

**PRINCE OF SONGKLA UNIVERSITY
FACULTY OF ENGINEERING**

Midterm Examination: Semester II
Date: 26, December 2004
Subject: 230 – 591 Special Topics in Chem. Eng I
(Computational Methods in Chem. Eng)

Academic year: 2004
Time: 9.00-12.00
Room: R 300

ทฤษฎีในการสอบ โทษขั้นต่ำ คือ ปรับตกในรายวิชาที่ทฤษฎี และพักการเรียน **1** ภาคการศึกษา

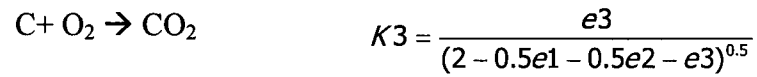
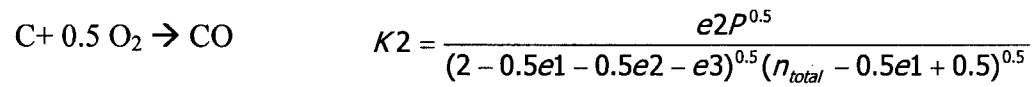
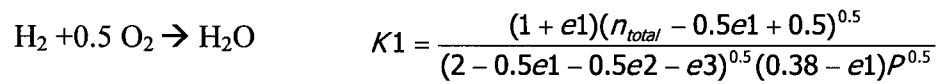
- **Only hand written note in 1 A4 is allowed**
 - There are 5 pages of the exam not include the cover page
 - Identify each page with your name or at least your code
 - If need to write the answers at the back of each page, please identify the problem number
 - Writing clearly and concisely will be your advantage. Explanation of your answer is required.
-

Name _____ code _____

Problem Number	Score
1	30
2	30
3	30
4	30
5	30
Total	150

Dr. Kulchanat Kapilakarn

1 [30 points] The following three reactions occur in a coal gasifier



e_1 , e_2 , and e_3 represent the number of moles of H_2 used in reactions 1, 2 and 3, respectively.

1.1 Set up the equations of $f_1(e_1, e_2, e_3)$, $f_2(e_1, e_2, e_3)$ and $f_3(e_1, e_2, e_3)$ used in Newton-Raphson method.

1.2 Show algorithm of solving e_1 , e_2 and e_3 by Newton-Raphson method.

2 [30 points] The outflow chemical from completely mixed reactor is measured as

t, min	0	2	4	6	8	12	16	20
C, mg/m ³	0	20	30	40	60	72	70	50

For an outflow of $Q = 12 \text{ m}^3/\text{min}$, you can estimate the mass of chemical that exits the reactor from $t = 0$ to $t = 20$.

2.1 Write the formula and algorithm of using trapezoidal rule to estimate the mass.

2.2 Can we use Simpson's 1/3 rule to estimate the mass and why?

2.3 Write formula and algorithm of using Simpson's 1/3. If your answer in (2.2) is "No", what are your assumptions to solve the problem?

3 [30 points] The modified Euler method can be written in Runge-Kutta format as:

$$k_1 = f(y_i, t_i)h$$

$$k_2 = f(y_i + k_1, t_i + h)h$$

$$y_{i+1} = y_i + (k_1 + k_2) / 2 \quad (a)$$

$$\text{If } dy/dt = f(y,t) = -\lambda y \quad (b)$$

$$y(0) = y_0 \quad \lambda \text{ is a positive constant}$$

3.1 Write out equation (a) for equation (b) with the step size h .

3.2 What is the approximate maximum integration step h that you could use with the Euler method to maintain a stable solution?

4 [30 points] Consider $dy/dt = f(y,t) = -\lambda \sin y + e^{-t}$, $y(0) = y_0$ (c)

4.1 Apply the implicit Euler method, $y_{i+1} = y_i + dy_{i+1} / dt * h$ to equation (c).

4.2 Use Euler to estimate y_{i+1} and calculate y_{i+1} from (4.1).

4.3 Write algorithm to solve this problem.

- 5 [30 points] Using the shooting method and modify Euler integration to solve

$$a \frac{d^2 y}{dx^2} - b \frac{dy}{dx} - y + x = 0$$
 when coefficients **a** and **b** are positive real numbers. The boundary

condition for the equation are $y(0) = y_0$ and $y(20) = y_{20}$. Write the algorithm to solve the problem.