M. Tech. –II (Chemical Engineering) (CBCS – 2015 Course) :
WINTER - 2018
SUBJECT : MODELLING & SIMULATION OF CHEMICAL PROCESSES

Day : Monday
Date : 19/11/2018

W-2018-3157

Time : 11.00 AM TO 02.00 PM
Max. Marks : 60

N.B.:

1) All questions are **COMPULSORY**.
2) Figures to the right indicate **FULL** marks.
3) Use of non-programmable **CALCULATOR** is allowed.
4) Answers to both the sections should be written in **SEPARATE** answer books.

SECTION – I

Q.1 **a)** Consider CSTR of perfectly mixed liquid where component A reacts reversibly to form product component B **[05]**

$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$.

Write the total and component continuity equation.

b) Consider jacketed tubular reactor in which the reaction $A \xrightarrow{k_1} B$ takes place. Assume that no radial gradients are present in velocity, concentration or temperature. Heat can be transferred from the process fluid reactants and products at temperature T to the metal wall of the reactor at temperature T_m. The heat is subsequently transferred to the cooling water. Write the energy equation for the tubular reactor. **[05]**

OR

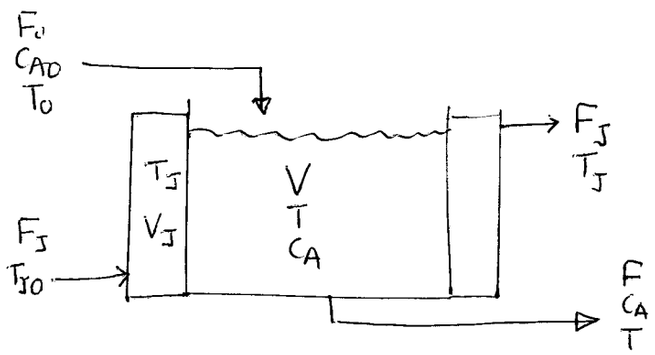
Discuss the following equations used in the formulation of models: **[10]**

i) Equations of state
ii) Chemical equilibrium
iii) Phase equilibrium

Q.2 Consider a non-isothermal CSTR in which temperature can change with time. An irreversible exothermic reaction is carried out in a single perfectly mixed CSTR **[10]**

$A \xrightarrow{k} B$.

The reaction is n^{th} order in reactant A and has a heat of reaction λ. Negligible heat losses and constant densities are assumed.



Develop a mathematical model stating:

i) Reactor total continuity
ii) Reactor component continuity
iii) Reactor energy equation
iv) Jacket energy equation considering perfectly mixed cooling jacket

OR

P.T.O.

a) Develop a mathematic model for mixing vessel with reaction $A + B \underset{k_R}{\overset{k_F}{\rightleftharpoons}} C + D$. **[05]**

b) Discuss simple modeling principles that must be observed while constructing a mathematical model. **[05]**

Q.3 Develop a mathematical model for three CSTR in series with variable holdups. Assume that reaction is n^{th} order in reactant A. Check the degree of freedom of the system and comment whether system is sufficiently specified or under specified. **[10]**

OR

Develop (a) steady state and (b) practical mathematical model for multicomponent flash drum. Draw a neat sketch and clearly mention the assumptions made. **[10]**

SECTION – II

Q.4 a) What is density function theory? How it is used in simulation? **[05]**

b) Why vibrational analysis is important in simulation? **[05]**

OR

a) How to define basic sets in simulation? What is their importance? **[05]**

b) What is the importance of molecular dynamics? **[05]**

Q.5 How parameter sensitivity analysis is done? Why it is important in modeling and simulation? **[10]**

OR

What are the solution methods for initial value problems? How they are used in simulation and optimization? **[10]**

Q.6 What are deterministic and stochastic approaches in process modeling and simulation? Explain in detail. **[10]**

OR

What is Fuzzy logic? How it is used in process modeling and simulations? **[10]**

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