B.Tech. VIII Semester

Mid Term Examination, April 2019

Subject: **Modeling and Simulation in Chemical Engineering** Max. Marks: **30**

Course No. **ChBC – 84** Time: **1 hour 30 minutes**

Note: **Attempt ALL the questions and make necessary suitable assumptions**

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Course Outcomes

1. Identify the terms involved in inventory rate equation of mass, energy and momentum
2. Recall the basic concepts involved in modeling and simulation
3. Apply conservation of mass, momentum and energy equations to engineering problems.
4. Develop model equations for chemical engineering systems
5. Solve the model equations and chemical engineering problems using numerical techniques

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1. a. Express the rate of quantity interms of (i) Inlet/outlet rate (ii) Generation rate (iii) Accumulation rate. — 02 [CO1]

   b. Dust evolves at a rate of 0.3 kg/ h in a foundry which has the dimensions of 20 m x 8 m x 4 m. According to ILO (International Labor Organization) standards, the dust concentration should not exceed 20 mg/ m^3 to protect workers' health. Determine the volumetric flow rate of ventilating air to meet the standards of ILO. — 02 [CO2, CO3]

   c. Air at atmospheric pressure and 95 ^oC flows at 20 m/s over a flat plate of naphthalene 80 cm long in the direction of flow and 60 cm wide. Experimental measurements report the molar concentration of naphthalene in the air, C_A, as a function of distance x from the plate as follows: — 06 [CO2, CO5]

x, (cm)	0	10	20	30	40	50
C_A, (mol/m^3)	0.127	0.094	0.078	0.064	0.056	0.044

   Determine the molar flux of naphthalene from the plate surface under steady conditions by using least squares method. (Data: Diffusion coefficient of naphthalene (A) in air (B) at 25°C= 0.52×10^{-5} m^2/s)

2. a. List and discuss the basic steps involved in the development of steady-state macroscopic balances. 02 [CO2]

b. Derive the momentum generation as a result of pressure force for steady state flow in a pipe. 03 [CO1, CO2]

c. The following parallel reactions take place in an isothermal constant volume CSTR 05 [CO3]

$$A \rightarrow 2B \quad r = k_1 C_A \quad k_1 = 1.3\ s^{-1}$$

$$3A \rightarrow C \quad r = k_2 C_A \quad k_2 = 0.4\ s^{-1}$$

Pure A is fed to the reactor at a concentration of 350 mol/m^3

(i). Determine the residence time required to achieve 85% convection of species A under steady conditions

(ii). Determine the concentration of species B and C

3. a. It is required to cool a gas composed of 75 mole % N_2, 15 mole % CO_2 and 10 mole % O_2 from 800 °C to 200 °C. Determine the cooling duty of the heat exchanger if the heat capacity expressions are in the form. C_p (J/(mol* K)) = a + bT + CT^2 + dT^3 05 [CO2, CO3]

Species	A	b X 10^2	c X 10^5	d X 10^9
N_2	28.882	-0.1570	0.8075	-2.8706
O_2	25.460	1.5192	-0.7150	1.3108
CO_2	21.489	5.9768	-3.4987	7.4643

b. A liquid feed to a jacketed CSTR consists of 2000 mol/m^3 of *A* and 2400 mol/m^3 of *B*. A second-order irreversible reaction takes place as A+B →2C. The rate of reaction is given by $r = kC_A C_B$, where the reaction rate constant at 298 K is $k = 9.15 \times 10^{-5}$ m^3 / (mol * min). The reactor operates isothermally at 65^{O}C. (i) Calculate the residence time required to obtain 80% conversion of species A. (ii) What should be the volume of the reactor if species *C* are to be produced at a rate of 820 mol/min? 05 [CO1, CO3]

B.Tech. VIII Semester Max Marks: 30 Time: 1hr 30 min. 1

Department of Chemical Engineering

Modeling & simulation in chemical Engineering

ANSWER KEY - Mid Term, Apr 2019 25-04-2019

1.a. (i) Inlet/outlet rate $= \begin{cases} (\text{Flux})(\text{Area}) & \text{if flux is constant} \\ \iint_A \text{flux } dA & \text{if flux is Position dependent} \end{cases}$

(ii) Generation rate $= \begin{cases} (\mathcal{R})(\text{volume}) & \text{if } \mathcal{R} \text{ is constant} \\ \iiint_V \mathcal{R}\, dV & \text{if } \mathcal{R} \text{ is Position dependent} \end{cases}$

(iii) Let ρ be the mass density and φ be the quantity per unit mass. Thus,

$$\text{Total quantity of } \varphi = \iiint_V \rho\varphi\, dV$$

and the rate of accumulation is given by

$$\text{Accumulation rate} = \frac{d}{dt}\left(\iiint_V \rho\varphi\, dV\right),$$

If φ is independent of Position, Accumulation rate $= \frac{d}{dt}(m\varphi)$ where m is the total mass within the system.

1.b. Given,

Rate of dust evolves = Rate of generation of dust $= 0.3\,kg/h$,

Dimensions $= 20m \times 8m \times 4m$

(volume of foundry) V

The dust conc^n shd not exceed $= C_f$ (or) $C_0 = 20\frac{mg}{m^3} = 20\times10^{-6}\frac{kg}{m^3}$

on basis of dust, material balance of dust,

$$\begin{pmatrix}\text{Rate of I/P}\\ \text{of dust}\end{pmatrix} - \begin{bmatrix}\text{Rate of O/P}\\ \text{of dust}\end{bmatrix} + \left(\text{Rate of generation of dust}\right) = \begin{Bmatrix}\text{Rate of accumulation}\\ \text{of dust}\end{Bmatrix}$$

Assume process is steady state, so, no accumulation term and Initial conc^n of dust is equal to zero $= c_i = 0$

so, $c_i q_i - C_0 Q_0 + RV = 0$

$$(-20\times10^{-6}\times Q_0) + 0.3 = 0$$

$$Q_0 = \frac{0.3}{20\times10^{-6}} = \boxed{15{,}000\, m^3/h}$$

$\downarrow$

volumetric flow rate of ventilating air to meet the standards

1.C.

x, cm	CA, mol/m³	$y_i = \log CA$	$x_i y_i$	x_i^2
0	0.117	-0.932	0	0
5	0.105	-0.979	-4.89	25
15	0.085	-1.071	-16.06	225
25	0.069	-1.161	-29.03	625
35	0.057	-1.244	-43.54	1225
45	0.047	-1.328	-59.76	2025
$\Sigma x = 125$		$\Sigma y_i = -6.714$	$\Sigma x_i y_i = -158.28$	$\Sigma x_i^2 = 4125$

least square

$$\Sigma y = NC + m\Sigma x$$

$$\Sigma xy = b\Sigma x + m\Sigma x^2$$

$$m = \frac{(n)(\Sigma x_i y_i) - (\Sigma x_i)(\Sigma y_i)}{n(\Sigma x_i^2) - (\Sigma x_i)^2} \quad b = \frac{(\Sigma y_i)(\Sigma x_i^2) - (\Sigma x_i)(\Sigma x_i y_i)}{n(\Sigma x_i^2) - (\Sigma x_i)^2}$$

$$\log C_A = -0.0088x - 0.94$$

$n = 6$

$m = -0.0088$

$b = -0.94$

By logorithmic Principles

$$\ln C_A = 2.303 \log C_A$$

$$\frac{\ln C_A}{2.303} = -0.0088x - 0.94$$

$$\ln C_A = 2.303(-0.0088x - 0.94)$$

$$\ln C_A = -0.02004x - 2.1648$$

$$C_A = e^{-0.02004x} e^{-2.1648}$$

$$C_A = 0.115 e^{-0.02004x}$$

$$\frac{dC_A}{dx} = 0.115 \frac{de^{-0.02004x}}{dx}$$

$$\frac{dC_A}{dx} = 0.115(-0.02004)e^{-0.2004x}$$

$$\frac{de^{ax}}{dx} = ae^{ax}$$

$$\left.\frac{dC_A}{dx}\right|_{x=0} = -0.0023e^{-0.2004x}\Big|_{x=0}$$

$$\left.\frac{dC_A}{dx}\right|_{x=0} = -0.0023 \times 1 = -0.0023 \ (\text{mol/m}^3)/\text{cm}$$

$$= -0.0023 \times 10^2 \ \text{mol/m}^4$$

$$\left.\frac{dC_A}{dx}\right|_{x=0} = -0.23 \ \text{mol/m}^4$$

$$J_{Ax}\Big|_{x=0}$$

2.a. The basic steps in the development of steady-state macroscopic balances are as follows:

→ Define your system
→ If possible, draw a simple sketch
→ List the assumptions
→ Write down the inventory rate equation for each of the basic concepts relevant to the problem
→ Use engineering correlations to evaluate the transfer coefficients
→ Solve the algebraic equations.

2.b. Momentum Generation As a Result of Pressure Force

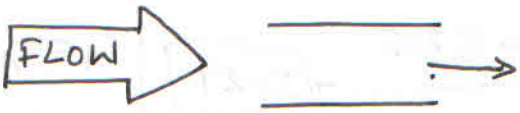

Fig: Flow through a pipe

Consider the steady flow of an incompressible fluid in a pipe. The rate of mechanical energy required to pump the fluid is given by

$$\dot{W} = F_D \langle v \rangle = Q|\Delta P|$$

since the volumetric flow rate, Q, is the product of average velocity, $\langle v \rangle$, with the cross-sectional area, A

$$A|\Delta P| = F_D = 0$$

According to conservation of mass

$$\dot{m}_{in} = \dot{m}_{out}$$

$$(\rho v A)_{in} = (\rho v A)_{out}$$

Assume $A_{in} = A_{out}$ + $\rho = const$

$$v_{in} = v_{out}$$

for steady state

$$\begin{pmatrix}\text{Rate of} \\ \text{momentum} \\ \text{in}\end{pmatrix} - \begin{pmatrix}\text{Rate of} \\ \text{mom. out}\end{pmatrix} + \begin{pmatrix}\text{Rate of} \\ \text{mom. generation}\end{pmatrix} = 0$$

$$(\dot{m} v)_{in} - \left[(\dot{m} v)_{out} + F_D\right] + \mathcal{R} A L = 0$$

where,
$\mathcal{R}$ = Rate of momentum generation per unit volume. ~~Not~~

Note that rate of momentum transfer from the fluid to the pipe wall manifests itself as a drag force.

$$\mathcal{R}(AL) - F_D = 0$$

Rate of momentum generation per unit volume is equal to the pressure gradient.

$$F_D = A\Delta P$$

$$\mathcal{R}(AL) = A\Delta P$$

$$\mathcal{R} = \frac{|\Delta P|}{L}$$

2c. $A \rightarrow 2B$, $r = k_1 C_A$, $k_1 = 1.3\ s^{-1}$

$3A \rightarrow C$, $r = k_2 C_A$, $k_2 = 0.4\ s^{-1}$

Given,

$C_{Ain} = 350\ mol/m^3$

$X_A = 0.85$

$\tau = ?$

Assumptions:-

① $(C_i)_{out} = (C_i)_{sys} \rightarrow$ perfect mixing

② $V = const. \Rightarrow Q_{in} = Q_{out} = Q$

(i) For species 'A' :- $QC_{Ain} - QC_A - (k_1 C_A + 3k_2 C_A)V = 0$

$$\tau = \frac{C_{Ain} - C_A}{k_1 C_A + 3k_2 C_A} \Rightarrow \frac{350 - 52.5}{(1.3 \times 52.5 + 3 \times 0.4 \times 52.5)} = \boxed{2.27\ sec}$$

$C_A = C_{Ain}(1 - X_A)$

$C_A = 350(1 - 0.85)$

$\boxed{C_A = 52.5\ mol/m^3}$

(ii)

For species 'B' :- $QC_{Bin} - QC_B + 2k_1 C_A V = 0$

$$\tau = \frac{C_B - C_{Bin}}{2k_1 C_A} \Rightarrow 2.27 \times 2 \times 1.3 \times 52.5 = C_B$$

$$\boxed{C_B = 309.86\ mol/m^3}$$

For species 'C'

$QC_{Cin} - QC_C + k_2 C_A V = 0$

$$\tau = \frac{C_C - C_{Cin}}{k_2 C_A}$$

$$C_C = 2.27 \times 0.4 \times 52.5$$

$$\boxed{C_C = 47.67\ mol/m^3}$$

3.a. Assumptions

1. Ideal gas behavior.
2. changes in kinetic and Potential energies are negligible.
3. Pressure drop in the heat exchanger is negligible.

Since $\dot{n}_{int} = 0$ and there is no chemical reaction,

$$\dot{n}_{in} = \dot{n}_{out} = \dot{n}$$

$$\dot{Q}_{int} = \dot{n}\left(\int_{T_{ref}}^{T_{out}} \hat{C}_p dT - \int_{T_{ref}}^{T_{in}} \hat{C}_p dT\right) = \dot{n}\left(\int_{T_{in}}^{T_{out}} \hat{C}_p dT\right)$$

$$\hat{Q}_{int} = \int_{T_{in}}^{T_{out}} \hat{C}_p dT$$

where $\hat{Q}_{int} = \dot{Q}_{int}/\dot{n}$, $T_{in} = 1073\,K$, and $T_{out} = 473\,K$.

The molar heat capacity of the gas stream, $\hat{C}_P$, can be calculated by multiplying the mole fraction of each component by the respective heat capacity and adding them together

$$\hat{C}_p = \sum_{i=1}^{3} I_i (a_i + b_i T + c_i T^2 + d_i T^3)$$

$$= 27.431 + 0.931\times10^{-2} T + 0.009\times10^{-5} T^2 - 0.902\times10^{-9} T^3$$

$$\hat{Q}_{int} = \int_{473}^{1073} \hat{C}_p dT = -20522.84\ J/mol$$

3.b. Assumptions

1. As a result of Perfect mixing, concentrations of the species within the reactor are uniform, i.e., $(C_i)_{out} = (C_i)_{sys}$.

(i) Since the reactor volume is constant, the inlet and outlet volumetric flow rates are the same and equal to Q. Therefore, the inventory rate equation for conservation of species A

$$Q(C_A)_{in} - QC_{A_{sys}} - (kC_{A_{sys}} C_{B_{sys}}) V_{sys} = 0$$

$$\tau = \frac{(C_A)_{in} - C_A}{kC_A C_B}$$

the extent of reaction can be calculated as

$$\xi = \frac{(C_A)_{in}}{(-\alpha_A)} X_A = \frac{(2000)(0.8)}{1} = 1600\ mol/m^3$$

$$c_A = (c_A)_{in} + \alpha_A \xi = 2000 - 1600 = 400 \text{ mol/m}^3$$
$$c_B = (c_B)_{in} + \alpha_B \xi = 2400 - 1600 = 800 \text{ mol/m}^3$$
$$c_C = (c_C)_{in} + \alpha_C \xi = (2)(1600) = 3200 \text{ mol/m}^3$$

$$\tau = \frac{2000 - 400}{(9.15 \times 10^{-5})(400)(800)} = 54.6 \text{ min}$$

(ii) The reactor volume, V, is given by

$$V = \tau Q$$

The volumetric flow rate can be determined from the production rate of species C,

$$c_C Q = 820 \Rightarrow Q = \frac{820}{3200} = 0.256 \text{ m}^3/\text{min}$$

Hence, the reactor volume is

$$V = (54.6)(0.256) = 14 \text{ m}^3$$