M. TECH. –II (CHEMICAL ENGINEERING) (CBCS – 2015 COURSE) : SUMMER - 2018

SUBJECT : MODELLING & SIMULATION OF CHEMICAL PROCESSES

Day : **Monday** **S-2018-3019** Time : **11.00 AM TO 02.00 PM**
Date : **11/06/2018** 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)** Write the component continuity equations for a CSTR and tubular reactor with reversible reaction $A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$. **[05]**

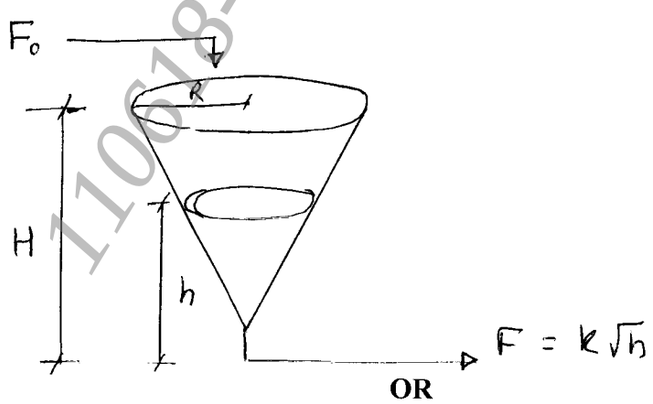
b) What are the principles of formulation of any mathematical model? **[05]**

OR

a) Consider a CSTR with a cooling coil inside the tank that can remove the exothermic heat of reaction λ. The reaction is $A \xrightarrow{k_1} B$, where the rate of heat generation due to reaction is the rate of consumption of A times λ. **[05]**
$Q_G = -\lambda\, VC_A\, k$.
Develop a mathematical model.

b) Compare and contrast the following: **[05]**
i) Lumped parameter Vs. Distributed parameter model
ii) Steady state Vs. Dynamic model.

Q.2 A fluid of constant density ρ is pumped into a cone-shaped tank of total volume $H\pi R^2/3$. The flow out of the bottom of the tank is proportional to the square root of height h of liquid in the tank. Derive the equations describing the system. **[10]**



OR

Consider a continuous stirred tank reactor (CSTR) in which following reaction is carried out **[10]**

$$A + B \underset{k_1'}{\overset{k_1}{\rightleftharpoons}} C + D$$

$$C + B \underset{k_2'}{\overset{k_2}{\rightleftharpoons}} E$$

$$A + E \underset{k_3'}{\overset{k_3}{\rightleftharpoons}} F$$

Develop a mathematical model for CSTR.

P.T.O.

Q.3 Develop a mathematical model for non-ideal distillation column with NC components, non equimolar overflow and inefficient trays. Clearly state the assumptions and define Murphree vapor phase efficiency. **[10]**

OR

Develop a mathematical model for batch reactor. Consider that first order consecutive reaction takes place in the reactor. **[10]**

$A \xrightarrow{k_1} B \xrightarrow{k_2} C$.

It is required to state the following equations while formulating the model:

i) Total continuity equation.
ii) Component continuity equation for A and B.
iii) Energy equation of process and metal wall.
iv) Heating phase – total continuity and energy equation of steam vapor.

SECTION – II

Q.4 What are Ab-initio methods of simulation? Explain in detail. **[10]**

OR

Define ensembles and fluctuations in simulation. What is ensemble averaging? How it is used in simulation? **[10]**

Q.5 Why parameter estimation is important? What are the methods of parameter estimation? **[10]**

OR

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

Q.6 What is statistical determination theory? How it is used in process modeling and simulation? **[10]**

OR

What is genetic algorithm? How it is used in process modeling and simulation? **[10]**

* * * *