## Code No: R41084

# IV B.Tech I Semester Supplementary Examinations, February/March - 2018 <br> COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING 

Time: $\mathbf{3}$ hours

Max. Marks: 75

## Answer any FIVE Questions <br> All Questions carry equal marks <br> *****

1 a) A polynomial $y=a_{0}+a_{1} x+a_{2} x_{2}+a_{3} x_{3}$ passes through point $(3,2),(4,3),(5,4)$ and $(6,6)$ in an $x-y$ coordinate System. Setup the system of equations and solve it for coefficients $a_{0}$ to $a_{3}$ by Gaussian elimination.
b) Find the molar volume of ammonia gas at 56 atm and 450 K using the Redlich Kwong equation of state, $\mathrm{Tc}=405.5 \mathrm{~K}, \mathrm{p}_{\mathrm{c}}=111.3 \mathrm{~atm}, \mathrm{a}=4.2527, \mathrm{~b}=0.02590$; units of a and b correspond to v in $\mathrm{l} / \mathrm{g}$ mol. Use Excel method.

2 Develop an algorithm to calculate vapor composition, liquid composition and liquid flow rates obtained after a P-T flashing of a given saturated feed liquid mixture of three components., its mole composition and Antoine's constants. termination criteria for flashing is $\sum_{1}^{3} \frac{F Z i}{(F-G) K i+G}=1$ where, $\mathrm{K}_{\mathrm{i}}=\mathrm{P} / \mathrm{Vp}_{\mathrm{i}}$

3 a) Frame mathematical expressions for MIXR, REAC, SEPR citing with few examples.
b) Explain the process simulation for Ammonia process with vapor-liquid equilibria and a purge stream.

4 a) Carbon dioxide from a fermentation process contains 1 mol percent ethyl alcohol. The alcohol needs to be removed by contact with water at 358C and 1 atm . The gas flow rate is $400 \mathrm{lbmol} / \mathrm{h}$ and the water stream is $620 \mathrm{lbmol} / \mathrm{h}$ and contains 0.02 mol percent alcohol. Determine the compositions out of the absorption column if you model it with 10 stages.
b) With a suitable example, explain the short cut methods used in multicomponent distillation.

5 a) Derive the design equation for Plug flow reactor from fundamentals, clearly stating the assumptions made.
b) Discuss about chemical reactors with mass transfer limitations using MATLAB.

6 a) A horizontal annulus is 27 ft long. The outside radius of the inner cylinder is 0.495 in , the inner radius of outer radius is 1.1 in . A $60 \%$ of aqueous soln. of sucrose $\left(\mathrm{C}_{12} \mathrm{H}_{22} \mathrm{O}_{\mathrm{n}}\right)$ is to be pumped through the annulus at $20{ }^{\circ} \mathrm{C}$. At this temperature the fluid density is $80.3 \mathrm{lb} / \mathrm{ft}$ and its viscosity is $136.8 \mathrm{lb} / \mathrm{ft} / \mathrm{hr}$. What is the volume rate of flow when the impressed pressure drop is 5.39 psi ?
b) Obtain the shell balance equation for laminar flow of liquid in an annulus. Also derive the expression for velocity profile in it.

7 a) Solve for the drag on a cylinder in a flowing stream with a uniform velocity profile upstream. Solve for Reynolds number from 1 to 100. Far from the cylinder use neutral boundary conditions (this will mimic an infinite domain). How does the qualitative behavior of the solution change with Reynolds number?
b) What are the various FEMLAB boundary conditions used in serpentine mixer? [3]

8 a) Discuss with an example the heat conduction in a hole using MATLAB.
b) Enlist the steps involved during dispersion in micro fluidic devices.

