National Institute of Technology Hamirpur
Department of Chemical Engineering

B. Tech.: 7th Semester

End Semester Theory Examination 2020

CHD-411: Process Modeling and Simulation

Date: 7th December 2020 | Time: 14:00 to 16:00 | Max. Marks: 50

Note: *(i) Answer all the questions (ii) Write proper valid assumptions, (iii) while solving the problems intermediate steps are very-very important, (iii) Make necessary assumptions for missing data, if any.*

Q.1(a) Explain the difference between lumped parameter model and distributed parameter model with appropriate examples. **5**

(b) Write any four constitutive relationships with proper explanation of terms and units. **2**

Q.2 Explain the Linearization technique and apply it to Arrhenius equation. **4**

Q.3 What is the meaning of degrees of freedom for any processing system? The mathematical model of a stirred tank heater is given by **5**

$$A\frac{dh}{dt} = F_i - F$$

$$Ah\frac{dT}{dt} = F_i(T_i - T) + \frac{Q}{\rho C_p}$$

where A, ρ and C_p are parameters with given constant values. How many degrees of freedom are there?

Q.4(a) Develop the mathematical model for a batch reactor with volume $V(\,ft^3)$ where the following reactions take place: **6**

$$A \xrightarrow[\lambda_1]{k_1} B \xrightarrow[\lambda_2]{k_2} C$$

$$A \xrightarrow[\lambda_3]{k_3} D$$

where $k_{1,}\, k_2, k_3$ and $\lambda_{1,}\, \lambda_2, \lambda_3$ are rate constants and heat of reactions, respectively. The fluid properties such as density and specific heat capacity are constant. All the reactions are endothermic and have first-order kinetics. The reacting mixture is heated by steam of 150 psig, which flows through a jacket around the reactor with a rate of $F_J(lb/\text{min})$.

(b) Model a mixing tank with two feed streams, as shown below in figure 1. Assume that there are two components, A and B. C represents the concentration of A. (C_1 is the mass concentration of A in stream 1 and C_2 is the mass concentration of A in stream 2). **6**

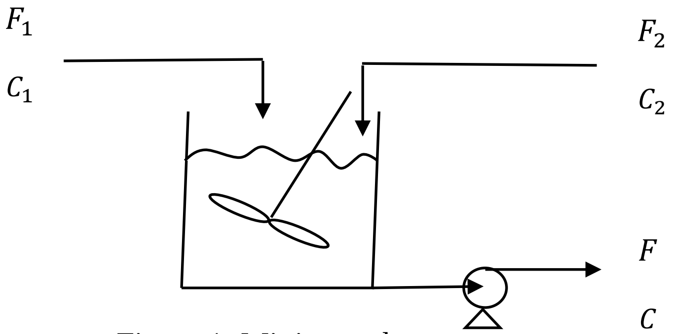

Figure 1: Mixing tank

Model the following cases:

a) Constant volume, constant density.
b) Constant volume, density varies linearly with concentration.
c) Variable volume, density varies linearly with concentration.

Q.5(a) Consider a CSTR with a second-order reaction. Assume that the rate of reaction (per unit volume) is proportional to the square of the concentration of the reacting component. Assuming constant volume and constant density, write the modeling equation. The rate constant is, $k = 0.32 ft^3 lbmol^{-1} min^{-1}$, the volume of the reactor is, $V = 5 ft^3$ and the inlet volumetric flow rate is $F = 1\, ft^3/min$. Calculate the steady-state concentration of reacting component if the steady-state inlet concentration is $C_{is} = 1.25\ lbmol ft^{-3}$. 6

(b) A component material balance around a chemical reactor yields the following steady-state equation 6

$$0 = \frac{F}{V} C_{in} - \frac{F}{V} C - kC^3$$

Where $\frac{F}{V} = 0.1\ min^{-1}, C_{in} = 1 \frac{lbmol}{ft^3}$ and $k = 0.05 \frac{ft^6}{lbmol^2 min}$

a) How many steady-state solutions are there?
b) Write two different direct substitution methods and assess the convergence of each.
c) Perform two iterations of Newton's method using an initial guess of $C = 1.0$.

Q.6 Consider an exothermic, irreversible first order reaction which takes place in a real plug flow reactor as shown in Figure 2. To remove the heat of reaction λ, a cooling jacket surrounds the reactor. The coolant enters in opposite direction of the feed (counter-current). Feed velocity *v(m/s)*, concentration of reactant C_A(mol/m^3), coolant temperature T_c and coolant velocity v_c can all vary with time and axial position *z*. The diffusive flux of A, N_A (mol/s.m^2) is given by Fick's law as 10

$$N_A = -D_A \frac{\partial C_A}{\partial z}$$

where D_A $(m^2/s)$is diffusion coefficient due to both diffusion and turbulence in fluid flow. The cross sectional area of the reactor is *A* (m^2). The density and heat capacity for both reaction mixture and coolant are constant. Carry out mass balance and energy balance for both reactor and coolant sections. Also, assume the necessary variable and parameters, if not given in the question.

$$A \xrightarrow{k} B$$

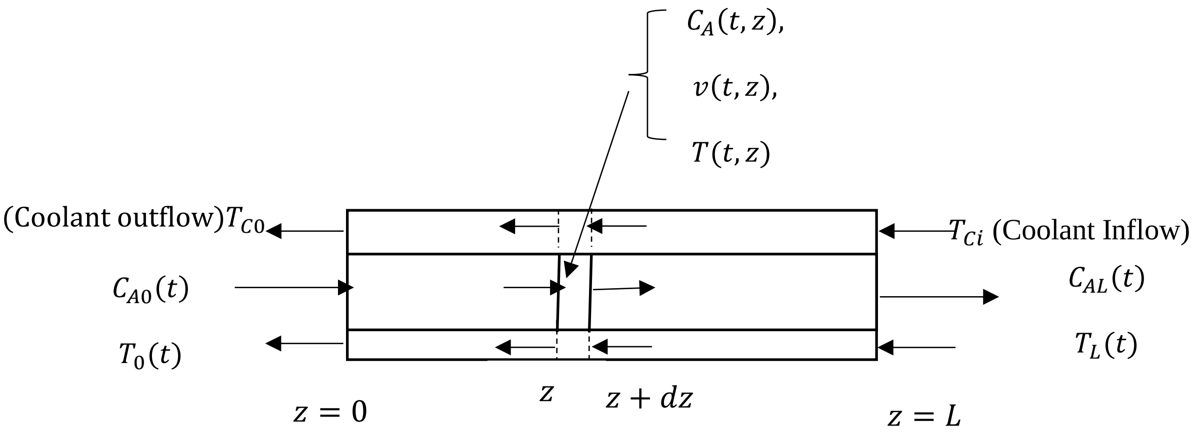

Figure 2: Plug flow reactor with counter-current cooling jacket