Reg. No.										

MANIPAL INSTITUTE OF TECHNOLOGY

MANIPAL

A Constituent Institution of Manipal University

V SEMESTER B.TECH. (CHEMICAL ENGINEERING)

END SEMESTER EXAMINATIONS, NOV/DEC 2016

SUBJECT: COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING [CHE 3105]

REVISED CREDIT SYSTEM
(05/12/2015)

Time: 3 Hours MAX. MARKS: 50

Instructions to Candidates:

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

1A. **10**

Find the temperature distribution inside a square plate taking $\Delta x = \Delta y = 0.25$ if it follows the model

$$\pi^2 \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \qquad 0 \le x \le 1, \quad 0 \le y \le 1$$

With the boundary conditions of

$u(x,0) = 0$ $\quad u(x,1) = 2(1-x^2)$ $\quad 0 \le x \le 1$

$u(0,y) = \sin(\pi y)$ $\quad u(1,y) = e^{\sin(\pi y)}$ $0 \le y \le 1$

Use Gauss Seidel method

1B. **10**

Constant volume batch reactor with reaction A → B and 2nd order reaction can be modeled as

$$\frac{dX_A}{dt} = kC_{A0}(1 - X_A)^2$$

if $kC_{A0}=10^{-4}$ L/(mol-s), Calculate the time required to reach 90% conversion using composite Simpson's 1/3rd rule with n=5

2A. **16**

Find the Prandtl number of methane at 118 K using the data given below

T (K)	105	110	115	120
Cp (kJ/mol.K)	0.034853	0.035378	0.036016	0.036786

T (K)	91	100	105	120
μ (μPa.s)	3.6388	3.9976	4.1951	4.3034

T (K)	110	115	120	125
K (W/m.K)	11.350	12.062	12.811	13.604

2B. Discuss the importance of computational methods in engineering with applications **4**

3A.	Consider a continuous stirred tank reactor of diameter 1.25 m and height 2.6 m which is 80% filled initially with pure water at 20^{o}C. At time t=0, 15% salt solution at 25^{o}C is entering the CSTR with a mass flow rate of 15 kg/min and leaves at 10 kg/min. The CSTR is heated using steam at 250^{o}C in a coil with overall heat transfer coefficient 189 W/m^{2}K and effective heat transfer area 1.1 m^{2}. Calculate the concentration and temperature of the stream leaving the CSTR after 3 minutes using Runge-Kutta 4th order method.	**20**
4A.	Use Colebrook equation to calculate the friction factor for flow of a fluid in a pipe with $\varepsilon/D = 10^{-4}$ and $N_{Re} = 10^{5}$ $f = \frac{1}{[0.86\ln(\frac{\frac{\varepsilon}{D}}{3.7} + \frac{2.51}{N_{Re}\sqrt{f}}]^{2}}$ Use Regula Falsi method	**14**
4B.	The analysis of a two-stage distillation column to separate 1-butene from a mixture of 1-butene, butadiene and propane has resulted in the following coefficient matrix A, $A = \begin{bmatrix} 1 & 1 & 1 \\ 0.04 & 0.54 & 0.26 \\ 0.93 & 0.24 & 0 \end{bmatrix}$ Estimate the Dominant eigen value and Dominant eigen vector using Power method	**6**
5A.	Discuss the Convergence and Algorithm to solve a non-linear equation using Newton-Raphson method	**6+4**
5B.	One dimensional transient heat conduction is taking place in a large flat steel plate of 3 cm thickness. If the plate is initially kept at 15^{o}C and it is assumed that heat transfer is significant only in the *x*-direction, find the temperatures after 1 second if Δx =0.5 cm if left and right faces are maintained at 50^{o}C and 75^{o}C respectively at any instant of time. Given thermal diffusivity of steel 1.88*10^{-5} m^{2}/s. Use implicit method	**10**