BACHELOR OF ENGINEERING IN CHEMICAL ENGINEERING

4 TH YEAR 1 ST SEMESTER

MATHEMATICAL MODELING IN CHEMICAL ENGINEERING

TOTAL MARKS: 100

TIME: THREE HOURS

50 MARKS FOR EACH PART

USE SEPARATE ANSWER SCRIPT FOR EACH PART

PART -I

ANSWER ANY TWO QUESTIONS

ALL QUESTIONS CARRY EQUAL MARKS

ASSUME MISSING DATA, IF ANY

REFERENCE: EX/CHE/T/412/2017

1.Thetemperature distribution in a tapered conical cooling fin is described by the following differential equation which has been non dimensionalized.

$$\frac{d^2u}{dx^2} + \left(\frac{2}{x}\right)\left(\frac{du}{dx} - pu\right) = 0$$

Where u= temperature ($0 \le u \le 1$),x=axial distance ($0 \le x \le 1$), and p is a nondimensional parameter that describes the heat transfer and geometry.

$$p = \frac{hL}{k}\sqrt{1 + \frac{4}{2m^2}}$$

Where h = a heat transfer co-efficient, k = thermal conductivity, L = length or height of the cone, and m = the slope of the cone wall. The equation has boundary conditions

$U(x=0) = 0$ $\quad u(x=1) = 1$

Formulate the finite difference equations for the differential equation above.

2. The following system is a classic example of stiff ODE's in the solution of chemical reaction kinetics

$Dc_1/dt = -0.013c_1 - 1000c_1c_3$

$Dc_2/dt = -2500bc_2c_3$

$Dc_3/dt = -.013\ c_1 - 1000c_1c_3 - 2500c_2c_3$

Initial conditions: $c_1(0) = c_2(0) = 1 \quad c_3(0) = 0$

Use implicit Euler method to solve the ODE's for two iterations only.

3. Use Liebmann's method (Gauss Seidel) method to solve for the temperature of a square heated plate with upper boundary condition of 150^0C, the left condition of 75^0C, right boundary condition of 50^0C and bottom boundary condition 0^0C. The Laplacian elliptic partial differential equation model describes the heat transfer phenomenon quite accurately.

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

4.Solve the following tridiagonal system with the Thomas algorithm:

$$2.04T_1 - T_2 = 40.8$$

$$-T_1 + 2.04T_2 - T_3 = 0.8$$

$$-T_2 + 2.04T_3 - T_4 = 0.8$$

$$-T_3 + 2.04T_4 = 200.8$$

B. CHEM ENGG. 4TH YEAR 1ST. SEM. EXAM. - 2017

MATHEMATICAL MODELLING IN CHEMICAL ENGINEERING

Time: three hour

PART II **Full marks: 50**

Answer any two questions
Assume any missing data
All questions carry equal marks
Symbols have usual significance
Draw labeled schematic of the problem wherever needed
Clearly state all the assumptions, boundary and initial conditions

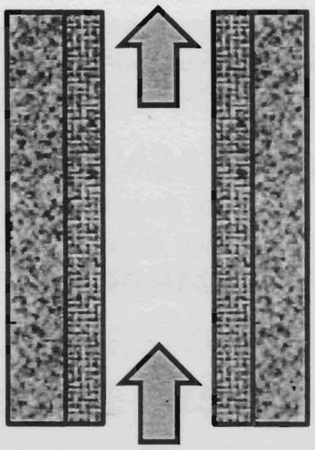
1) A heat exchanger network consists of four streams. Data for each stream is given in the following table. Assume 20 °C temperature of approach.

Stream No.	Condition	FCP	Inlet temp. °C	Outlet temp. °C
1	HOT (H1)	1000	250	120
2	HOT (H2)	4000	200	100
3	COLD (C1)	3000	90	150
4	COLD (C2)	6000	130	190

In order to design heat exchanger network based on stream data calculate the following:

a) Energy availability calculations for each stream based on first law of thermodynamics.
b) Why heat exchanger network cannot be designed without applying the second law of thermodynamics?
c) Calculate total energy demand.
d) Draw temperature interval diagram considering 20°C approach temperature difference.
e) Draw combined hot and cold utility diagram showing amount of energy transferred in each temperature interval.
f) Draw energy cascade diagram to identify the pinch condition if any.
g) If pinch condition exists, calculate pinch temperatures for hot and cold streams and the average pinch temperature.
h) Calculate minimum heating and cooling utilities required.
i) Write the significance of pinch condition.
j) Perform stream matching above pinch to Calculate number of heat exchangers above pinch
k) Calculate number of hot utility above pinch
l) Repeat steps (j) to (l) for calculations below pinch.

2) The following figure represents a vertical flue duct, heating wall, and coke bed assembly in a coke oven plant.



Preheated coke oven gas is burnt at the bottom of the flue duct and the burnt gas is entering the duct at a temperature T_1 and leaving from the top. Gas flows through the duct with steady mass flow rate of $\dot{m}$. The equivalent diameter of flow passage is D. The walls are initially at T_W which is much lower than the inlet gas temperature. Assume 2-D conduction transient conduction in walls and convection from flue gas to the inner surface of the wall. Heat from the hot gas it transferred to heating wall and then to the coke bed where carbonization takes place. The height of the duct is H, thickness of the wall is L and coke bed thickness Lc.

Thermo-physical properties of gas and the wall materials are:
Gas: ρ,μ,α,k,Cp (with subscript 'g')
Wall: ρ,α,k,Cp (with subscript 'w')
Coke bed: ρ,α,k,Cp (with subscript 'c')
Based on the above mentioned description of the problem, write the model equations as required below.

a) Write unsteady state energy balance equation for the flue gas.
b) Write unsteady state 2-D conduction equation for heat wall.
c) Write proper boundary conditions at gas solid interface
d) Write boundary condition at wall-coke bed interface
e) Write proper energy balance equation for coke bed
f) Write finite difference formulations of model equations
g) Write a suitable algorithm to solve for thermal dynamics of gas flow, heating wall and the coke bed.

ANY NUMERICAL SOLUTION TO THE PROBLEM IS NOT REQUIRED

3) Derive overall mass balance equation and component balance equation for a tapered tube geometry.

Water is flowing into a well starred tank at 150 kg/hr and methanol is being added at at 30kg/hr. The resulting solution is leaving the tank at 120 kg/hr. Due to effective stirring; the concentration of the outlet solution is same as that in the tank. Initially the tank contains 100 kg of fresh water. The rate of input and output are same thereafter. Calculate outlet mass fraction of methanol after 1.0 hr.

Draw a labeled schematic of the problem. All steps of calculations are to be provided. Draw the proper information flow diagram needed. Comment on limitation of the model so developed for this particular problem.

4) Draw a schematic of dry well and wet well assembly in a typical PHWR nuclear power plant. Identify the components therein. Write the sequence of scenario of incidences happen after break in PHT loop Write model equations for dry well and vent shaft. . Derive model equation for vent clearing stage.

5) Draw a labeled schematic of a belt cooling arrangement for solidification of molten sulfur. Write the mathematical model equations for thermal analysis of the problem. Write proper boundary conditions and equation for solid-liquid interface. Explain how these model equations with boundary conditions may be solved numerically to obtain required length of the belt cooler.