Reg. No.										

MANIPAL INSTITUTE OF TECHNOLOGY

MANIPAL

A Constituent Institution of Manipal University

V SEMESTER B.TECH. (CHEMICAL ENGINEERING)

END SEMESTER EXAMINATIONS, JAN 2017

SUBJECT: COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING [CHE 3105]

REVISED CREDIT SYSTEM

Time: 3 Hours MAX. MARKS: 100

Instructions to Candidates:

- Answer **ALL** the questions.
- Missing data may be suitably assumed.

1A. The following data represents the activity coefficient versus mole fraction for the system acetone(1) – dichloroethylene(20). Use Least Square regression to fit the data to **10**

$$x_1 = a + b\gamma_1 + c\gamma_2$$

x1	0.023	0.053	0.357	0.516	0.883	0.979
γ1	0.608	0.711	0.854	0.917	0.987	1
γ2	0.993	0.974	0.934	0.891	0.781	0.694

1B. The van der Waals equation to calculate fugacity is given by **10**

$$\ln f = \frac{b}{V-b} - \frac{2a}{RTV} + \ln\frac{RT}{V-b}$$

Find the molar volume of ethylene at 373 K. The following data apply:

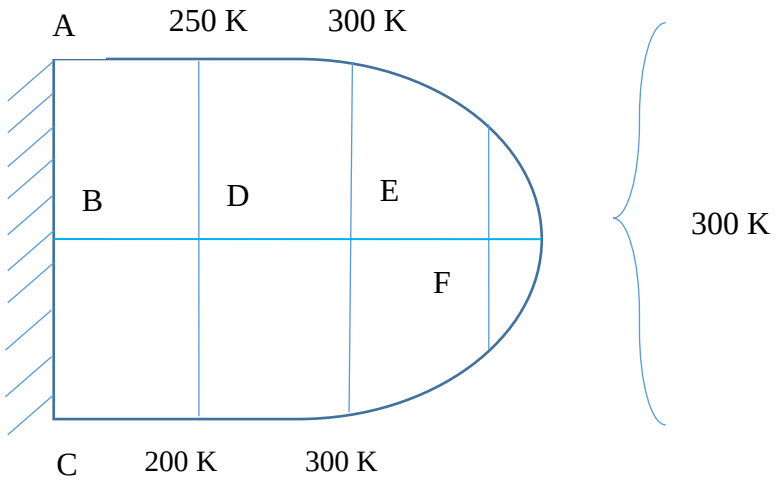
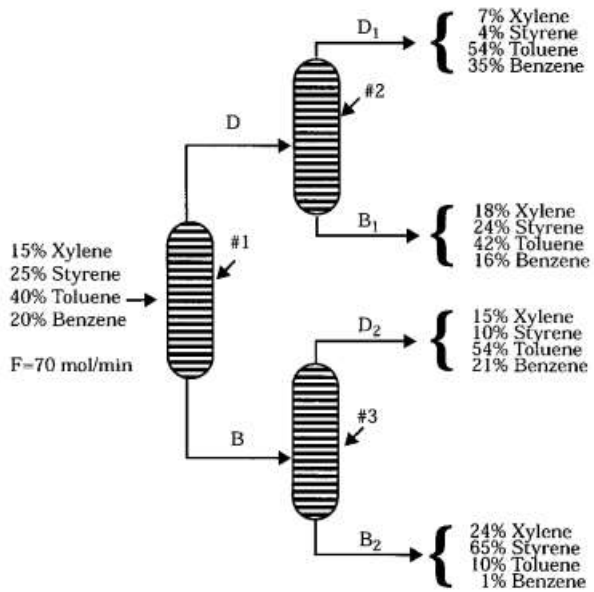
a = 0.0453 J m^3/mol^2, b = 0.0000571 m^3/mol, fugacity = 73.7 bar, R = 8.314.

Use Newton Raphson method.

2. The differential equation for diffusion and second order reaction in a spherical catalyst pellet is given by: **20**

$$D\left(\frac{d^2C}{dr^2} + \frac{2}{r}\frac{dC}{dr}\right) - kC^2 = 0$$

It is assumed that pellet is isothermal and therefore the rate constant is also fixed. D is effective binary diffusivity of A within the catalyst pallet. The concentration at surface of spherical pellet is 1 mol/m^3.The boundary conditions are: At r=1cm: C_A=1 and at r=0:

	C_A=10. The radius of pellet is 1 cm. Take rate constant k=10^{-3} m^3/mol-s and D=10^{-9} m^2/s. determine concentration of species A at r = 0.8cm of catalyst pallet	
3.	Find the temperatures at the interior nodes and at the insulated boundary for a flat plate shown in figure. The entire curved edge is kept at 300K Take Δx = 2 cm, Δy = 3 cm, α1= 1, α2 = 0.9, β1 = β2 = 0.8  	**20**
4A.	Find the flow rates D and B correct up to 3 decimal points  	**10**
4B.	In an attempt to understand the mechanism of the depolarization process in a fuel cell, an electro-kinetic model for mixed oxygen-methanol current on platinum was developed in the laboratory at FAMU. A very simplified model of the reaction developed suggests a functional relation in an integral form. To find the time required for 50% of the oxygen to be consumed, the time, T(s) is given by	**10**

	$$T = -\int_{1.22*10^{-6}}^{0.61*10^{-6}} \frac{6.73x + 4.3025 * 10^{-7}}{2.316 * 10^{-11}x}$$ Find the time required for 50% of the oxygen to be consumed. Use Romberg Integration	
5.	One dimensional transient heat conduction is taking place in a large flat steel plate of 2 cm thickness. If the initial temperatures (^{0}C) within the plate are given as $$u\,(x, 0) = 100 \sin \frac{\pi x}{2}$$ Find the temperatures as a function of x and t if both faces are maintained at 0^0C at any instant of time. Given α = 0.1515. Use Crank-Nicolson method	**20**