Reg. No.										

MANIPAL INSTITUTE OF TECHNOLOGY

MANIPAL

(A constituent unit of MAHE, Manipal)

B.TECH. (CHEMICAL ENGINEERING)

END SEM EXAMINATIONS, November 2018

SUBJECT:COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING [CHE 3105]

REVISED CREDIT SYSTEM, **DATE: 21/11/2018**

Time: 3 Hours **Instructions to Candidates** **MAX MARKS: 50**

- Answer all questions **FULLY**.
- Missing data may be suitable assumed.

1A Solve for X by Gauss Elimination method when AX =B **4**

A>>					B>>	
	2	3	1	3		-4
	1	2	3	2		1
	3	1	2	3		-3
	3	4	5	3		-6

1B Thermistors are temperature-measuring devices based on the principle that the thermistor material exhibits a change in electrical resistance with a change in temperature. For a 10K3A Betatherm thermistor the relationship between the resistance R of the thermistor and the temperature is given by **3**

$$\frac{1}{T} = 1.129241\times10^{-3} + 2.341077\times10^{-4}\ln(R) + 8.775468\times10^{-8}\{\ln(R)\}^3$$

T is in Kelvin. Use the Newton-Raphson method to find the resistance R at 18.99°C. Take initial guess as R= 7,500 make 2 iterations

1C **3**

$$0 = \frac{1}{\sqrt{f}} + 2.0\log\left(\frac{\varepsilon}{3.7D} + \frac{2.51}{\mathrm{Re}\sqrt{f}}\right)$$

Calculate the friction factor with above equation using regular Falsi method if ϵ/D =0.0001 and Re =100,000. Use lower and upper limits as 0.02 and 0.05 respectively. Make 2 iterations.

2A The concentration of salt in a soap maker is givens as a function of time **6**

$\frac{dx}{dt} = 37.5 - 3.5x$,

Where x is the salt concentration. At time t =0, the salt concentration is 50 g/L. Using RK4 method find the concentration after 0.2 minutes. Use time step as 0.1 mins

2B Tom starts a bike from rest (zero speed) and travels at velocity at different time as given below. Find the distance travelled using Trapezoidal Rule **4**

t(min)	0	2	4	6	8	10	12	14	16	18	20
v(km/hr)	0	60	108	150	174	192	120	66	30	12	0

3A (8)

$$q = Q_m \frac{K_a C_{eq}}{1 + K_a C_{eq}}$$

The above Langmuir adsorption equation is to be fitted to the following data using linear regression. The problem can be converted to linear regression by plotting C_{eq}/q versus C_{eq}. Hence find the values of K_a (L/mg) and Q_m (mg/g).

C_{eq}(mg/L)	0.64	1.28	3.30	6.77	10.00	14.72	17.86	21.08
q(mg/g)	4.46	8.38	12.58	14.49	16.51	15.28	16.88	18.25

3B (2)

The vapor pressure of water increase with temperature. The values are tabulated below.

T °C	30	40	50	60
p_v (mm Hg)	31.8	55.3	92.5	149.4

Find the vapor pressure at 35 ^{0}C using Newton's Forward interpolation

4A (4)

Solve the system of simultaneous non-linear equations using Newton-Raphson method

$2x^2 + 3xy + y^2 = 3$

$4x^2 + 2xy + y^2 = 30$

Given $x_o = -3$, $y_o = 2$. Make 1 iteration.

4B (6)

The spread of a medicine in human bloodstream and gastrointestinal (GI) tract is described by the following set of two differential equations:

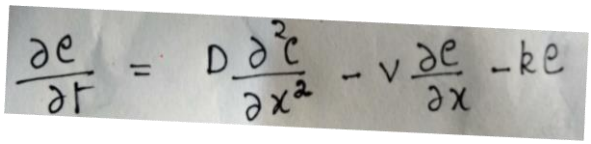
$$\frac{dx}{dt} = 3t^2 - 0.7x$$

$$\frac{dy}{dt} = 0.7x - 0.02y$$

x(t) and y(t) represent the distributions in the gastrointestinal tract and bloodstream, respectively. At t = 0, x = y = 0. Determine the profiles up to t = 2. $\Delta t = 1$. Use RK4 method.

5 (10)

Solve the equation for flow with reaction in a PFR using finite difference implicit method



where C is concentration in water (mol/L), t is time (s), v is pore water flow velocity (m/s), x is distance (m), D is the hydrodynamic dispersion coefficient (m^2/s), k is the first order reaction constant

The length of reactor is 1 m. dx= 0.25 m, dt =1 s. At time t=0, the initial concentration is 0 at all nodes except left boundary where the boundary condition is concentration is 1 mol/L. The other end of the rod has zero dispersion boundary condition.

Pore Velocity = 0.5 m/s, k=0.1 s^{-1}, Dispersion coefficient D = 0.2m/s^2, Take dx =0.25 m, Find the concentrations at the nodes at time =1 seconds.