*Ref. No.* Ex/PG/ChE/T/128C/2019

# M. CHEMICAL ENGINEERING 1st YEAR 1ST SEMESTER EXAMINATION, 2019
## SUBJECT: MODELLING AND SIMULATION OF CHEMICAL PROCESSES

Time: Three hours Full Marks 100

Answer question 1 and any three from the rest .

State all the assumptions. Assume any missing data.

| No. of Questions | | Marks |
|---|---|---|
| 1.(a) | (i)Explain the difference between a simulation and design problem<br>(ii)Consider that X and Y are the input and output variable matrix of a process G of an existing plant. Using the same process model G=g[X,Y,t], explain the difference between Simulation, Identification and Control problems. | (2+3) |
| 1(b) | (i)Consider single-stage multi-component isothermal flash distillation. Draw the process and define the variables. The feed temperature, composition, equilibrium temperature and pressure are known. Write the generalized model equations.<br>(ii)For composition independent equilibrium constant K values, simplify the model equations for the simulation of percent vaporization ($\psi$), liquid and gas phase composition.<br>(iii) Draw the information flow diagram for isothermal flash and write the algorithm of the numerical technique to be used for solving the percent vaporization ($\psi$).<br>(iv) A 100 kmol/h feed consisting of 10,20,30,40 mol% of Propane, n-butane, n pentane and n hexane, respectively is isothermally flash distilled at a constant pressure and temperature. At a flash temperature 366.5 K and 689.5 kPa the $K_i$ values (independent of composition) for Propane, n butane n pentane and n hexane are 4.2, 1.75, 0.74 and 0.34, respectively. Calculate the percent vaporization and liquid and vapor phase compositions using the algorithm in question (iii). (show the iteration wise results and convergence). | (20) |

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<tr><th>No. of Questions</th><th></th><th>Marks</th></tr>
<tr><td>2.</td><td>

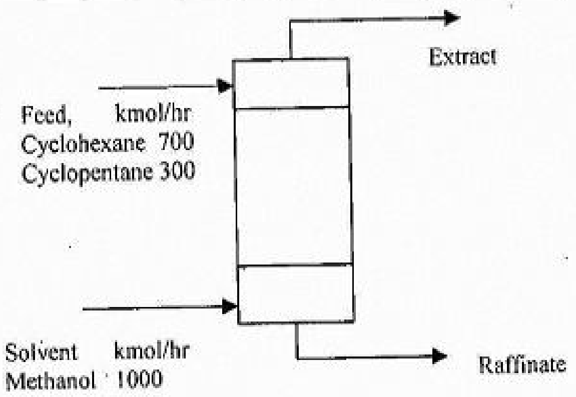


Fig.1 Schematic of an extractor

A mixture of cyclohexane (1) and cyclopentane (2) is to be separated by liquid-liquid extraction at 25°C with methanol (3). Phase equilibria $(K_i = \frac{\gamma_{iL}^{II}}{\gamma_{iL}^{I}})$ for this system may be predicted by NRTL or UNIQUAC equation.

It is desired to calculate the product rates, composition, and inter-stage flow rates and compositions for the conditions given in Fig.1 for N=3 equilibrium stage. Use Tomich method to model and simulate the process.

(i)Define variables and develop the model equations. Derive the matrix form. Draw the information flow diagram. Name the numerical techniques to be used for solving the equations and write the algorithm to solve the equations numerically.

(ii) Calculate the inter-stage flow rates considering temperature and composition independent K values: $K_1$=0.1, $K_2$=2 and $K_3$=0.5.

</td><td>(2+3)<br><br>(20)</td></tr>
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| 3. | Consider a multicomponent distillation column having 3 equilibrium stages, a partial condenser, a partial reboiler. The saturated liquid feed consisting of 3 components is introduced at the middle plate. Use Napthali Sandhlom procedure to model the system.<br>(i)Write the MESH equations of conservation of mass (M), energy (H) and of equilibrium (E) (for the above specific case). Group them by stage/tray. Use common notations. What is the number of equations?<br>(ii) Define the output variable matrix and function matrix.<br>(iii) In order to evaluate the corrections to the output variables use Newton Raphson technique. Show the formulation of Jacobian matrix. What is the structure of Jacobian matrix? Write the solution algorithm.<br>(iv)How do you compute the initial guesses? | (25) |
| 4. | Consider an isothermal tubular reactor with axial mixing (TRAM) with irreversible second order chemical reaction ($r_A=-kC_A^2$).<br>The non-dimensonalized steady state species balance equation and boundary conditions are as follows<br>$\frac{1}{Pe}\frac{d^2y}{dx^2}-\frac{dy}{dx}-Da\,y^2=0$<br>$\frac{dy}{dx}=Pe(y-1)$ at x = 0<br>$\frac{dy}{dx}=0$ at x = 1 | |

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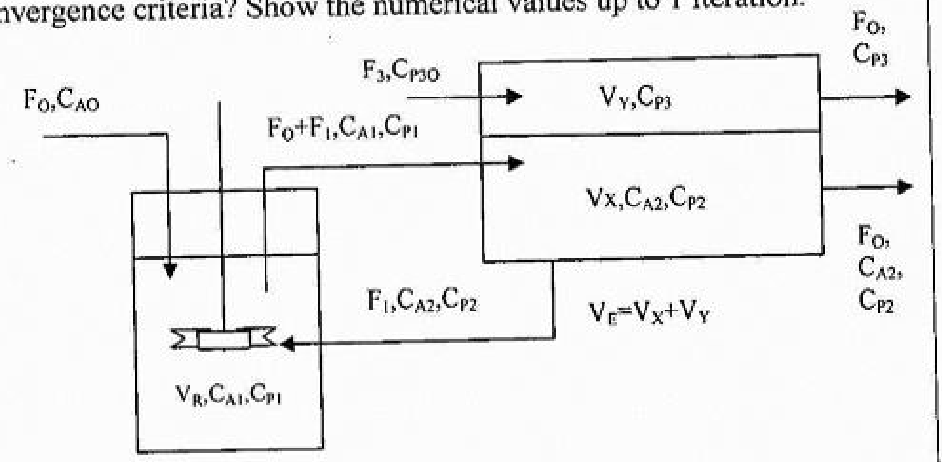
| 5. | Where Pe is the Peclet number for mass transfer and Da is the Damkholer number.Use finite difference technique to solve the equation.<br>(i)Discretise the governing equations with N internal grid points. Incorporate the boundary conditions.<br>(ii)Write the matrix form for N=3 (four grid point equispaced) for Pe=5, Da=2. Evaluate the coefficient matrix. What is the form of the matrix?<br>(iii)Write the algorithm to solve y at different grid points. What is the convergence criteria? Show the numerical values up to 1 iteration.<br><br><br>Fig.2 Integrated reactor and liquid -liquid extractor<br><br>Often it is necessary to extract a product, which impedes a reaction in a CSTR. This is accomplished with an integrated liquid-liquid extraction unit (refer to Fig. 2). Consider a CSTR with reaction $A \longrightarrow P$<br>The kinetics exhibit inhibition by the product: $-r_A = r_p = k_1 C_A/[1+C_p/K_I]$, where $k_1$ is the reaction constant and $K_I$ is the inhibition constant.<br>(i) Develop the transient model equations for the CSTR and integrated extractor. | (25) |

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| | (ii)Values of inlet feed rate and composition to CSTR, inlet solvent rate and composition to extractor are known. $V_R$ and $V_E$ are known. You are asked to simulate the product rate of the extractor and the conversion fraction, product produced/reactant fed for a fixed recycle ratio. Identify the variable matrix and function matrix. Write the step by step algorithm for solving the simultaneous ODEs using Crank Nicholson technique. (iii)How do you check the steady state solution from the above method of solution? (iv)Write down the steady state balance equation for the CSTR and the integrated extractor. Write the algorithm to solve algebraic equations. | (25) |
| 6. | Consider an isothermal catalytic packed bed reactor with spherical porous catalyst. Reactant 'A' simultaneously diffuses through the catalyst and reacts. Consider a first order reaction. (i)Consider Ws is the rate of consumption of reactant A per catalyst at any axial position of the packed bed at any time and $n_d$ is the number density of the catalyst. Develop the species (A) balance equation for the packed bed including Ws which is a function of local species concentration ($C_A\alpha$). What kind of equation is it? (ii) In order to evaluate Ws it is required to consider a single spherical porous catalyst and evaluate the radial concentration profile of species A. Derive the isothermal species balance equation and write the boundary conditions. Use convective boundary condition at r=R: $-D_{eff}\, dC_A/dr=kc(C_A-C_{A\alpha})$ and at r=0, $dC_A/dr=0$ Non dimensionalize the equation and boundary conditions. (iii)Discretize the derived nondimensional equation in part (ii) using finite difference using N internal equally spaced grid points. What is the discretized form of governing equation at r=0, i=1? Incorporate the boundary conditions. Derive the matrix form for solving the concentration profile. (iv) Write the algorithm for solving the matrix. (v)How do you numerically evaluate Ws? | (25) |