Registration Number:

MANIPAL UNIVERSITY

Vth Semester B.Tech (Chemical Engineering)

END SEMESTER EXAMINATION – NOV/DEC 2015

SUBJECT: Computational Methods for Chemical Engineers (CHE 311)

Time: 3 hrs **Max. Marks: 100**

- **Instructions to students**
  1. **Answer any FIVE FULL questions.**
  2. **Make suitable Assumption if required**
  3. **Answer should be correct to three places of decimal**

1	**A**	Write the algorithm of Regula falsi method to find the root of a non-linear equation	**4**
1	**B**	Determine the temperature distribution on the surface of a 4×4 cm^2 rectangular slab under steady state as shown in figure. T(x,0)=250 K, T(0,y)=280 K, T(4,y)= 275 K and T(x,4)=300 K.Take Δx = 1cm and Δy=1 cm	**8**
1	**C**	Use Multivariable Newton Raphson method find the value of x_1 and x_2 $f_1(x) = (2{x_1}^2 + {x_2}^2 - 8) = 0$ $f_2(x) = ({x_1}^2 - {x_2}^2 + x_1x_2 - 4) = 0$	**8**
2	**A**	Below is given the FT-IR (Fourier Transform Infra Red) data of a 1:1 (by weight) mixture of ethylene carbonate (EC) and dimethyl carbonate (DMC). Absorbance P is given as a function of wavenumber, m. Regress the above data to a second order polynomial P = a + b*m +c*m^2	**10**

Wavenumber *m* (cm-1)	804.184	827.326	846.611	869.753	889.038	892.895	900.609
Absorbance *P*	0.1591	0.0439	0.005	0.0073	0.0448	0.0649	0.1204

2	**B**	For the given reaction, $H_2O \longrightarrow H_2 + 0.5\ O_2$ The mole fraction 'x' of H_2O that dissociates can be represented by $$K = \frac{x}{1-x}\sqrt{\frac{2P_t}{2+x}}$$ Where K is the reaction equilibrium constant and Pt is the total pressure of the mixture. If P_t = 3 atm and K = 0.05 determine the value of 'x'.	**10**
3	**A**	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 $$T = -\int_{1.22\times10^{-6}}^{0.61\times10^{-6}} \left(\frac{6.73x + 4.3025\times10^{-7}}{2.316\times10^{-11}\,x}\right)dx$$ Find the time required for 50% of the oxygen to be consumed. Use single segment Trapezoidal rule and Simpson's 1/3rd rule. Compare the results. Find the true error, Et.	**10**
3	**B**	The specific volume of a superheated steam is listed in steam tables for various temperatures. For example, at a pressure of 3000 lb/in^2 , absolute. Determine 'v' at T=750°F.	**10**

T (^{o}F)	700	720	740	760	780
V ft^{3}lbm^{-1}	0.0977	0.12184	0.1406	0.15509	0.16643

4	**A**	Write a note on the importance of numerical methods in chemical engineering.	**5**
4	**B**	Discuss the different types of errors emcountered in numerical methods	**5**
4	**C**	For the reactions, A ⟷ B, A ⟷ D, B ⟷ C, B ⟷ D and C ⟷ D, in a batch reactor under constant pressure and temperature determine the equilibrium concentration of each component $-0.2\ C_A + 0.55\ C_B - 0.1\ C_C + 0.052\ C_D = 0$ $0.45\ C_B + 0.81\ C_C - 0.11\ C_D = 0$	**10**

		$0.3\ C_A + 0.8\ C_B + 0.04\ C_C - 0.1\ C_D = 0$ Constraint:- The concentration of all species must sum to one	
5		A rod of steel is subjected to a temperature of 100° C on the left end and 25° C on the right end. If the rod is of length 0.05 m, use Crank-Nicolson method to find the temperature distribution in the rod from t = 0 to t = 6 seconds. Use $\Delta x = 0.01$m, $\Delta t = 3$s. Given $k = 54\ W\ m^{-1}\ K^{-1}$ $\rho = 7800\ kg\ m^{-3}$ $Cp = 490\ J\ kg^{-1}\ K^{-1}$. The initial temperature of the rod is 20° C.	**20**
6		A vertical, cylindrical tank is filled with hot water at 80°C. The tank is insulated at the bottom alone and is exposed on its vertical sides and top to air at 25°C . The diameter of the tank is 50 cm and its height is 100 cm. The overall heat transfer coefficient, U, is 120 W/(m. K). Neglect the metal wall of the tank and assume water in the tank is perfectly mixed (i. e., uniform temperature). Calculate the elapsing time until the temperature drops to T = 30°C. Use R-K 4^{th} order method with h = 10^oC	**20**