2013-14
M.TECH. (SUMMER SEMESTER) EXAMINATION
(Chemical Engineering)
Mathematical Methods in Chemical Engineering
(CH-612)

Maximum Marks: 60 CREDIT 04 Duration: Three Hours

Answer the questions in the order stated in the question paper. Assume suitable data if missing. Notations used have their usual meaning.

Q.No. Question M.M.

1(a) State and explain what do you understand by orthonormal and orthogonal vectors. [05]

OR

1(a') Categorize the following equations in terms of linear/non linear/homogenous/non homogenous.

(i) \( \frac{dx}{dt} = k \sin \omega t - x \)

(ii) \(-k \frac{d^2 T}{dx^2} = \mu \left( \frac{V}{b} \right) \)

1(b) Find whether the following sets of vectors are dependent or independent: [10]

(a) \((2,0,4)^t, (2,0,8)^t, (2,1,3)^t, (4,1,5)^t\)

(b) \((2,1,4)^t, (6,3,12)^t\)

OR

1(b') if \(d(u,v) = \sum |u_i - v_i|\) is a suitable metric on \(\mathbb{R}^n\) then,\(d(u,v) = \sum |u_i - v_i|\) should satisfy the axioms for all vectors in \(\mathbb{R}^n\), take \(u = (1,1,2,0)^t\) and \(v = (2,2,1,0)^t\)

State and check that all the axioms are satisfied here with.

Contd......2
2. Solve the following differential equation
\[
\frac{dx}{x + t} = \frac{dy}{y} = \frac{dt}{t + y^2}
\]

OR

2'. For the following general Pfaffian Differential Equation obtain the general solution.
\[
\sum_{i=1}^{n} (F_i \partial x_i) = 0
\]

3. Find the values of \( x, y \) and \( z \) so that the following function is an optimum.
\[
F(x, y, z) = xyz
\]
Subject to the following constraint
\[
G(x, y, z) = xy + 2xz + 2yz - 108
\]

4. A fluid of concentration \( C_{A1} \) flows at a rate of \( q_1 \) into a tank where the component A in the fluid decomposes by first order reaction. Initially the tank contains \( V_0 \) of the fluid with a concentration of \( C_{A0} \). With the ideal stirring condition, the reacting mixture flows out at a rate \( q \). Suggest a step by step mathematical treatment for the above problem and develop an expression for the outlet concentration as a function of time.
Answer all the questions. Assume suitable data if missing. Notations used have their usual meaning.

Q.No.  
1(a). With the help of a neat diagram explain briefly the steps involved in solid-fluid heterogeneous catalytic reactions. [05]

1(b). What is catalyst deactivation and what are its different modes? Name various strategies which are adopted to offset the decline in activity of catalyst in continuous flow reactors? Describe any one of them in detail. [10]

OR

1'(a). Write a short note on adsorption and its types. Derive the Langmuir adsorption isotherm equation for multi-component adsorption. [05]

1'(b). To remove oxides of nitrogen (assumed to be NO) from automobile exhaust, a scheme has been proposed that uses unburned carbon monoxide (CO) in the exhaust to reduce the NO over a solid catalyst, according to the reaction

\[ \text{CO} + \text{NO} \rightarrow \text{Products (N}_2, \text{ CO}_2) \]

Experimental data for a particular solid catalyst indicate that the reaction rate can be well represented over a large range of temperatures by

\[ -r_N = \frac{kP_N P_C}{(1 + K_1 P_N + K_2 P_C)^2} \]

where $P_N =$ gas phase partial pressure of NO

$P_C =$ gas phase partial pressure of CO

$k, K_1, K_2 =$ Coefficients depending on temperature

Contd.......2
Propose an adsorption-surface reaction-desorption mechanism that will explain the experimentally observed kinetics. A certain engineer thinks that it would be desirable to operate with a very large stoichiometric excess of CO to minimize catalytic reactor volume. Do you agree or disagree? Explain.

2. The catalytic oxidation of carbon monoxide is taking place in the presence of a Pt catalyst in a fluidized bed reactor. The rate of reaction of CO ($-r_{CO}$) varies with the concentration of CO as shown in Fig. 1, and the stoichiometry of this oxidation reaction is given by:

$$CO + \frac{1}{2}O_2 \rightarrow CO_2 ; \epsilon_{CO} \neq 0$$

Develop the dynamic model of this fluidized bed reactor and show that at most three steady states may exist. Assume that excess oxygen is used. Also carry out the stability analysis of this system and describe in detail the procedure to remove the low and intermediate conversion steady states.

![Graph showing variation of oxidation rate of CO with its concentration](image)

**Figure 1:** Variation of oxidation rate of CO with its concentration

3(a). Calculate the mass flux of reactant A to a single catalyst pellet 1 cm in diameter suspended in a large body of liquid. The reactant is present in dilute concentrations, and the reaction is considered to take place instantaneously at the external pellet surface (i.e., $C_{AS} = 0$). The bulk concentration of the reactant is 1.0 $M$, and the free-

Contd.…….3
system liquid velocity is 0.1 m/s. The kinematic viscosity is 0.5 centistoke (1 centistoke = $10^{-6}$ m$^2$/s), and the liquid diffusivity of A is $10^{-10}$ m$^2$/s.

3(b). Develop the performance equation of a packed bed reactor operating at steady state and sustaining a mass transfer limited reaction. Also find the expression for concentration profile assuming negligible dispersion in axial direction.

OR

3'. In many heterogeneous reactions, the gas-phase reactant reacts with a species contained in an inert solid matrix. One such reaction is encountered in the regeneration of fouled catalyst particles, e.g., oxygen reacts with carbon present in catalyst particles (say spherical shaped) that have been deactivated by fouling. Carbon is first removed from the outer edge of the pellet and then in the final stages of the regeneration from the center core of the pellet. Using the principles of shrinking core model and the quasi steady state assumption, find the expression for time that is required to consume all the carbon present in the fouled spherical catalyst pellet.

4(a). What is Weisz-Prater criterion and why is it used? Using this criterion, estimate the Thiele modulus and effectiveness factor for an elementary heterogeneous catalytic reaction $A \rightarrow B$, which is occurring in a spinning basket reactor containing two different-sized pellets. The reactor is operating at sufficiently high rotation speeds that external mass transfer resistance can be neglected. How small should the pellets be made to virtually eliminate all internal diffusion resistance (say $\eta = 0.95$)? The results of two experimental runs made under identical conditions are as given in Table 1.

### Table 1: Results of experimental runs made under identical conditions

<table>
<thead>
<tr>
<th>Run No.</th>
<th>Measured Rate (mol/g cat.s) $\times 10^3$</th>
<th>Pellet Radius (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.0</td>
<td>0.01</td>
</tr>
<tr>
<td>2</td>
<td>15.0</td>
<td>0.001</td>
</tr>
</tbody>
</table>

4(b). Write a short note about the two parameter models used to describe real reactors. How are these parameters evaluated?
Answer all the questions.  
All parts of a question should be answered in a proper sequence.  
Notations used have their usual meaning.

Q.No. | Question                                                                                                                                                                                                 | M.M.  
--- | ---                                                                                                                                                                                                     | ---  
1(a) | Discuss briefly three important regions of flow if vapour and liquid phases are flowing in a horizontal and in a vertical tube.                                                                  | [04]  
1(b) | Define and discuss the following dimensionless numbers in the study of transfer operations:                                                                                                               | [04]  
   (i) Jakob number (ii) Biot number (iii) Prandtl number and (iv) Schmidt number                                                                                                                             |               
1(c) | Derive an expression to determine the thickness of thermal boundary layer, $\delta$, when liquid is flowing in a tube and heated from outside.                                                          | [07]  
2(a) | Discuss with the help of a neat diagram of experimental set-up, the procedure of calculating boiling heat transfer coefficient for pure liquids.                                                     | [09]  
2(b) | Enumerate recent techniques of enhancement of boiling heat transfer coefficient? Explain three methods to achieve the same.                                                                                | [06]  

OR

2'(a) | How do the various parameters affect the performance of a finned surface? Explain them clearly.                                                                                                         | [05]  
2'(b) | Discuss the mechanism of enhanced boiling heat transfer.                                                                                                                                               | [05]  
   A steel tube is fitted with transverse circular steel fins of constant cross section, It has the following dimensions:                                                                                   |               
   i) Tube O.D. = 58 mm (ii) Fin dia. = 70 mm (iii) Fin thickness = 2.84 mm and (iv) No. of fins = 245/m.                                                                                             |               

Contd......2
2(c) Determine the heat loss per unit length of the tube when surface temperature is 380K and the surrounding temperature is 280K. The heat transfer coefficient between the fin and gas is 35 W/m²K and thermal conductivity is 48 W/m K.

3(a) How will you select an industrial heat exchanger for a process industry? Explain them clearly with suitable reasons.

3(b) Briefly discuss applications of any two thermal fluids in process industries?

OR

3(b') Discuss the design and applications of Spiral Tube heat exchanger for chemical industries.

3(c) Explain clearly the effect of feed temperature, and steam pressure at the performance of an evaporator

OR

3(e') What are important parameters which affect studies of heat transfer and pressure drop in a fluidised/packed bed.

4(a) Predict the diffusion coefficient of acetone in water at 30 °C and 60 °C using Wilke-Chang equation. The experimental value is reported to be 1.30x10⁻⁹ m²/s at 30 °C. The other data are as follows:

(i) Viscosity of water at 30°C = 0.88 x 10⁻³ Pa-s.
(ii) Viscosity of water at 60°C = 0.53 x 10⁻³ Pa-s.
(iii) Association parameter for water = 2.65

4(b) An ethanol-water solution in the form of a stagnant film of 2.0mm thickness at 300 K is in contact at one surface with an organic solvent in which ethanol is soluble and water is insoluble. At point 1, the cone. of ethanol is 17.0 wt. % and solution density ρ₁ is 971.8 kg/m³. At point 2, the cone. of ethanol is 6.5 wt. % and ρ₂ = 987.5 kg/m³. The ethanol diffusivity is 0.78 x 10⁻⁹ m²/s. Calculate the flux at steady state.
Answer all the questions. Assume suitable data if missing. Notations used have their usual meaning. Use of transport phenomena equations is allowed.

Q.No.  Question  M.M.
1. Consider a series of \( m \) CSTRs in which an irreversible liquid phase reaction: \( A \rightarrow B \) \((-r_A = kC_A^n)\), is taking place. Flow control valves are installed on the outlet of each reactor and follow the relationship \( F_i = f(V_i) \), where \( F_i \) is the volumetric flow rate from \( i^{th} \) reactor and \( V_i \) is the holdup in \( i^{th} \) reactor. The process is isothermal, however, the holdup in each CSTR is varying depending on the net flow in the reactor. Develop the dynamic model of this system and specify the assumptions used. [15]

OR

1'. Consider a single component vaporizer sketched in Fig. 1. The liquid is fed at a volumetric flow rate \( F_0 \) into a pressurized tank to hold the liquid level in the tank. Heat is added at a rate \( Q \) to hold the desired pressure in the tank by vaporizing the liquid at a rate \( W_p \) (mass per time). Heat losses and the mass of the tank walls are assumed negligible. Gas is drawn off the top of the tank at a volumetric flow rate \( F_v \). Develop the dynamic model of this vaporizer. Assume that the vapour phase behaves as an ideal gas and its dynamics can be neglected. The relationships between inlet flow and holdup, and the heat input and pressure are respectively given by:

\[
Q = f_1(P) \quad \text{and} \quad F_0 = f_2(V_L)\]

Contd......2
2. A radial flow reactor with its inner walls coated with a catalytic agent is shown in Fig. 2. An isothermal gaseous phase first order catalytic reaction \( \text{A} \rightarrow \text{B} \) is taking place on the inner surface of the walls. The volumetric flow rate and the reactant concentration of the feed are \( v_0 \) and \( C_{A_0} \), respectively. The flow between the plates is laminar, and the steady state and isothermal conditions are prevailing. Develop the model equation for this reactor along with relevant conditions. It should be noted that the velocity will not be constant along radial direction. The density of the fluid mixture may be assumed to be constant throughout the system.

Figure 2: Radial flow reactor
3(a). Develop the maximum gradient model of a packed bed adsorber by assuming that the process of adsorption is fast and that the local equilibrium exists near the solid particles; the equilibrium relation follows a linear relationship between the solid phase composition and solute composition. Also specify the relevant ICs and BCs.

3(b). A Newtonian fluid of constant density and viscosity is contained in a very long horizontal square duct of cross sectional area $a^2$ and length $L$. Initially the fluid is at rest and at time $t=0$, a pressure gradient $(P_0-P_f)/L$ is impressed on the system. Develop the model equation describing the transient velocity profile of flowing fluid. Also state the relevant assumptions and associated conditions used.

OR

3'. Consider the steady flow of a Newtonian fluid over a sharp edged and very thin plate as shown in Fig. 3. The velocity and temperature of the fluid away from the boundary layer are denoted by $U_\infty$ and $T_\infty$, respectively. The fluid properties are assumed to be constant and the viscous dissipation can be neglected. Develop the transport phenomena based microscopic model for the flow in boundary layer. Also carry out the scaling of resultant equations and order of magnitude analysis to extract the maximum information without solving the equations.

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**Figure 3: Boundary layer flow over a sharp edged thin plate**

Contd......4
4. Develop the mathematical models for any two of the following systems. Also state the relevant assumptions and allied conditions.

(i) Start-up operation of a double pipe heat exchanger with a counter current flow arrangement (hot fluid is flowing in the inner pipe and the cold fluid is flowing the outer pipe).

(ii) Unsteady state axial dispersion model of a tubular chemical reactor running under isothermal conditions.

(iii) Dissolution of a spherical pill inside stomach.