เลขที่นั่งสอบ

มหาวิทยาลัยเทคโนโลยีพระจอมเกล้าธนบุรี

การสอบกลางภาคการเรียนที่ 2 ปีการศึกษา 2550

ข้อสอบวิชา ChE 343 Chemical Engineering Kinetics & Reactor Design

ภาควิชาวิศวกรรมเคมี ปีที่ 3 (หลักสูตรสองภาษา)

สอบวันที่ 19 ธันวาคม 2550 เวลา 9:00-12:00

หมายเหตุ

- ข้อสอบมีทั้งหมด 5 ข้อ
- อนุญาตให้ใช้เครื่องคำนวณได้
- ไม่อนุญาตให้นำเอกสารเข้าห้องสอบ

(รศ. ดร. วิโรจน์ บุญอำนวยวิทยา)
ผู้ออกข้อสอบ

(ผศ. ดร. อัศวิน มีชัย)
ผู้ออกข้อสอบ

ข้อสอบนี้ผ่านการประเมินจากภาควิชาวิศวกรรมเคมีแล้ว

(รศ. ดร. อนวัช สังข์เพ็ชร)
หัวหน้าภาควิชา

ชื่อนักศึกษา					รหัส
ข้อ 1 (20)	ข้อ 2 (20)	ข้อ 3 (20)	ข้อ 4 (20)	ข้อ 5 (20)	รวม

1. We got data from three separate batch experiments using the reactants with the same initial concentrations of $C_{A0}= C_{B0}= C_{C0}=10$ mol/L. The reactions consumed the reactants and occurred in different orders of reaction. Determine the rate constant, and order of reaction for each experiment using the data obtained.

Time (min)	C_A(mol/L)	C_B(mol/L)	C_C(mol/L)
0	10.0	10.0	10.0
2	9.9	9.0	5.0
4	9.8	8.2	3.3
6	9.7	7.4	2.5
8	9.6	6.7	2.0
10	9.5	6.1	1.7
12	9.4	5.4	1.4
14	9.3	5.0	1.2
16	9.2	4.5	1.1
18	9.1	4.0	1.0
20	9.0	3.6	0.9

2. From the lab data given below, what reactor between CSTR and PFR would require the smaller volume to achieve a conversion of 60%. The molar flow rate of the feed A is 5 mol/s.

x	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.85
$-r_A$	0.0053	0.0052	0.0050	0.0045	0.0040	0.0033	0.0025	0.0018	0.0013	0.0010

3. The homogeneous liquid reaction

$$CH_3COOH_5C_2 + OH^- \xrightarrow{k} + CH_3COO^- + C_2H_5OH$$

is irreversible with the reaction rate $-r_A = kC_AC_B \quad (kmol \cdot m^{-3} \cdot s^{-1})$
where $k = 1.54\ m^3 \cdot kmol^{-1} \cdot s^{-1}$

The reaction is performed isothermally and continuously in a CSTR with the space time 600 s. Concentrations of A, B at the input are $C_{A0} = C_{B0} = 0.01\ kmol \cdot m^{-3}$.

3.1 Find the conversion at the steady state.
3.2 If the concentration of B, $C_B = 0.25\ kmol \cdot m^{-3}$, find the concentration at the steady state.

4. The elementary irreversible gas reaction

$$A(g)+B(g) \rightarrow C(g,l)$$

is carried out isothermally in a PFR in which there is no pressure drop. As the reaction proceeds the partial pressure of C builds up and a point is reached at which C begins to condense. The vapor pressure of C is 0.4 atm. What is the rate of reaction at the point at which C first starts to condense. The feed is equal molar in A and B, there are no inerts or other species entering the reactor and the total pressure at the entrance is 2 atm.

Additional Information

$$C_{A0} = 0.02\ mol\ /\ dm^3$$
$$k_A = 100\ \mathrm{dm^3 \cdot mol^{-1} \cdot min^{-1}}$$

5. For the following parallel gas phase reactions with D and U as desired and undesired products, respectively.

$$A + B \rightarrow D, \qquad r_D = k_D C_A^{1.5} C_B$$

$$A + B \rightarrow U, \qquad r_U = k_U C_A^{2}$$

Given the rate law above for each reaction and the activation energy $E_D = 10{,}000$ kcal/mol and $E_U = 17{,}500$ kcal/mol. Suggest all possible choices of reactor and conditions that minimize the unwanted product (U).

Ideal Gas Constant and Conversion Factors

B

Ideal Gas Constant

$$R = \frac{8.314\ \text{kPa} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}} \qquad R = \frac{1.987\ \text{Btu}}{\text{lb mol} \cdot {}^\circ\text{R}}$$

$$R = \frac{0.73\ \text{ft}^3 \cdot \text{atm}}{\text{lb mol} \cdot {}^\circ\text{R}} \qquad R = \frac{8.3144\ \text{J}}{\text{mol} \cdot \text{K}}$$

$$R = 0.082\ \frac{\text{dm}^3 \cdot \text{atm}}{\text{mol} \cdot \text{K}} = \frac{0.082\ \text{m}^3 \cdot \text{atm}}{\text{kmol} \cdot \text{K}} \qquad R = \frac{1.987\text{cal}}{\text{mol} \cdot \text{K}}$$

Volume of Ideal Gas

1 lb mol of an ideal gas at 32°F and 1 atm occupies 359 ft^3.
1 g mol of an ideal gas at 0°C and 1 atm occupies 22.4 dm^3.

$$C_A = \frac{P_A}{RT} = \frac{y_A P}{RT}$$

where C_A = concentration of A, mol/dm^3
R = ideal gas constant, $\text{kPa} \cdot \text{dm}^3/\text{mol} \cdot \text{K}$
T = temperature, K
P = pressure, kPa
y_A = mole fraction of A

Volume

1 cm^3	= 0.001 dm^3
1 in^3	= 0.0164 dm
1 fluid oz	= 0.0296 dm^3
1 ft^3	= 28.32 dm^3
1 m^3	= 1000 dm^3
1 U.S. gallon	= 3.785 dm^3

$$\left(1\ \text{ft}^3 = 28.32\ \text{dm}^3 \times \frac{1\ \text{gal}}{3.785\ \text{dm}^3} = 7.482\ \text{gal}\right)$$

Length

1 Å	= 10^{-8} cm
1 dm	= 10 cm
1 μm	= 10^{-4} cm
1 in.	= 2.54 cm
1 ft	= 30.48 cm
1 m	= 100 cm

Pressure

1 torr (1 mmHg)	=	0.13333 kPa
1 in. H_2O	=	0.24886 kPa
1 in. Hg	=	3.3843 kPa
1 atm	=	101.33 kPa
1 psi	=	6.8943 kPa
1 megadyne/cm^2	=	100 kPa

Energy (Work)

1 kg·m^2/s^2	=	1 J
1 Btu	=	1055.06 J
1 cal	=	4.1841 J
1 L·atm	=	101.34 J
1 hp·h	=	2.6806×10^6 J
1 kWh	=	3.6×10^6 J

Temperature

°F	=	1.8 × °C + 32
°R	=	°F + 459.69
K	=	°C + 273.16
R	=	1.8 × K
°Réamur	=	1.25 × °C

Mass

1 lb	=	454 g
1 kg	=	1000 g
1 grain	=	0.0648 g
1 oz (avoird.)	=	28.35 g
1 ton	=	908,000 g

Viscosity

1 poise = 1 g/cm·s

Rate of change of energy with time

1 watt = 1 J/s

1 hp = 746 J/s

Force

1 dyne = 1 g·cm/s^2

1 Newton = 1 kg·m/s^2

1 Newton/m^2 = 1 Pa

Work

Work = Force·Distance

1 Joule = 1 Newton·meter = 1 kg m^2/s^2 = 1 Pa·m^3

Gravitational conversion factor

Gravitational constant

$$g = 32.2 \text{ ft/s}^2$$

American Engineering System

$$g_c = 32.174 \frac{(\text{ft})(\text{lb}_m)}{(\text{s}^2)(\text{lb}_f)}$$

SI/cgs System

$$g_c = 1 \text{ (Dimensionless)}$$

Numerical Techniques A

A.1 Useful Integrals in Reactor Design

Also see http://www.integrals.com

$$\int_0^x \frac{dx}{1-x} = \ln\frac{1}{1-x} \tag{A-1}$$

$$\int_0^x \frac{dx}{(1-x)^2} = \frac{x}{1-x} \tag{A-2}$$

$$\int_0^x \frac{dx}{1+\varepsilon x} = \frac{1}{\varepsilon}\ln(1+\varepsilon x) \tag{A-3}$$

$$\int_0^x \frac{1+\varepsilon x}{1-x}\,dx = (1+\varepsilon)\ln\frac{1}{1-x} - \varepsilon x \tag{A-4}$$

$$\int_0^x \frac{1+\varepsilon x}{(1-x)^2}\,dx = \frac{(1-\varepsilon)x}{1-x} - \varepsilon\ln\frac{1}{1-x} \tag{A-5}$$

$$\int_0^x \frac{(1+\varepsilon x)^2}{(1-x)^2}\,dx = 2\varepsilon(1+\varepsilon)\ln(1-x) + \varepsilon^2 x + \frac{(1+\varepsilon)^2 x}{1-x} \tag{A-6}$$

$$\int_0^x \frac{dx}{(1-x)(\Theta_B - x)} = \frac{1}{\Theta_B - 1}\ln\frac{\Theta_B - x}{\Theta_B(1-x)} \qquad \Theta_B \neq 1 \tag{A-7}$$

$$\int_0^x \frac{dx}{ax^2+bx+c} = \frac{-2}{2ax+b} + \frac{2}{b} \qquad \text{for } b^2 = 4ac \tag{A-8}$$

$$\int_0^x \frac{dx}{ax^2+bx+c} = \frac{1}{a(p-q)}\ln\left(\frac{q}{p}\cdot\frac{x-p}{x-q}\right) \qquad \text{for } b^2 > 4ac \tag{A-9}$$

$$\int_0^W (1-\alpha W)^{1/2}\,dW = \frac{2}{3\alpha}\left[1-(1-\alpha W)^{3/2}\right] \tag{A-10}$$

where p and q are the roots of the equation.

$$ax^2 + bx + c = 0 \qquad \text{i.e., } p, q = \frac{-b \mp \sqrt{b^2 - 4ac}}{2a}$$

$$\int_0^x \frac{a+bx}{c+gx}\,dx = \frac{bx}{g} + \frac{ag-bc}{g^2} \ln \frac{c+gx}{c} \tag{A-11}$$

A.2 Equal-Area Graphical Differentiation

There are many ways of differentiating numerical and graphical data. We shall confine our discussions to the technique of equal-area differentiation. In the procedure delineated below we want to find the derivative of y with respect to x.

This method finds use in Chapter 5

1. Tabulate the (y_i, x_i) observations as shown in Table A-1.
2. For each *interval*, calculate $\Delta x_n = x_n - x_{n-1}$ and $\Delta y_n = y_n - y_{n-1}$.

TABLE A-1

x_i	y_i	Δx	Δy	$\dfrac{\Delta y}{\Delta x}$	$\dfrac{dy}{dx}$
x_1	y_1				$\left(\dfrac{dy}{dx}\right)_1$
		$x_2 - x_1$	$y_2 - y_1$	$\left(\dfrac{\Delta y}{\Delta x}\right)_2$	
x_2	y_2				$\left(\dfrac{dy}{dx}\right)_2$
		$x_3 - x_2$	$y_3 - y_2$	$\left(\dfrac{\Delta y}{\Delta x}\right)_3$	
x_3	y_3				$\left(\dfrac{dy}{dx}\right)_3$
		$x_4 - x_3$	$y_4 - y_3$	$\left(\dfrac{\Delta y}{\Delta x}\right)_4$	
x_4	y_4				$\left(\dfrac{dy}{dx}\right)_4$
		$x_5 - x_4$	$y_5 - y_4$	$\left(\dfrac{\Delta y}{\Delta x}\right)_5$	
x_5	y_5		etc.		

3. Calculate $\Delta y_n / \Delta x_n$ as an estimate of the *average* slope in an interval x_{n-1} to x_n.
4. Plot these values as a histogram versus x_i. The value between x_2 and x_3, for example, is $(y_3 - y_2)/(x_3 - x_2)$. Refer to Figure A-1.

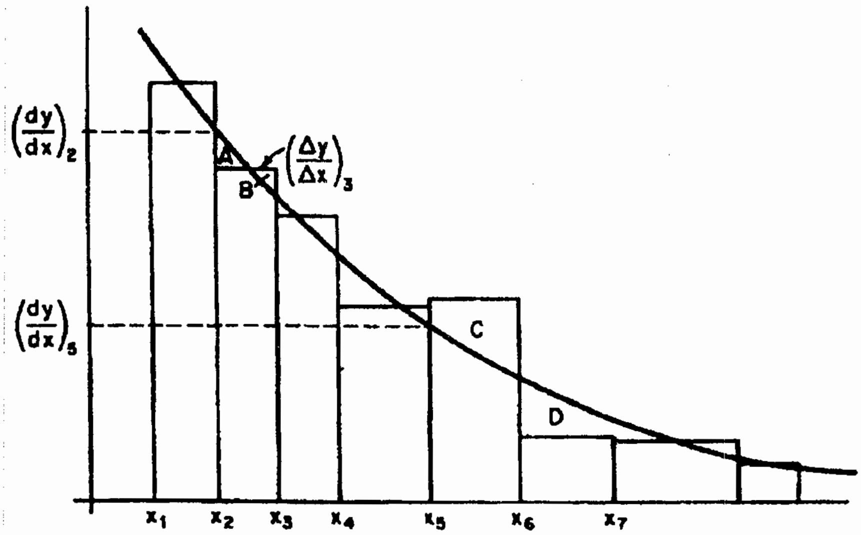

Figure A-1 Equal-area differentiation.

5. Next draw in the *smooth curve* that best approximates the *area* under the histogram. That is, attempt in each interval to balance areas such as those labeled A and B, but when this approximation is not possible, balance out over several intervals (as for the areas labeled C and D). From our definitions of Δx and Δy we know that

$$y_n - y_1 = \sum_{i=2}^{n} \frac{\Delta y}{\Delta x_i} \Delta x_i \tag{A-12}$$

The equal-area method attempts to estimate dy/dx so that

$$y_n - y_1 = \int_{x_1}^{x_n} \frac{dy}{dx}\, dx \tag{A-13}$$

that is, so that the area under $\Delta y/\Delta x$ is the same as that under dy/dx, *everywhere possible.*

6. Read estimates of dy/dx from this curve at the data points $x_1, x_2, \ldots$ and complete the table.

An example illustrating the technique is given on the CD-ROM.

Differentiation is, at best, less accurate than integration. This method also *clearly indicates bad data* and allows for compensation of such data. Differentiation is only valid, however, when the data are presumed to differentiate *smoothly*, as in rate-data analysis and the interpretation of transient diffusion data.

A.3 Solutions to Differential Equations

Methods of solving differential equations of the type

$$\frac{d^2y}{dx^2} - \beta y = 0 \tag{A-14}$$

can be found in such texts as *Applied Differential Equations* by M. R. Spiegel (Upper Saddle River, N.J.: Prentice Hall, 1958, Chap. 4; a great book even though it's old) or in *Differential Equations* by F. Ayres (Schaum Outline Series, McGraw-Hill, New York, 1952). One method of solution is to determine the characteristic roots of

$$\left(\frac{d^2}{dx^2} - \beta\right)y = (m^2 - \beta)y \tag{A-15}$$

which are

$$m = \pm\sqrt{\beta} \tag{A-16}$$

Solutions of this type are required in Chapter 12

The solution to the differential equation is

$$y = A_1 e^{-\sqrt{\beta}x} + B_1 e^{+\sqrt{\beta}x} \tag{A-17}$$

where A_1 and B_1 are arbitrary constants of integration. It can be verified that Equation (A-17) can be arranged in the form

$$y = A \sinh\sqrt{\beta}x + B\cosh\sqrt{\beta}x \tag{A-18}$$

Equation (A-18) is the more useful form of the solution when it comes to evaluating the constants A and B because $\sinh(0) = 0$ and $\cosh(0) = 1.0$. As an exercise you may want to verify that Equation (A-18) is indeed a solution to Equation (A-14).

A.4 Numerical Evaluation of Integrals

In this section we discuss techniques for numerically evaluating integrals for solving first-order differential equations.

1. *Trapezoidal rule* (two-point) (Figure A-2). This method is one of the simplest and most approximate, as it uses the integrand evaluated at the limits of integration to evaluate the integral:

$$\int_{X_0}^{X_1} f(X)\,dX = \frac{h}{2}[f(X_0) + f(X_1)] \tag{A-19}$$

when $h = X_1 - X_0$.

2. *Simpson's one-third rule* (three-point) (Figure A-3). A more accurate evaluation of the integral can be found with the application of Simpson's rule:

$$\int_{X_0}^{X_2} f(X)\,dX = \frac{h}{3}[f(X_0)+4f(X_1)+f(X_2)] \qquad \text{(A-20)}$$

where

$$h = \frac{X_2 - X_0}{2} \qquad X_1 = X_0 + h$$

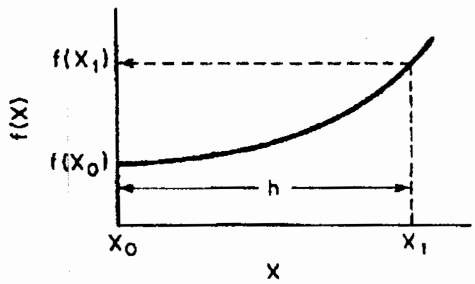

Figure A-2 Trapezoidal rule illustration.

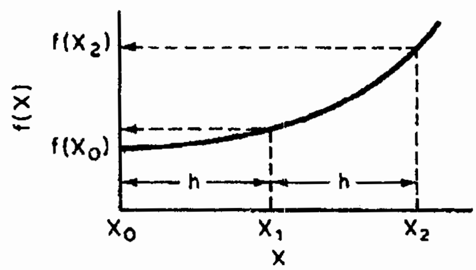

Figure A-3 Simpson's three-point rule illustration.

3. *Simpson's three-eighths rule* (four-point) (Figure A-4). An improved version of Simpson's one-third rule can be made by applying *Simpson's second rule*:

$$\int_{X_0}^{X_3} f(X)\,dX = \tfrac{3}{8}h[f(X_0)+3f(X_1)+3f(X_2)+f(X_3)] \qquad \text{(A-21)}$$

where

$$h = \frac{X_3 - X_0}{3} \qquad X_1 = X_0 + h \qquad X_2 = X_0 + 2h$$

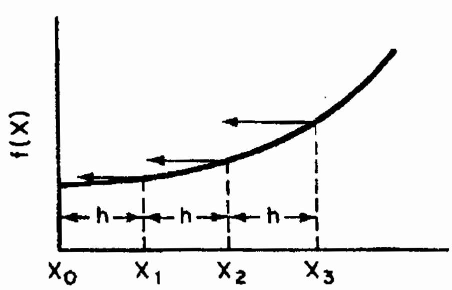

Figure A-4 Simpson's four-point rule illustration.

4. *Five-point quadrature formula:*

$$\int_{X_0}^{X_4} f(X)\,dX = \frac{h}{3}(f_0+4f_1+2f_2+4f_3+f_4) \qquad \text{(A-22)}$$

where

$$h = \frac{X_4 - X_0}{4}$$

5. For $N + 1$ points, where $(N/3)$ is an integer,

$$\int_{X_0}^{X_N} f(X)\, dX = \tfrac{3}{8} h [f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + \cdots + 3f_{N-1} + f_N] \quad \text{(A-23)}$$

where

$$h = \frac{X_N - X_0}{N}$$

6. For $N + 1$ points, where N is even,

$$\int_{X_0}^{X_N} f(X)\, dX = \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 4f_{N-1} + f_N) \quad \text{(A-24)}$$

where

$$h = \frac{X_N - X_0}{N}$$

These formulas are useful in illustrating how the reaction engineering integrals and coupled ODEs (ordinary differential equation(s)) can be solved and also when there is an ODE solver power failure or some other malfunction.

A.5 Software Packages

Instructions on how to use POLYMATH, MatLab, and ASPEN can be found on the CD-ROM.

For the ordinary differential equation solver (ODE solver), contact:

POLYMATH
CACHE Corporation
P.O. Box 7939
Austin, TX 78713-7379

Aspen Technology, Inc.
10 Canal Park
Cambridge, Massachusetts
02141-2201 USA
E-mail: info@aspentech.com
Website: http://www.aspentech.com

Matlab
The Math Works, Inc.
20 North Main Street, Suite 250
Sherborn, MA 01770

Maple
Waterloo Maple Software
766884 Ontario, Inc.
160 Columbia Street West
Waterloo, Ontario, Canada N2L3L3

A critique of some of these software packages (and others) can be found in *Chemical Engineering Education*, Vol. XXV, Winter, p. 54 (1991).