



MANIPAL INSTITUTE OF TECHNOLOGY
MANIPAL

A Constituent Institution of Manipal University

Reg. No.

V SEMESTER B.TECH. (CHEMICAL ENGINEERING)

MAKE UP EXAMINATIONS, DECEMBER 2017

SUB: COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING [CHE 3105]

REVISED CREDIT SYSTEM

21/12/2017, 2-5 PM

Time: 3 Hours

MAX. MARKS: 50

Instructions to Candidates:

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

1A. Discuss the classification of partial differential equations with example **3**

1B. The friction factor f depends on the Reynolds number for turbulent flow in a smooth pipe according to the following relationship:

$$\frac{1}{\sqrt{f}} = -0.4 + \sqrt{3} \ln(Re\sqrt{f})$$

Find the friction factor for $Re = 10^5$ by using Secant method. Take $f_{i-1} = 0.005$ and $f_i = 0.01$

2A The rate of an enzymatic reaction is given by the following expression:

$$r = \frac{k \cdot S}{K_m + S}$$

The problem of estimating k and K_m can be converted to linear regression by inverting the above expression and defining: $x = 1/[S]$, $y = 1/r$. The following data was obtained in the lab:

[S]	1.233	0.540	0.442	0.258	0.198	0.162	0.130	0.128
r	5.970	3.319	2.253	2.547	1.493	1.182	1.095	0.869

Obtain $y_0 = a_0 + a_1 x$ and find the values of k and K_m .

2B What is the importance of the Numerical Methods in Chemical Engineering? **3**

3. A rectangular plate $9 \times 12 \text{ cm}^2$ is subjected to steady state two-dimensional heat transfer. Find the temperatures at all interior nodes taking $\Delta x = \Delta y = 3 \text{ cm}$. The boundary conditions are given by, $T(x, 0) = 250 \text{ K}$, $T(0, y) = 300 \text{ K}$, $T(9, y) = 420 \text{ K}$ and $T(x, 12) = 480 \text{ K}$ 10

4. 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

$$T = - \int_{1.22 \times 10^{-8}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx$$

Find the time required for 50% of the oxygen to be consumed. Use Romberg Integration

5. The rate of cooling of a body can be expressed as

$$\frac{dT}{dt} = -k(T - T_a)$$

where T =temperature of the body ($^{\circ}\text{C}$), T_a =temperature of the surrounding medium ($^{\circ}\text{C}$), and k is the proportionality constant (min^{-1}). Thus, this equation specifies that the rate of cooling is proportional to the difference in temperature between the body and the surrounding medium. If a metal ball heated to 90°C is dropped into water that is held at a constant value of $T_a=20^{\circ}\text{C}$, use Runge Kutta 4th order method to compute the temperature after 10 minutes if $k=0.25 \text{ min}^{-1}$. Use step size of 2 minute 10