PRINCE OF SONGKLA UNIVERSITY
FACULTY OF ENGINEERING

Midterm Examination: Semester II — Academic year: 2004
Date: 26, December 2004 — Time: 9.00-12.00
Subject: 230 – 591 Special Topics in Chem. Eng I
(Computational Methods in Chem. Eng) — Room: R 300

ทุจริตในการสอบ โทษขั้นต่ำ คือ ปรับตกในรายวิชาที่ทุจริต 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

Midterm 230-591 I Name____________________________Code___________

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

$H_2 + 0.5\ O_2 \rightarrow H_2O$ $$K1 = \frac{(1+e1)(n_{total} - 0.5e1 + 0.5)^{0.5}}{(2 - 0.5e1 - 0.5e2 - e3)^{0.5}(0.38 - e1)P^{0.5}}$$

$C + 0.5\ O_2 \rightarrow CO$ $$K2 = \frac{e2P^{0.5}}{(2 - 0.5e1 - 0.5e2 - e3)^{0.5}(n_{total} - 0.5e1 + 0.5)^{0.5}}$$

$C + O_2 \rightarrow CO_2$ $$K3 = \frac{e3}{(2 - 0.5e1 - 0.5e2 - e3)^{0.5}}$$

e1, e2, and e3 represent the number of moles of H_2 used in reactions 1, 2 and 3, respectively.

1.1 Set up the equations of f1(e1,e2,e3), f2(e1,e2,e3) and f3(e1,e2,e3) used in Newton- Raphson method.

1.2 Show algorithm of solving e1, e2 and e3 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 m^3/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:

$k_1 = f(y_i, t_i)h$

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

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

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

$y(0) = y_0$ λ 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 $a\frac{d^2y}{dx^2} - b\frac{dy}{dx} - y + x = 0$ 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.