kK_AK_B(P_AP_B - P_C/K)}{(1 + K_AP_A + K_BP_B)^2} \quad \text{unit of } -r_A \text{ is mol/g-cat h}$$

At 270°C, k = 0.00665 mol/g-cat h, $K_A = K_B = 0.131$ atm^{-1}, K = 14.7exp[-(28.6T- 9740)/RT] atm^{-1} where T[=] K, R = 1.987 cal/mol K. For an equimolar feed of A and B at a total rate of 2520 mol/h, calculate

(a) equilibrium conversion at 136 atm and 270°C. (10%)

(b) mass of catalyst required to convert 20% of A. (unit on rate constants are consistent) (20%)