

ชื่อ _____

รหัส _____

PRINCE OF SONGKLA UNIVERSITY
FACULTY OF ENGINEERING

Final Examination: Semester II

Academic year: 2004

Date: 1, March 2005

Time: 13.30 – 16.30

Subject: 230 – 591 Special Topics in Chem. Eng 1

(Computational Methods in Chem. Eng)

Room: R 200

ทฤษฎีในการสอบ โทษขั้นต่ำ คือ ปรับตกในรายวิชาที่ทฤษฎี และพักการเรียน 1 ภาคการศึกษา

- ข้อสอบมีทั้งหมด 5 ข้อรวม 6 หน้า ให้นักศึกษาตรวจสอบความเรียบร้อย และเขียนชื่อก่อนลงมือทำ
ข้อสอบ

- อนุญาตให้นำข้อมูลจดด้วยลายมือตัวเองลงในกระดาษขนาด A4 จำนวน 1 แผ่น และเครื่อง
คำนวณเข้าห้องสอบได้เท่านั้น
- อนุญาตให้ทำข้อสอบด้านหลังได้

ข้อ	คะแนน
1	25
2	25
3	30
4	30
5	30
รวม	140

อาจารย์กุลชนารุ กปิลกาญจน์

ผู้ออกข้อสอบ

1 (25 points) Consider heat conduction without convection problem:

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right) + Q = 0$$

1.1. What is the geometric type of PDE for this problem?

Answer _____

1.2 Give the method that you prefer to solve this problem and show how to solve.

1.3 Give the method that is not suitable to solve this problem, and give the reasons why it does not work?

2 (25 points) Answer the questions from the following MATLAB code:

```
%
clear %line1
T0=150;Ti=30;Ta=30;h=2;dr=0.1;dt=0.2;roCp=2;B=0.2;r0=0.5;r1=2;a=0.01; %line2
tmax =1000; %line3
n=(r1-r0)/dr+1; %line4
errt=1; %line5
it=1; %line6
r=r0; %line7
time(it) =0; %line8
while and ((it <=tmax),(errt>10^(-5))) %line9
    for i=1:n %line10
        temp(1,i)=Ti; %line11
        r(i)=r0+(i-1)*dr; %line12
    end %line13
    % point 1 %line14
    temp(it,1)=T0; %line15
    dTdt(it,1)=0; %line16
    % point 2 - point n-1 %line17
    for j =2:n-1 %line18
        dT1(it,j)=(temp(it,j)-temp(it,j-1))/dr; %line19
        dT2(it,j)=(temp(it,j+1)-2*temp(it,j)+temp(it,j-1))/dr^2; %line20
        dTdt(it,j)=(a*dT2(it,j)+(a/r(j))*dT1(it,j))-2*h/B/roCp*(temp(it,j)-Ta); %line21
    end %line22
    %point n %line23
    dTdt(it,n)=0-2*h/B/roCp*(temp(it,n)-Ta); %line24
    % next step of time %line25
    it=it+1; %line26
    time(it) = time(it-1)+dt; %line27
    for j=1:n %line28
        temp(it,j)=temp(it-1,j)+dt*dTdt(it-1,j); %line29
        err(j)=abs(temp(it,j)-temp(it-1,j)); %line30
    end %line31
    errt=max(err); %line32
end %line33
plot(time,temp(:,1),time,temp(:,5),time,temp(:,n)) %line34
```

2.1 What is the geometric type of this PDE?

Answer _____

2.2 What is the method solved for this problem? **Answer** _____

2.3 What is the meaning of the statement in line 9 ?

Answer _____

2.4 What is the meaning of the statement in line 10 ?

Answer _____

2.5 What is the meaning of the statement in line 11 ?

Answer _____

2.6 Three- point approximation (difference table) of $\mathbf{dT/dt}$ brings 2nd order of error ($O(\Delta t^2)$).
Show how to apply this approximation instead of the use in the code.

2.7 Why, sometimes, the system is not stable when \mathbf{dt} is smaller than the given \mathbf{dt} ?

3. (30 points) A mixture of benzene and toluene are to be separated in a flash tank. The pressure in the flash tank is 760 mm Hg. The units for Antoine's equation are mm Hg and °C for pressure and temperature, respectively.

$$x_B P_{\text{sat B}} + x_T P_{\text{sat T}} = P$$

$$\ln(P_{\text{sat B}}) = A1 - B1/(T+C1)$$

$$\ln(P_{\text{sat T}}) = A2 - B2/(T+C2)$$

The process engineer wants to set the operating temperature which gives the highest purity toluene in the liquid phase (x_T). For this problem,

- 3.1 Write the objective function and all constraints.
- 3.2 Show how to get the desired temperature for this process (do not need to calculate the final answer).

4 (30 points) A chemical plant can produce at most 3×10^6 L/ day of a solution at the most profit. Three sources are available at different process and supply rates. Each source also has a different concentration of an impurity that must be kept below a minimum level. The data for the three sources are summarized in the following table.

	Source 1	Source 2	Source 3	Required
Profit (\$/L)	0.50	1.00	1.20	
Supply (10^5 L/day)	20	10	5	≤ 30
Concentration (mg/L)	135	100	75	≤ 100

4.1 Write the objective function, constraints and standard form.

4.2 Use Simplex method to determine the amount from each source to meet the requirements.

5. (30 points) Write the algorithm to fit experimental data (x_1, x_2, y) with the given equation:

$$y = a_0 + a_1x_1 + a_2x_1^2x_2 + a_3x_2 \text{ nonlinear equation } f(x_1, x_2, y) \text{ by using Gauss-Newton method.}$$

And what is the objective function of the problem? (Hint: sum of the squares of the residuals is required)