



MANIPAL INSTITUTE OF TECHNOLOGY
MANIPAL

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V SEMESTER B.TECH. (CHEMICAL ENGINEERING)

END SEMESTER EXAMINATIONS, NOVEMBER 2017

SUBJECT: COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING [CHE 3105]

REVISED CREDIT SYSTEM
(17/11/2017)

Time: 3 Hours

MAX. MARKS: 50

Instructions to Candidates:

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

1A. Derive the Secant Method formula to find the root of an equation 3

1B. Acetone has a Vapour Pressure-Temperature relationship as given by,

$$P = \exp\left(C_1 + \frac{C_2}{T} + C_3 \ln(T) + C_4 T^{C_5}\right)$$

where, $C_1=69.006$, $C_2=-5599.6$, $C_3=-7.0985$, $C_4=6.2237 \times 10^{-6}$ and $C_5=2$. Calculate the temperature using Secant Method if the corresponding Vapour Pressure is 65000 Pa. Take $T_{i-1} = 300$ K and $T_i = 400$ K 7

2. Consider the density-temperature data for Acetaldehyde

T (K)	300	301	303	304	307	308	310
Rho (mol/dm ³)	3.941242	3.938763	3.933776	3.931269	3.923691	3.921146	3.916027

- i. Use Least Square regression to fit the data in to a second order polynomial and find the temperature at 306 K 4
- ii. Use Lagrange's Interpolation and estimate the temperature at 306 K 4
- iii. Discuss the results 2

3A Write the algorithm to estimate the solution of a system of linear equations using LU factorization method 3

- 3B Methane and oxygen react in the presence of a catalyst to form formaldehyde. Consider the heat capacity data for methane as $f(T)$ where T is in K. calculate the amount of heat needed to raise the temperature of 100 moles of methane from 300 to 900 K at constant pressure

$$f(T) = 4.568 - 8.975 \times 10^{-3}T + 3.631 \times 10^{-5}T^2 - 3.407 \times 10^{-8}T^3 + 1.091 \times 10^{-11}T^4$$

Use Romberg Integration

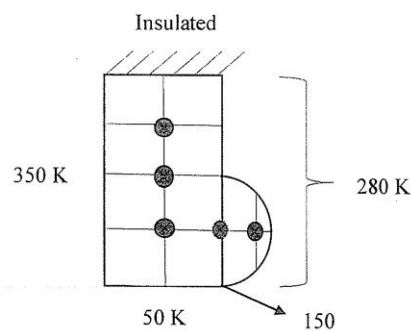
4. The dynamic model for a system of two non-interacting tanks is given by

$$A \frac{dh_1}{dt} = F_i - k_1 \sqrt{h_1}$$

$$A \frac{dh_2}{dt} = k_1 \sqrt{h_1} - k_2 \sqrt{h_2} + F_d$$

Where the cylindrical tank diameters are 0.15 m each, orifice constant $k_1 = k_2 = 3 \times 10^{-4}$. Determine the liquid level in both the tanks after two minutes taking step size of one minute, if $F_i = F_d = 8.333 \times 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $h_1(0) = 0.38 \text{ m}$ and $h_2(0) = 0.31$

5. Find the steady state temperature distribution on a two-dimensional plate as shown in figure



Take $\alpha_1 = 0.8$, $\alpha_2 = 0.2$, $\beta_1 = \beta_2 = 0.6$ and $\Delta x = \Delta y$.