MODELING SIMULATION & OPTIMIZATION
(CHEN 4103)

Time Allotted : 3 hrs **Full Marks : 70**

Figures out of the right margin indicate full marks.

Candidates are required to answer Group A and any 5 (five) from Group B to E, taking at least one from each group.

Candidates are required to give answer in their own words as far as practicable.

Group – A
(Multiple Choice Type Questions)

1. Choose the correct alternative for the following: **10 × 1 = 10**

(i) A and B are reacting where, B is a valuable chemical. An ideal distribution of chemicals would involve
(a) using excess B (b) using excess A
(c) using an inert species C
(d) using stoichiometric amounts of A and B.

(ii) For transport of free flowing solids we can use:
(a) Apron conveyor (b) Belt conveyor
(c) Pneumatic conveyor (d) Flight conveyor.

(iii) Selectivity in zeolite adsorbents is controlled by
(a) adsorption equilibrium (b) adsorption temperature
(c) adsorption pressure (d) molecular sieving.

(iv) Distillation column pressure is generally set according to
(a) nature of the components
(b) cooling water temperature in condenser
(c) reboiler heat duty (d) boiling point of light key.

(v) Outer approximation method is valid for
(a) nonlinear optimization problem
(b) linear optimization problem
(c) optimization problem with saddle point
(d) either (a) or (c).

(vi) Initial basic solution in a simplex method is obtained for the
(a) coefficient to the variable in the constraints
(b) coefficient to the variable in the objective function
(c) slack variable
(d) process variable.

(vii) For developing heads upto 3200 ft we should use a
(a) diaphragm pump (b) centrifugal pump
(c) plunger pump (d) peristaltic pump.

(viii) For a reactive distillation operation which type of tray is most suitable?
(a) Bubble cap (b) Valve (c) Sieve (d) Linde.

(ix) For an objective function f(x) the function is called positive semidefinite if
(a) $x^T\nabla^2 f(x)x > 0$ (b) $x^T\nabla^2 f(x)x \leq 0$
(c) $x^T\nabla^2 f(x)x \geq 0$ (d) $x^T\nabla^2 f(x)x < 0$.

(x) Equality constraints for any distillation process optimization problem mainly consists of
(a) mass balance, energy balance and product purity
(b) environmental regulations, energy balance and product purity
(c) mass balance, utility capacity and product purity
(d) mass balance, energy balance and equilibrium equations.

Group – B

2. (a) What are the characteristics of a flowsheet module? Which flowsheeting algorithm is generally followed in simulation softwares like ASPEN, DWSIM etc.?

(b) Suppose the following table is obtained after calculation of output flow rates in a distillation column separating Benzene, Toluene and Xylene:

Component	Input flow	Top output flow	Bottom output flow
Benzene	100 mol	97 mol	1 mol
Toluene	100 mol	95 mol, 2 mol Benzene	5 mol
Xylene	100 mol	7 mol	93 mol
Heat	20,000 kJ	13,000 kJ	7,000 kJ

Write an expression for Benzene top outflow as a linear function of input flows of all the components.

(3 + 1) + 8 = 12

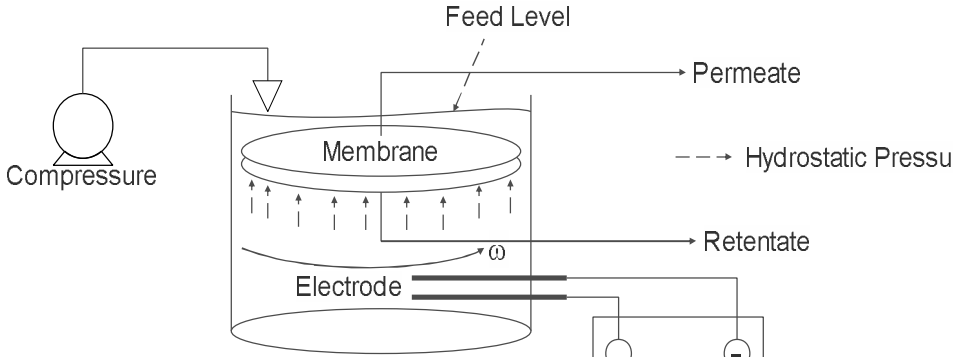

Fig. 1

Fig.1 shows a membrane separation process, where the trans-membrane pressure was generated through compressing the feed (dissolved A and B) within the module drum. To avoid fouling a battery is connected to electrodes inserted within the feed drum. However, the battery operation is intermittent depending on the membrane performance judged by the permeate flux over time. The flux (J) and running time (t) is related as $J=J_0\exp(-t)$. Battery energy calculation is given by = Volt × Amp-Hour. Compressor energy involved in the process is E_C, where this energy consumption is proportional to the trans-membrane pressure. When the membrane is kept in washing the compressor is being switched off. In washing the battery may or may not be operated depending on the extent of fouling. Develop a MINLP model for the entire process considering minimum energy consumption as an objective function. Based on the optimization model discussed above provide the algorithm for outer approximation. Membrane can't be operated for more than 3 h and the volume concentration factor can't be more than 2. The rejection must be in between 80-85%, when the concentration of A in the feed can't be more than 50 ppm. If it is found that the steady state flux achieved within 2 h, the voltage has to be increased by 20%.

(8 + 4) =12

3. (a) A vapour feed is being fed to a catalytic tubular reactor from where a vapour product is coming out. The feed contains some inerts which negatively impact the catalyst performance. The reaction is highly exothermic. The cost of separation of the inerts from feed is Rs. 2000/g while the cost of separation from the product is Rs. 500/g. Draw the flow-sheet of the process and justify it.

(b) A pump is to be installed in a pipeline to pump 400 gpm of liquid water to a distance of 300 ft. There are 2 control valves in the pipeline and at one point, the pipeline is elevated by 5 ft. The pump draws water from the surface of a tank open to atmosphere and the discharge pressure is fixed to be 1000 psi. What horsepower pump will be required?

6 + 6 = 12

Group – C

4. (a) What are the assumptions of the ideal PFR reaction model?

(b) What are the main types of reactor models available in simulation softwares like ASPEN and DWSIM? Explain each model and its applicability in reactor design.

3 + (3 + 6) = 12

5. (a) What is the significance of attainable region in reactor network synthesis? What is meant by a non-convex attainable region?

(b) For the reaction scheme given below, write the equations that need to be solved for constructing a PFR trajectory. How can a PFR trajectory be expanded?

$$A \overset{k_1, k_2}{\Leftrightarrow} B \overset{k_3}{\rightarrow} C$$

$$2A \overset{k_4}{\rightarrow} D$$

(3 + 2) + (3 + 4) = 12

Group – D

6. (a) What type of distillation column (tray/packed) will you select for an operation which involves: i) systems with large temperature fluctuations ii) large column diameter iii) fouling liquids?

(b) In case of a liquid-liquid extraction operation which type of equipment will you select for i) operation which requires only a few theoretical stages ii) operation requiring large number of stages.

(c) Mention four important factors which influence the selection of the type of dryer.

6 +2 + 4= 12

7. (a) Briefly explain the algorithm for selection of condenser type and setting distillation column pressure.

(b) Write a note on membrane separation by gas permeation.

8 + 4 = 12

Group – E

8. (a) Minimize the function $f(x) = x^4 - x + 1$ using Newton's method taking the starting point for optimum search at x=3 (show atleast 2 iterations).

(b) The production cost of a chemical A is Rs. 1000/kg and chemical B is Rs. 1200/kg. It has been seen that chemical A in a day can't be produced more than 34 kg and B in day can't be produced more than 14 kg per day. The hours and manpower consideration for the production of chemical A and B are given below.

Hours Consideration:

A requires 2 hrs per kg and B requires 3 hrs per kg production. The total production cost can't be more than 60 hrs.

Manpower Consideration:

A requires 10 people per kg and B requires 5 people per kg production. The total employee strength there is 200 and some of them may be transferred to other production if the plant doesn't have any requirement.

Using simplex method find out the production amount per day for A and B with the minimum production cost.

3 + 9 =12

9.