Chapter-5 - Ismail Tosun

RATE OF GENERATION IN MASS TRANSPORT :- ①

→ Stoichiometry of a chemical Reaction :- Balancing of a chemical ~~reaction~~ equation is based on the conservation of mass for a closed thermodynamic system.

→ If a chemical reaxⁿ takes place in a closed container, the mass does not change even if there is an exchange of energy with the surroundings.

→ Consider a reaxⁿ b/w nitrogen and hydrogen to form ammonia, i.e., $N_2 + 3H_2 \longrightarrow 2NH_3$

Assume,
If $A_1 = N_2$, $A_2 = H_2$ and $A_3 = NH_3$ then we can express as $A_1 + 3A_2 = 2A_3$

→ It is convenient to write all the chemical species on one side of the eqn and give a +ve sign to the species regarded as the products of the reaxⁿ. Thus

$$2A_3 - A_1 - 3A_2 = 0 \quad (or) \quad \boxed{\sum_{i=1}^{s} \alpha_i A_i = 0} \quad — ①$$

where,
α_i = stoichiometric coefficient of i^{th} chemical species. +ve for pdts & −ve for reactants

s = Total number of species in the reaction.

A_i = chemical symbol for the i^{th} chemical species.

→ Each chemical species, A_i, is the some of the chemic[al el]ements, E_j such that

$$A_i = \sum_{j=1}^{t} \beta_{ji} E_j \quad — ②$$

where,
β_{ji} → No. of chemical elements E_j in the chemical species A_i

t → Total no. of chemical elements

Sub. of (2) in (1) (19)

$$\sum_{i=1}^{s} \alpha_i \left(\sum_{j=1}^{t} \beta_{ji} E_j \right) = \sum_{j=1}^{t} \left(\sum_{i=1}^{s} \alpha_i \beta_{ji} \right) E_j = 0 \quad \text{--- (3)}$$

(or)

$$\boxed{\sum_{i=1}^{s} \alpha_i \beta_{ji} = 0} \quad \text{for } j = 1, 2, 3, \ldots$$

Balance chemical reaction

(5.1) consider the reaxn btn N_2 & H_2 to form NH_3

$$\alpha_1 N_2 + \alpha_2 H_2 + \alpha_3 NH_3 = 0$$

show how one can apply to balance this equation.

Sol: If $A_1 = N_2$, $A_2 = H_2$ & $A_3 = NH_3$

$$\alpha_1 A_1 + \alpha_2 A_2 + \alpha_3 A_3 = 0$$

If we let $E_1 = N \ (j=1)$, $E_2 = H \ (j=2)$

For $j=1$ $\quad \alpha_1 \beta_{11} + \alpha_2 \beta_{12} + \alpha_3 \beta_{13} = 0$

For $j=2$ $\quad \alpha_1 \beta_{21} + \alpha_2 \beta_{22} + \alpha_3 \beta_{23} = 0$

$$\alpha_1(2) + \alpha_2(0) + \alpha_3(1) = 0$$

$$\alpha_1(0) + \alpha_2(2) + \alpha_3(3) = 0$$

$$\alpha_1 = -\frac{1}{2}\alpha_3, \quad \alpha_2 = -\frac{3}{2}\alpha_3$$

Assume, $\alpha_3 = 2$, $\alpha_1 = -1$, $\alpha_2 = -3$

$$-N_2 - 3H_2 + 2NH_3 = 0$$

(or)

$$\boxed{N_2 + 3H_2 = 2NH_3}$$

The law of combining properties:-

$$\boxed{\varepsilon = \frac{n_i - n_{i0}}{\alpha_i}}$$,

or

$$\varepsilon = \frac{n_{i0} - n_i}{-\alpha_i}$$

ε = molar extent of reax^n

n_i = no. of moles of ith chemical species

n_{i0} = Initial no. of moles of ith chemical species.

α_i = stoichiometric coefficient of ith chemical species.

Molar Extent of Reaction (ε):- is qty that measures the extent in which the reax^n proceeds.

Rearrangement of above eqn gives

$$\boxed{n_i = n_{i0} + \alpha_i \varepsilon}$$

→ Note that once 'ε' has been determined, the no. of moles of any chemical species participating in the reax^n can be determined.

→ The molar extent of the reax^n shd not be confused with the fractional conversion variable 'X', which can only take values btn 0 and 1.

→ The molar extent of the reax^n is an extensive property measured in moles and its value can be greater than unity. And molar extent is unique for a given reax^n.

→ It is also important to note that the fractional conversion may be different for each of the reacting species, i.e.,

$$\boxed{X_i = \frac{n_{i0} - n_i}{n_{i0}}}$$

comparison of above two eqns

$$\boxed{\varepsilon = \frac{n_{i0}}{(-\alpha_i)} x_i}$$

the total no. of moles, n_T, of a reacting mixture at any instant can be calculated by the summation of overall species.

$$\boxed{n_T = n_{T_0} + \bar{\alpha}\varepsilon}$$, n_{T_0} = Initial total no. of moles

$$\boxed{\bar{\alpha} = \sum_i \alpha_i}$$

(5.2)

(5.3)

→ molar concn of the i^{th} species, C_i is defined by

$$\boxed{C_i = \frac{n_i}{V}}$$ mol/m³

we know,
so, $n_i = n_{i0} + \alpha_i \varepsilon$, divide by volume 'V' gives

$$C_i = C_{i0} + \alpha_i \xi, \quad \boxed{\xi = \frac{\varepsilon}{V}}$$

C_{i0} = Initial molar concn of i^{th} species

ξ = Intensive extent of reacn in moles per unit volume

so, $$\boxed{\xi = \frac{C_{i0}}{(-\alpha_i)} x_i}$$

The total molar concn, C, of a reacting mixture at any instant can be calculated by summation of overall species, $\boxed{C = C_0 + \bar{\alpha}\xi}$

C_0 = Initial total molar concn

When more than one reaction takes place in a reactor, then,

$$\boxed{n_{ij} = n_{ij_0} + \alpha_{ij}\varepsilon_j}$$

when,

n_{ij} = No. of moles of i^{th} species in j^{th} reac^n

n_{ij_0} = No. of initial moles of i^{th} species in j^{th} reac^n

α_{ij} = stoichiometric coefficient of i^{th} species in the j^{th} reac^n.

ε_j = Extent of the j^{th} reacn

Summation of overall reac^{n}s taking place in a reactor gives

$$\boxed{\sum_j n_{ij} = \sum_j n_{ij_0} + \sum_j \alpha_{ij}\varepsilon_j}$$

(or)

$$\boxed{n_i = n_{i_0} + \sum_j \alpha_{ij}\varepsilon_j}$$

Rate of Reaction :-

The rate of chemical reaction r is defined as

$$\boxed{r = \frac{1}{V}\frac{d\varepsilon}{dt}}$$

where, V = volume physically occupied by the reacting fluid

Note that the reaction rate has the units of moles reacted per unit time per unit volume of the reaction mixture.

The reaction rate expression, r, has the following characteristics

→ It is an intensive property
→ It is independent of reactor type
→ It is independent of a process

Change in the molar extent of the reaction can be related to the changes in no of moles of species 'i' by differentiating

$$\varepsilon = \frac{n_{i0} - n_i}{-\alpha_i} \quad (or) \quad \varepsilon = \frac{n_i - n_{i0}}{\alpha_i}$$

$$\boxed{d\varepsilon = \frac{dn_i}{\alpha_i}}$$

$$r = \frac{1}{V}\frac{1}{\alpha_i}\frac{dn_i}{dt}$$

$$\boxed{r = \frac{1}{\alpha_i} R_i}$$, R_i = Rate of generation of species 'i' per unit volume

$$\boxed{R_i = \alpha_i r}$$

–ve, if 'i' appears as reactant
+ve, if 'i' appears as pdt

Ex 5.5 For the reaction

$$3A \longrightarrow B + C$$

Express the reaction rate in terms of the time rate of change of species A, B, and C.

Sol:

$$r = \frac{1}{\alpha_i}\frac{1}{V}\frac{dn_i}{dt}$$

$$r = -\frac{1}{3}\frac{1}{V}\frac{dn_A}{dt} = \frac{1}{V}\frac{dn_B}{dt} = \frac{1}{V}\frac{dn_C}{dt}$$

if 'V' is constant, then

$$\boxed{r = -\frac{1}{3}\frac{dc_A}{dt} = \frac{dc_B}{dt} = \frac{dc_C}{dt}}$$

In case of several reactions, R_i is defined by

$$\boxed{R_i = \sum_j \alpha_{ij} r_j}$$

where, r_j = rate of j^{th} reaxn

→ The reaction rate is a function of temperature and concentration and is assumed to be the pdt of two functions.

$$r(T, c_i) = K(T) f(c_i)$$

$K(T)$ = rate const.

$$K(T) = A T^m e^{-E/RT}$$

E → Activation Energy
R → Gas const.
A → const.
m = 0 → Arhenius
m = ½ → Kinetic
m = 1 → Transition

5.2 A system containing 1 mole A_1, 2 mole A_2 and 7 mole A_3 undergoes the following reaction 5

$$A_1(g) + A_2(g) + \frac{3}{2} A_3(g) \rightarrow A_4(g) + 3A_5(g)$$

Det. the limiting reactant and fractional conversion with respect to each reactant if the reaction goes to completion.

Sol:

$n_i = n_{i0} + \alpha_i \epsilon$

species	$n_{i0}/(-\alpha_i)$
A_1	$1/-(-1) = 1$
A_2	$2/-(-1) = 2$
A_3	$7/-(-\frac{3}{2}) = 4.67$

The limiting reactant has the least +ve value of $n_{i0}/(-\alpha_i)$.

So, from above table, the limiting reactant is A_1.

→ Note that the least +ve value of $n_{i0}/(-\alpha_i)$ is also the greatest possible value of 'ϵ' since the reaction goes to completion, species 'A_1' will be completely depleted and $\epsilon = 1$.

And using Eqn $\boxed{\epsilon = \frac{n_{i0}}{(-\alpha_i)} X_i}$ calculate fractional conversion.

species	X
A_1	$1/1 = 1$
A_2	$1/2 = 0.5$
A_3	$1/4.67 = 0.21$

Ex 5.3 A system containing 3 mole A_1 and 4 mole A_2 undergoes the following reaction

$$2A_1(g) + 3A_2(g) \longrightarrow A_3(g) + 2A_4(g)$$

Calculate the mole fractions of each species if $\epsilon = 1.1$. What is the fractional conversion based on the limiting reactant.

$$n_1 = 3 - 2\epsilon = 3 - 2(1.1) = 0.8 \text{ mol}$$

$$n_2 = 4 - 3\epsilon = 4 - 3(1.1) = 0.7 \text{ mol}$$

$$n_3 = 0 + 1\epsilon = \boxed{1.1 \text{ mol}}$$

$$n_4 = 0 + 2\epsilon = \boxed{2.2 \text{ mol}}$$

$$\boxed{n_T = 4.8 \text{ mol}}$$

$x_1 = \frac{0.8}{4.8} = 0.167$, $x_2 = \frac{0.7}{4.8} = 0.146$, $x_3 = 0.229$, $x_4 = 0.458$

$$X = (n_{i_0} - n_i)/(n_{i_0})$$

$$X_{A_2} = \frac{4 - 0.7}{4} = \boxed{0.825} \rightarrow A_2 \rightarrow \text{limiting reactant}$$

species	$n_{i_0}/(\alpha_i)$
A_1	$3/(2) = 1.5$
A_2	$4/3 = 1.3$ ✓

(5.4) The following two reactions occur simultaneously in a batch reactor:

$$C_2H_6 = C_2H_4 + H_2$$

$$C_2H_6 + H_2 = 2CH_4$$

A mixture of 85 mole% C_2H_6 and 15% inerts is fed into a reactor and the reactions proceed until 25% C_2H_4 and 5% CH_4 are formed. Determine the % of each species in a reacting mixture.

Sol: Basis:- 1 mole of reacting mixture.

let ϵ_1 & ϵ_2 be the molar extents of the first & second reaxns resp. then the no. of moles of each species can be expressed as

$$n_{C_2H_6} = 0.85 - \epsilon_1 - \epsilon_2 \quad (\because n_i = n_{i0} + \sum_j \alpha_{ij}\epsilon_j)$$

$$n_{C_2H_4} = 0 + \varepsilon_1 = \varepsilon_1$$

$$n_{H_2} = 0 + \varepsilon_1 + 0 - \varepsilon_2 = \varepsilon_1 - \varepsilon_2$$

$$n_{CH_4} = 0 + 2\varepsilon_2 = 2\varepsilon_2$$

$$n_{inert} = 0.15$$

$$\boxed{n_T = 1 + \varepsilon_1}$$

Given $x_{C_2H_4} = \dfrac{\varepsilon_1}{1+\varepsilon_1} = 0.25 \Rightarrow \varepsilon_1 = \boxed{0.333}$

$x_{CH_4} = 0.05 = \dfrac{2\varepsilon_2}{1+\varepsilon_1} \Rightarrow \varepsilon_2 = \boxed{0.033}$

$$x_{C_2H_6} = \frac{0.85 - \varepsilon_1 - \varepsilon_2}{1+\varepsilon_1} = \boxed{0.363}$$

$$x_{H_2} = \frac{\varepsilon_1 - \varepsilon_2}{1+\varepsilon_1} = \boxed{0.225}$$

$$x_{inert} = \frac{0.15}{1+\varepsilon_1} = \boxed{0.112}$$

RATE OF GENERATION IN MOMENTUM TRANSPORT :-

→ In general, forces acting on a particle can be classified as surface forces and body forces. Surface forces, such as normal stresses (pressure) and tangential stresses, act by direct contact on a surface.

→ Body forces, however act at a distance on a volume. Those are Gravitational, electrical and electromagnetic forces.

→ For solid bodies Newton's second law of motion states that

$$\begin{pmatrix}\text{Summation of forces} \\ \text{acting on a system}\end{pmatrix} = \begin{pmatrix}\text{Time rate of change} \\ \text{of momentum of a system}\end{pmatrix} \quad (1)$$

→ in which forces acting on a system include both surface and body forces.

→ Eqn (1) can be extended to fluid particles by considering the rate of flow of momentum into and out of the volume element.

$$\begin{pmatrix}\text{Rate of} \\ \text{momentum} \\ \text{in}\end{pmatrix} - \begin{pmatrix}\text{Rate of} \\ \text{momentum} \\ \text{out}\end{pmatrix} + \begin{pmatrix}\text{summation of} \\ \text{forces acting} \\ \text{on a system}\end{pmatrix} = \begin{pmatrix}\text{Time rate of change} \\ \text{of momentum of a system}\end{pmatrix}$$

→ On the other hand, for a given system, the inventory rate eqn for momentum can be expressed as

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

compare above two eqns

$$\begin{pmatrix}\text{Rate of momentum} \\ \text{generation}\end{pmatrix} = \begin{pmatrix}\text{summation of forces} \\ \text{acting on a system}\end{pmatrix}$$

Pressure force (surface force)
&
Gravitational force (body force)

<u>Momentum generation as a result of Gravitational force</u> :- consider a basket ball player holding a ball in his/her hands. when he drops the ball, it starts to accelerate as a result of gravitational force. so,

Rate of momentum generation $= Mg$

Where,

M = mass of the ball

g = gravitational acceleration

$\therefore$ the rate of momentum generation per unit volume, $\boxed{R = \rho g}$

<u>Momentum generation as a result of Pressure force</u> :-

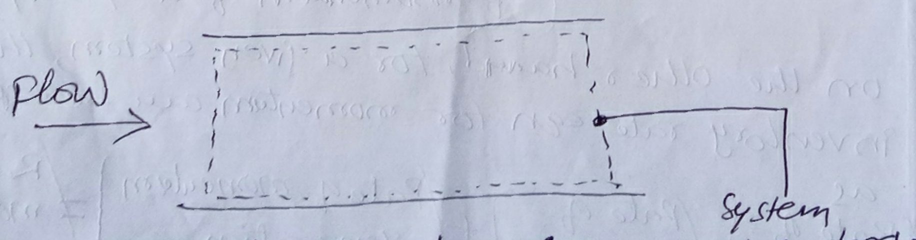

Fig: <u>Flow through a Pipe</u>

2

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

$$\text{Power} = \frac{\text{work}}{\text{Time}} = \frac{(\text{Force})(\text{distance})}{\text{time}} = F_D\langle v\rangle$$

$$\dot{W} = F_D\langle v\rangle = \phi\,\Delta P$$
$$= A\langle v\rangle\Delta P$$

$$\boxed{A\Delta P - F_D = 0}$$ ϕ = volumetric flow rate

According to conservation of mass

$$\dot{m}_{in} = \dot{m}_{out}$$ $\frac{kg\,m}{s^2} \cdot \frac{m}{s}$

$$(\rho VA)_{in} = (\rho VA)_{out}$$ $\frac{m^3}{s} \times \frac{kg}{m^2}$

Assume $A_{in} = A_{out}$ & ρ = const

$$V_{in} = V_{out}$$ $\frac{kg\,m}{s} \times \frac{s}{m}$

ρ

For steady state

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

$$(\dot{m}v)_{in} - \left((\dot{m}v)_{out} + F_D\right) + RAL = 0$$

$\frac{kg\,m}{s^2} \times \frac{1}{m^2} \times \frac{1}{m}$

$$W = \frac{kg\,m}{s^2} \times \frac{m}{s} = \frac{m^3}{s} \times \frac{kg\,m}{s^2} \times \frac{1}{m^2}$$

Pa
"
N/m²

$\frac{kg}{s} \times \frac{m}{s}$

$$\left(\frac{kg\,m}{s^2}\right) - \frac{kg\,m}{s^2} + \frac{kg\,m}{s^2} + \frac{kg\,m^2}{m^2 s^2} \times m$$

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Where,

$R =$ Rate of momentum generation per unit volume

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

$$R(AL) - F_D = 0$$

$$F_D = A\Delta P$$

$$R(AL) = A\Delta P$$

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

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

RATE GENERATION IN ENERGY TRANSPORT :-

The rate of energy generation per unit volume may be considered const. in most cases. If it is dependent on temperature, it may be expressed in various forms such as

$$R = \begin{cases} a + bT \\ R_0 e^{aT} \end{cases}, \quad a, b = \text{constants}$$

6

STEADY-STATE MACROSCOPIC BALANCES

The use of correlations in the determination of momentum, energy and mass transfer from one phase to another under steady-state conditions is covered in Chapter 4. Although some examples in Chapter 4 make use of steady-state macroscopic balances, systematic treatment of these balances for the conservation of chemical species, mass, and energy is not presented. The basic steps in the development of steady-state macroscopic balances are as follows:

- *Define your system:* A system is any region that occupies a volume and has a boundary.
- *If possible, draw a simple sketch:* A simple sketch helps in the understanding of the physical picture.
- *List the assumptions:* Simplify the complicated problem to a mathematically tractable form by making reasonable assumptions.
- *Write down the inventory rate equation for each of the basic concepts relevant to the problem at hand:* Since the accumulation term vanishes for steady-state cases, macroscopic inventory rate equations reduce to algebraic equations. Note that in order to have a mathematically determinate system the number of independent inventory rate equations must be equal to the number of dependent variables.
- *Use engineering correlations to evaluate the transfer coefficients:* In macroscopic modeling, empirical equations that represent transfer phenomena from one phase to another contain transfer coefficients, such as the heat transfer coefficient in Newton's law of cooling. These coefficients can be evaluated by using the engineering correlations given in Chapter 4.
- *Solve the algebraic equations.*

6.1 CONSERVATION OF CHEMICAL SPECIES

The inventory rate equation given by Eq. (1.1-1) holds for every conserved quantity φ. Therefore, the conservation statement for the mass of the ith chemical species under steady conditions is given by

$$\begin{pmatrix} \text{Rate of mass} \\ \text{of } i \text{ in} \end{pmatrix} - \begin{pmatrix} \text{Rate of mass} \\ \text{of } i \text{ out} \end{pmatrix} + \begin{pmatrix} \text{Rate of generation} \\ \text{of mass } i \end{pmatrix} = 0 \tag{6.1-1}$$

The mass of i may enter or leave the system by two means: (i) by inlet or outlet streams, (ii) by exchange of mass between the system and its surroundings through the boundaries of the system, i.e., interphase mass transfer.

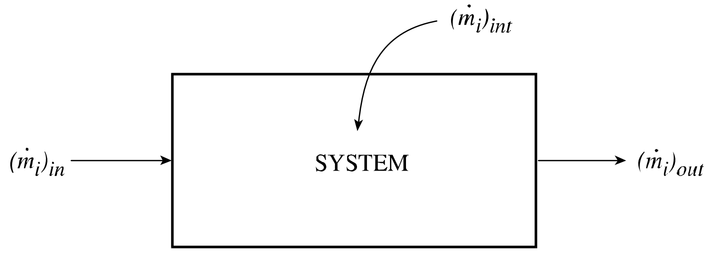


Figure 6.1. Steady-state flow system with fixed boundaries.

For a system with a single inlet and a single outlet stream as shown in Figure 6.1, Eq. (6.1-1) can be expressed as

$$\boxed{(\dot{m}_i)_{in} - (\dot{m}_i)_{out} \pm (\dot{m}_i)_{int} + \left(\sum_j \alpha_{ij} r_j\right) \mathcal{M}_i V_{sys} = 0} \tag{6.1-2}$$

in which the molar rate of generation of species i per unit volume, $\Re_i$, is expressed by Eq. (5.3-27). The terms $(\dot{m}_i)_{in}$ and $(\dot{m}_i)_{out}$ represent the inlet and outlet mass flow rates of species i, respectively, and $\mathcal{M}_i$ is the molecular weight of species i. The interphase mass transfer rate, $(\dot{m}_i)_{int}$, is expressed as

$$(\dot{m}_i)_{int} = A_M \langle k_c \rangle (\Delta c_i)_{ch} \mathcal{M}_i \tag{6.1-3}$$

where $(\Delta c_i)_{ch}$ is the characteristic concentration difference. Note that $(\dot{m}_i)_{int}$ is considered *positive* when mass is added to the system.

As stated in Section 2.4.1, the mass flow rate of species i, $\dot{m}_i$, is given by

$$\dot{m}_i = \rho_i \langle v \rangle A = \rho_i \mathcal{Q} \tag{6.1-4}$$

Therefore, Eq. (6.1-2) takes the form

$$\boxed{(\mathcal{Q}\rho_i)_{in} - (\mathcal{Q}\rho_i)_{out} \pm A_M \langle k_c \rangle (\Delta c_i)_{ch} \mathcal{M}_i + \left(\sum_j \alpha_{ij} r_j\right) \mathcal{M}_i V_{sys} = 0} \tag{6.1-5}$$

Sometimes it is more convenient to work on a molar basis. Division of Eqs. (6.1-2) and (6.1-5) by the molecular weight of species i, $\mathcal{M}_i$, gives

$$\boxed{(\dot{n}_i)_{in} - (\dot{n}_i)_{out} \pm (\dot{n}_i)_{int} + \left(\sum_j \alpha_{ij} r_j\right) V_{sys} = 0} \tag{6.1-6}$$

and

$$\boxed{(\mathcal{Q}c_i)_{in} - (\mathcal{Q}c_i)_{out} \pm A_M \langle k_c \rangle (\Delta c_i)_{ch} + \left(\sum_j \alpha_{ij} r_j\right) V_{sys} = 0} \tag{6.1-7}$$

where $\dot{n}_i$ and c_i are the molar flow rate and molar concentration of species i, respectively.

Example 6.1 The liquid phase reaction

$$A + 2B \rightarrow C + 2D$$

takes place in an isothermal, constant-volume stirred tank reactor. The rate of reaction is expressed by

$$r = kc_A c_B \qquad with \qquad k = 0.025\ \text{L/mol·min}$$

The feed stream consists of equal concentrations of species $\mathcal{A}$ and $\mathcal{B}$ at a value of 1 mol/L. Determine the residence time required to achieve 60% conversion of species $\mathcal{B}$ under steady conditions.

Solution

Assumption

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

Analysis

System: Contents of the reactor

Since the reactor volume is constant, the inlet and outlet volumetric flow rates are the same and equal to $\mathcal{Q}$. Therefore, the inventory rate equation for conservation of species $\mathcal{B}$, Eq. (6.1-7), becomes

$$\mathcal{Q}(c_B)_{in} - \mathcal{Q}(c_B)_{sys} - \left[2k(c_A)_{sys}(c_B)_{sys}\right]V_{sys} = 0 \qquad (1)$$

where $(c_A)_{sys}$ and $(c_B)_{sys}$ represent the molar concentration of species $\mathcal{A}$ and $\mathcal{B}$ in the reactor, respectively. Dropping the subscript "sys" and defining the residence time, τ, as $\tau = V/\mathcal{Q}$ reduces Eq. (1) to

$$(c_B)_{in} - c_B - (2kc_A c_B)\tau = 0 \qquad (2)$$

or,

$$\tau = \frac{(c_B)_{in} - c_B}{2kc_A c_B} \qquad (3)$$

Using Eq. (5.3-17), the extent of the reaction can be calculated as

$$\xi = \frac{(c_B)_{in}}{(-\alpha_B)} X_B = \frac{(1)(0.6)}{2} = 0.3\ \text{mol/L} \qquad (4)$$

Therefore, the concentrations of species $\mathcal{A}$ and $\mathcal{B}$ in the reactor are

$$c_A = (c_A)_{in} + \alpha_A \xi = 1 - 0.3 = 0.7\ \text{mol/L} \qquad (5)$$

$$c_B = (c_B)_{in} + \alpha_B \xi = 1 - (2)(0.3) = 0.4\ \text{mol/L} \qquad (6)$$

Substitution of the numerical values into Eq. (3) gives

$$\tau = \frac{1 - 0.4}{(2)(0.025)(0.7)(0.4)} = 42.9\ \text{min}$$

6.2 CONSERVATION OF MASS

Summation of Eq. (6.1-2) over all species gives the total mass balance in the form

$$\boxed{\dot{m}_{in} - \dot{m}_{out} \pm \dot{m}_{int} = 0} \tag{6.2-1}$$

Note that the term

$$\sum_i \Big(\sum_j \alpha_{ij} \, r_j \Big) \mathcal{M}_i = 0 \tag{6.2-2}$$

since mass is conserved. Equation (6.2-2) implies that the rate of production of mass for the entire system is zero. However, if chemical reactions take place within the system, an individual species may be produced.

On the other hand, summation of Eq. (6.1-6) over all species gives the total mole balance as

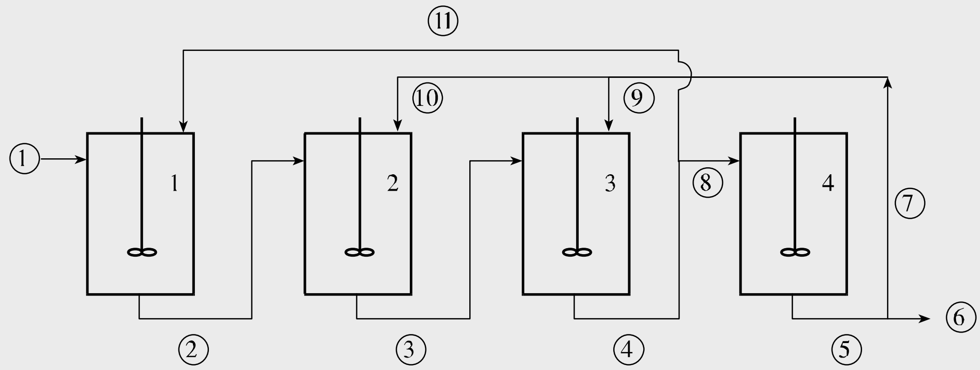
$$\boxed{\dot{n}_{in} - \dot{n}_{out} \pm \dot{n}_{int} + \Big[\sum_i \Big(\sum_j \alpha_{ij} \, r_j \Big) \Big] V_{sys} = 0} \tag{6.2-3}$$

In this case the generation term is not zero because moles are not conserved.

Example 6.2 A liquid phase irreversible reaction

$$A \rightarrow B$$

takes place in a series of four continuous stirred tank reactors as shown in the figure below.



The rate of reaction is given by

$$r = kc_A \qquad \text{with} \qquad k = 3 \times 10^5 \exp\Big(-\frac{4200}{T} \Big)$$

in which k is in h^{-1} and T is in degrees Kelvin. The temperature and the volume of each reactor are given as follows:

Reactor No	Temperature (°C)	Volume (L)
1	35	800
2	45	1000
3	70	1200
4	60	900

Determine the concentration of species $\mathcal{A}$ in each reactor if the feed to the first reactor contains 1.5 mol/L of $\mathcal{A}$ and the volumetric flow rates of the streams are given as follows:

Stream No	Volumetric Flow Rate (L/h)
1	500
7	200
9	50
11	100

Solution

Assumptions

1. Steady-state conditions prevail.
2. Concentrations of species within the reactor are uniform as a result of perfect mixing.
3. Liquid density remains constant.

Analysis

Conservation of total mass, Eq. (6.2-1), reduces to

$$\dot{m}_{in} = \dot{m}_{out} \tag{1}$$

Since the liquid density is constant, Eq. (1) simplifies to

$$\mathcal{Q}_{in} = \mathcal{Q}_{out} \tag{2}$$

Only four out of eleven streams are given in the problem statement. Therefore, it is necessary to write the following mass balances to calculate the remaining seven streams:

$$\mathcal{Q}_1 = \mathcal{Q}_6 = 500$$

$$500 + 100 = \mathcal{Q}_2$$

$$\mathcal{Q}_2 + \mathcal{Q}_{10} = \mathcal{Q}_3$$

$$\mathcal{Q}_3 + 50 = \mathcal{Q}_4$$

$$\mathcal{Q}_8 = \mathcal{Q}_5$$

$$\mathcal{Q}_5 = \mathcal{Q}_6 + 200$$

$$200 = 50 + \mathcal{Q}_{10}$$

Simultaneous solution of the above equations gives the volumetric flow rate of each stream as:

Stream No	Volumetric Flow Rate (L/h)
1	500
2	600
3	750
4	800
5	700
6	500
7	200
8	700
9	50
10	150
11	100

For each reactor, the reaction rate constant is

$$k = 3 \times 10^5 \exp\left[-\frac{4200}{(35+273)}\right] = 0.359\ \mathrm{h}^{-1} \qquad \text{for reactor \# 1}$$

$$k = 3 \times 10^5 \exp\left[-\frac{4200}{(45+273)}\right] = 0.551\ \mathrm{h}^{-1} \qquad \text{for reactor \# 2}$$

$$k = 3 \times 10^5 \exp\left[-\frac{4200}{(70+273)}\right] = 1.443\ \mathrm{h}^{-1} \qquad \text{for reactor \# 3}$$

$$k = 3 \times 10^5 \exp\left[-\frac{4200}{(60+273)}\right] = 0.999\ \mathrm{h}^{-1} \qquad \text{for reactor \# 4}$$

For each reactor, the conservation statement for species $\mathcal{A}$, Eq. (6.1-7), can be written in the form

$$(500)(1.5) + 100c_{A_3} - 600c_{A_1} - (0.359c_{A_1})(800) = 0$$

$$600c_{A_1} + 150c_{A_4} - 750c_{A_2} - (0.551c_{A_2})(1000) = 0$$

$$750c_{A_2} + 50c_{A_4} - 800c_{A_3} - (1.443c_{A_3})(1200) = 0$$

$$700c_{A_3} - 700c_{A_4} - (0.999c_{A_4})(900) = 0$$

Simplification gives

$$8.872c_{A_1} - c_{A_3} = 7.5$$

$$4c_{A_1} - 8.673c_{A_2} + c_{A_4} = 0$$

$$15c_{A_2} - 50.632c_{A_3} + c_{A_4} = 0$$

$$c_{A_3} - 2.284c_{A_4} = 0$$

The above equations are written in matrix notation[1] as

$$\begin{bmatrix} 8.872 & 0 & -1 & 0 \\ 4 & -8.673 & 0 & 1 \\ 0 & 15 & -50.632 & 1 \\ 0 & 0 & 1 & -2.284 \end{bmatrix} \begin{bmatrix} c_{A_1} \\ c_{A_2} \\ c_{A_3} \\ c_{A_4} \end{bmatrix} = \begin{bmatrix} 7.5 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Therefore, the solution is

$$\begin{bmatrix} c_{A_1} \\ c_{A_2} \\ c_{A_3} \\ c_{A_4} \end{bmatrix} = \begin{bmatrix} 8.872 & 0 & -1 & 0 \\ 4 & -8.673 & 0 & 1 \\ 0 & 15 & -50.632 & 1 \\ 0 & 0 & 1 & -2.284 \end{bmatrix}^{-1} \begin{bmatrix} 7.5 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0.115 & -0.004 & -0.002 & -0.003 \\ 0.054 & -0.119 & -0.002 & -0.053 \\ 0.016 & -0.036 & -0.021 & -0.025 \\ 0.007 & -0.016 & -0.009 & -0.449 \end{bmatrix} \begin{bmatrix} 7.5 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The multiplication gives the concentrations in each reactor as

$$\begin{bmatrix} c_{A_1} \\ c_{A_2} \\ c_{A_3} \\ c_{A_4} \end{bmatrix} = \begin{bmatrix} 0.859 \\ 0.402 \\ 0.120 \\ 0.053 \end{bmatrix}$$

6.3 CONSERVATION OF ENERGY

The conservation statement for *total* energy under steady conditions takes the form

$$\begin{pmatrix} \text{Rate of} \\ \text{energy in} \end{pmatrix} - \begin{pmatrix} \text{Rate of} \\ \text{energy out} \end{pmatrix} + \begin{pmatrix} \text{Rate of energy} \\ \text{generation} \end{pmatrix} = 0 \tag{6.3-1}$$

The first law of thermodynamics states that total energy can be neither created nor destroyed. Therefore, the rate of generation term in Eq. (6.3-1) equals zero.

Energy may enter or leave the system by two means: (*i*) by inlet and/or outlet streams, (*ii*) by exchange of energy between the system and its surroundings through the boundaries of the system in the form of heat and work.

For a system with a single inlet and a single outlet stream as shown in Figure 6.2, Eq. (6.3-1) can be expressed as

$$(\dot{E}_{in} + \dot{Q}_{int} + \dot{W}) - \dot{E}_{out} = 0 \tag{6.3-2}$$

where the interphase heat transfer rate, $\dot{Q}_{int}$, is expressed as

$$\dot{Q}_{int} = A_H \langle h \rangle (\Delta T)_{ch} \tag{6.3-3}$$

[1]Matrix operations are given in Section A.9 in Appendix A.

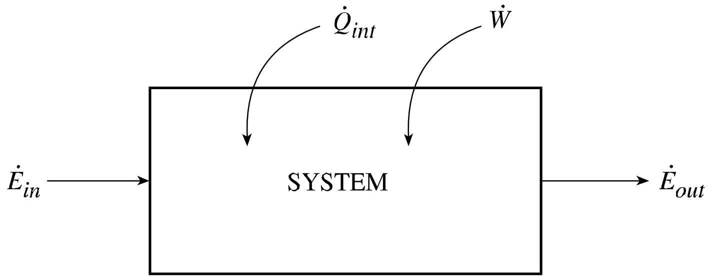


Figure 6.2. Steady-state flow system with fixed boundaries interchanging energy in the form of heat and work with the surroundings.

in which $(\Delta T)_{ch}$ is the characteristic temperature difference. Note that $\dot{Q}_{int}$ is considered positive when energy is added to the system. Similarly, $\dot{W}$ is also considered positive when work is done on the system.

As stated in Section 2.4.2, the rate of energy entering or leaving the system, $\dot{E}$, is expressed as

$$\dot{E} = \widehat{E}\dot{m} \tag{6.3-4}$$

Therefore, Eq. (6.3-2) becomes

$$(\widehat{E}\dot{m})_{in} - (\widehat{E}\dot{m})_{out} + \dot{Q}_{int} + \dot{W} = 0 \tag{6.3-5}$$

To determine the total energy per unit mass, $\widehat{E}$, consider an astronaut on the space shuttle *Atlantis*. When the astronaut looks at the earth, (s)he sees that the earth has an external kinetic energy due to its rotation and its motion around the sun. The earth also has an internal kinetic energy as a result of all the objects, i.e., people, cars, planes, etc., moving on its surface that the astronaut cannot see. A physical object is usually composed of smaller objects, each of which can have a variety of internal and external energies. The sum of the internal and external energies of the smaller objects is usually apparent as internal energy of the larger objects.

The above discussion indicates that the total energy of any system is expressed as the sum of its internal and external energies. Kinetic and potential energies constitute the external energy, while the energy associated with the translational, rotational, and vibrational motion of molecules and atoms is considered the internal energy. Therefore, total energy per unit mass can be expressed as

$$\widehat{E} = \widehat{U} + \widehat{E}_K + \widehat{E}_P \tag{6.3-6}$$

where $\widehat{U}$, $\widehat{E}_K$, and $\widehat{E}_P$ represent internal, kinetic, and potential energies per unit mass, respectively. Substitution of Eq. (6.3-6) into Eq. (6.3-5) gives

$$\left[\left(\widehat{U} + \widehat{E}_K + \widehat{E}_P\right)\dot{m}\right]_{in} - \left[\left(\widehat{U} + \widehat{E}_K + \widehat{E}_P\right)\dot{m}\right]_{out} + \dot{Q}_{int} + \dot{W} = 0 \tag{6.3-7}$$

The rate of work done on the system by the surroundings is given by

$$\dot{W} = \underbrace{\dot{W}_s}_{\text{Shaft work}} + \underbrace{(P\widehat{V}\dot{m})_{in} - (P\widehat{V}\dot{m})_{out}}_{\text{Flow work}} \tag{6.3-8}$$

In Figure 6.2, when the stream enters the system, work is done on the system by the surroundings. When the stream leaves the system, however, work is done by the system on the surroundings. Note that the boundaries of the system are fixed in the case of a steady-state flow system. Therefore, work associated with volume change is not included in Eq. (6.3-8).

Substitution of Eq. (6.3-8) into Eq. (6.3-7) and the use of the definition of enthalpy, i.e., $\widehat{H} = \widehat{U} + P\widehat{V}$, give

$$\boxed{\left[\left(\widehat{H} + \widehat{E}_K + \widehat{E}_P\right)\dot{m}\right]_{in} - \left[\left(\widehat{H} + \widehat{E}_K + \widehat{E}_P\right)\dot{m}\right]_{out} + \dot{Q}_{int} + \dot{W}_s = 0} \tag{6.3-9}$$

which is known as the *steady-state energy equation.*

The kinetic and potential energy terms in Eq. (6.3-9) are expressed in the form

$$\widehat{E}_K = \frac{1}{2}v^2 \tag{6.3-10}$$

and

$$\widehat{E}_P = gh \tag{6.3-11}$$

where g is the acceleration of gravity and h is the elevation with respect to a reference plane.

Enthalpy, on the other hand, depends on temperature and pressure. Change in enthalpy is expressed by

$$d\widehat{H} = \widehat{C}_P\,dT + \widehat{V}(1 - \beta T)\,dP \tag{6.3-12}$$

where β is the *coefficient of volume expansion* and is defined by

$$\beta = \frac{1}{\widehat{V}}\left(\frac{\partial \widehat{V}}{\partial T}\right)_P = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_P \tag{6.3-13}$$

Note that

$$\beta = \begin{cases} 0 & \text{for an incompressible fluid} \\ 1/T & \text{for an ideal gas} \end{cases} \tag{6.3-14}$$

When the changes in the kinetic and potential energies between the inlet and outlet of the system are negligible, Eq. (6.3-9) reduces to

$$\boxed{(\widehat{H}\dot{m})_{in} - (\widehat{H}\dot{m})_{out} + \dot{Q}_{int} + \dot{W}_s = 0} \tag{6.3-15}$$

In terms of molar quantities, Eqs. (6.3-9) and (6.3-15) are written as

$$\boxed{\left[\left(\widetilde{H} + \widetilde{E}_K + \widetilde{E}_P\right)\dot{n}\right]_{in} - \left[\left(\widetilde{H} + \widetilde{E}_K + \widetilde{E}_P\right)\dot{n}\right]_{out} + \dot{Q}_{int} + \dot{W}_s = 0} \tag{6.3-16}$$

and

$$\boxed{(\widetilde{H}\dot{n})_{in} - (\widetilde{H}\dot{n})_{out} + \dot{Q}_{int} + \dot{W}_s = 0} \tag{6.3-17}$$

6.3.1 Energy Equation Without a Chemical Reaction

In the case of no chemical reaction, Eqs. (6.3-9) and (6.3-16) are used to determine energy interactions. If kinetic and potential energy changes are negligible, then these equations reduce to Eqs. (6.3-15) and (6.3-17), respectively. The use of the energy equation requires the enthalpy change to be known or calculated. For some substances, such as steam and ammonia, enthalpy values are either tabulated or given in the form of a graph as a function of temperature and pressure. In that case enthalpy changes can be determined easily. If enthalpy values are not tabulated, then the determination of enthalpy depending on the values of temperature and pressure in a given process is given below.

6.3.1.1 *Constant pressure and no phase change* Since $dP = 0$, integration of Eq. (6.3-12) gives

$$\widehat{H} = \int_{T_{ref}}^{T} \widehat{C}_P \, dT \tag{6.3-18}$$

in which $\widehat{H}$ is taken as zero at T_{ref}. Substitution of Eq. (6.3-18) into Eq. (6.3-15) gives

$$\dot{m}_{in}\left(\int_{T_{ref}}^{T_{in}} \widehat{C}_P \, dT\right) - \dot{m}_{out}\left(\int_{T_{ref}}^{T_{out}} \widehat{C}_P \, dT\right) + \dot{Q}_{int} + \dot{W}_s = 0 \tag{6.3-19}$$

If $\widehat{C}_P$ is independent of temperature, Eq. (6.3-19) reduces to

$$\dot{m}_{in}\widehat{C}_P(T_{in} - T_{ref}) - \dot{m}_{out}\widehat{C}_P(T_{out} - T_{ref}) + \dot{Q}_{int} + \dot{W}_s = 0 \tag{6.3-20}$$

Example 6.3 It is required to cool a gas composed of 75 mole % N_2, 15% CO_2, and 10% O_2 from 800 °C to 350 °C. Determine the cooling duty of the heat exchanger if the heat capacity expressions are in the form

$$\widetilde{C}_P(\text{J/mol·K}) = a + bT + cT^2 + dT^3 \qquad T\ [=]\ \text{K}$$

where the coefficients a, b, c, and d are given by

Species	a	$b \times 10^2$	$c \times 10^5$	$d \times 10^5$
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

Solution

Assumptions

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

Analysis

System: Gas stream in the heat exchanger

Since $\dot{n}_{int} = 0$ and there is no chemical reaction, Eq. (6.2-3) reduces to

$$\dot{n}_{in} = \dot{n}_{out} = \dot{n} \tag{1}$$

Therefore, Eq. (6.3-19) becomes

$$\dot{Q}_{int} = \dot{n}\left(\int_{T_{ref}}^{T_{out}} \widetilde{C}_P \, dT - \int_{T_{ref}}^{T_{in}} \widetilde{C}_P \, dT\right) = \dot{n}\left(\int_{T_{in}}^{T_{out}} \widetilde{C}_P \, dT\right) \tag{2}$$

or,

$$\widetilde{Q}_{int} = \int_{T_{in}}^{T_{out}} \widetilde{C}_P \, dT \tag{3}$$

where $\widetilde{Q}_{int} = \dot{Q}_{int}/\dot{n}$, $T_{in} = 1073$ K, and $T_{out} = 623$ K.

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

$$\begin{aligned}\widetilde{C}_P &= \sum_{i=1}^{3} x_i(a_i + b_i T + c_i T^2 + d_i T^3) \\ &= 27.431 + 0.931 \times 10^{-2} T + 0.009 \times 10^{-5} T^2 - 0.902 \times 10^{-9} T^3 \end{aligned} \tag{4}$$

Substitution of Eq. (4) into Eq. (3) and integration give

$$\widetilde{Q}_{int} = -15{,}662 \text{ J/mol}$$

The minus sign indicates that heat must be removed from the gas stream.

6.3.1.2 *Constant pressure with phase change* When we start heating a substance at constant pressure, a typical variation in temperature as a function of time is given in Figure 6.3.

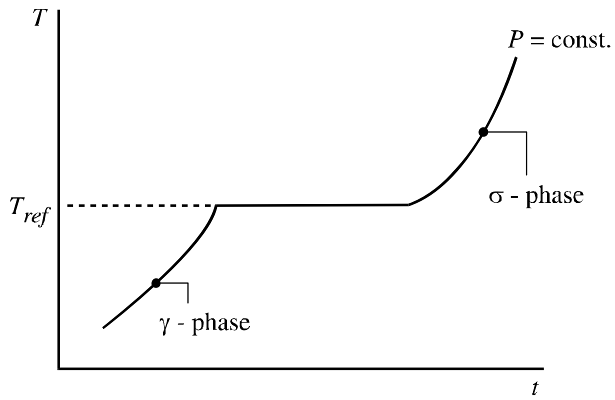


Figure 6.3. Temperature-time relationship as the substance transforms from the γ-phase to the σ-phase.

Conservation of Energy:-

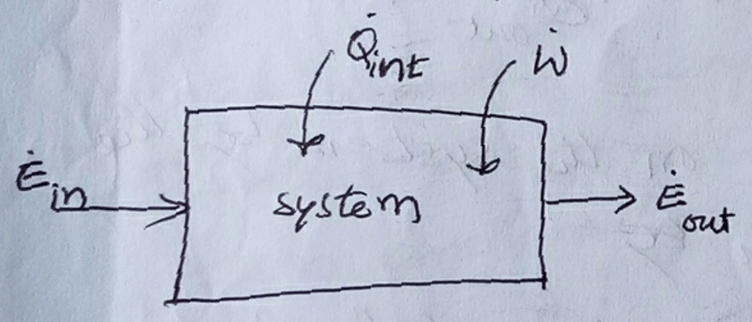
The conservation statement for total energy under steady conditions

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

According to first law of thermodynamics, total energy can neither be created nor destroyed. ∴ rate of generation term equals to zero.

Energy may enter (or) leave the system by two means ① By inlet/outlet streams

② by exchange of energy btw the system and its surroundings through the boundaries of the system in the form of heat and work.



For a system with a single inlet and outlet streams can be expressed as

$$(\dot{E}_{in} + \dot{Q}_{int} + \dot{W}) - \dot{E}_{out} = 0$$

Where,

$$\dot{Q}_{int} = A_H(h)(\Delta T)_{ch}$$

Note:- ① $\dot{Q}_{int}$ is considered +ve when energy is added to the system

② $\dot{W}$ is also considered +ve when work is done on the system.

we know, $\dot{E} = \hat{E}\dot{m}$

$\downarrow$

Rate of energy entering (or) leaving the system

$\hat{E}$ = Total energy per unit mass

$$(\hat{E}\dot{m})_{in} - (\hat{E}\dot{m})_{out} + \dot{Q}_{int} + \dot{W} = 0$$

Note:- Total energy of any system is expressed as the sum of its internal and External energies. kinetic & potential energies constitute the external energy, while the energy associated with the translational, rotational and vibration motion of molecules and atoms is considered as the internal energies.

$$\therefore \hat{E} = \hat{U} + \hat{E}_k + \hat{E}_p$$

$$\left[(\hat{U} + \hat{E}_k + \hat{E}_p)\dot{m}\right]_{in} - \left[(\hat{U} + \hat{E}_k + \hat{E}_p)\dot{m}\right]_{out} + \dot{Q}_{int} + \dot{W} = 0$$

the rate of work done on the system by the surroundings is given by

$$\dot{W} = \underset{\text{Shaft work}}{\underset{\downarrow}{\dot{W}_s}} + \underbrace{(P\hat{V}\dot{m})_{in} - (P\hat{V}\dot{m})_{out}}_{\text{Flow work}}$$

when the stream enter the system, work is done on the system by the surroundings. when the stream leaves the system, however, work is done by the system on the surroundings.

when the stream leaves the system, however (2)
work is done by the system on the surroundings.
Note that the boundaries of the system are
fixed in the case of a steady state flow system.
∴ work associated with volume change is not
included. & use of definition of Enthalpy
$\hat{H} = \hat{U} + P\hat{V}$

$$\left[(\hat{H} + \hat{E}_k + \hat{E}_p)\dot{m}\right]_{in} - \left[(\hat{H} + \hat{E}_k + \hat{E}_p)\dot{m}\right]_{out} + \dot{Q}_{int} + \dot{W}_s = 0$$

steady state energy equation. &

$$\hat{E}_k = \frac{1}{2}v^2, \quad \hat{E}_p = gh$$

Note:- when the changes in the kinetic and potential energies btw the inlet & outlet of the system are negligible.

$$(\hat{H}\dot{m})_{in} - (\hat{H}\dot{m})_{out} + \dot{Q}_{int} + \dot{W}_s = 0$$

In terms of molar quantities

$$(\hat{H}\dot{n})_{in} - (\hat{H}\dot{n})_{out} + \dot{Q}_{int} + \dot{W}_s = 0$$

I- Constant pressure and no phase change :- Energy eqn without chemical reaction.

$$dP = 0, \quad \hat{H} = \int_{T_{ref}}^{T} \hat{C}_p \, dT$$

in which $\hat{H}$ is taken as zero at T_{ref}

$$\dot{m}_{in}\left(\int_{T_{ref}}^{T_{in}} \hat{C}_p \, dT\right) - \dot{m}_{out}\left(\int_{T_{ref}}^{T_{out}} \hat{C}_p \, dT\right) +$$

$$\dot{Q}_{int} + \dot{W}_s = 0$$

If $\hat{C}_p$ is independent of temperature,

$$\dot{m}_{in}\hat{C}_p(T_{in} - T_{ref}) - \dot{m}_{out}\hat{C}_p(T_{out} - T_{ref})$$

$$+ \dot{Q}_{int} + \dot{W}_s = 0$$

Example 6.6 A liquid feed to a jacketed CSTR consists of 2000 mol/m^3 $\mathcal{A}$ and 2400 mol/m^3 $\mathcal{B}$. A second-order irreversible reaction takes place as

$$A + B \rightarrow 2C$$

The rate of reaction is given by

$$r = kc_A c_B$$

where the reaction rate constant at 298 K is $k = 8.4 \times 10^{-6}$ m^3/mol·min, and the activation energy is 50,000 J/mol. The reactor operates isothermally at 65 °C. The molar heat capacity at constant pressure and the standard heat of formation of species $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ at 298 K are given as follows:

Species	$\widetilde{C}_P^o$ (J/mol·K)	$\Delta \widetilde{H}_f^o$ (kJ/mol)
$\mathcal{A}$	175	−60
$\mathcal{B}$	130	−75
$\mathcal{C}$	110	−90

a) Calculate the residence time required to obtain 80% conversion of species $\mathcal{A}$.
b) What should be the volume of the reactor if species $\mathcal{C}$ are to be produced at a rate of 820 mol/min?

Solution

Assumptions

1. As a result of perfect mixing, concentrations of the species within the reactor are uniform, i.e., $(c_i)_{out} = (c_i)_{sys}$.
2. Solution nonidealities are negligible, i.e., $\overline{C}_{P_i} = \widetilde{C}_{P_i}$; $\Delta H_{rxn} = \Delta H^o_{rxn}$
3. There is no heat loss from the reactor.

Analysis

System: Contents of the reactor

a) Since the reactor volume is constant, the inlet and outlet volumetric flow rates are the same and equal to $\mathcal{Q}$. Therefore, the inventory rate equation for conservation of species $\mathcal{A}$, Eq. (6.1-7), becomes

$$\mathcal{Q}(c_A)_{in} - \mathcal{Q}(c_A)_{sys} - \left[k(c_A)_{sys}(c_B)_{sys}\right] V_{sys} = 0 \tag{1}$$

where $(c_A)_{sys}$ and $(c_B)_{sys}$ represent the molar concentrations of species $\mathcal{A}$ and $\mathcal{B}$ in the reactor, respectively. Dropping the subscript "sys" and dividing Eq. (1) by the volumetric flow rate, $\mathcal{Q}$, gives

$$\tau = \frac{(c_A)_{in} - c_A}{kc_A c_B} \tag{2}$$

Using Eq. (5.3-17), the extent of reaction can be calculated as

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

Therefore, the concentrations of species $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ in the reactor are

$$c_A = (c_A)_{in} + \alpha_A \xi = 2000 - 1600 = 400 \text{ mol/m}^3 \tag{4}$$

$$c_B = (c_B)_{in} + \alpha_B \xi = 2400 - 1600 = 800 \text{ mol/m}^3 \tag{5}$$

$$c_C = (c_C)_{in} + \alpha_C \xi = (2)(1600) = 3200 \text{ mol/m}^3 \tag{6}$$

If k_1 and k_2 represent the rate constants at temperatures of T_1 and T_2, respectively, then

$$k_2 = k_1 \exp\left[-\frac{\mathcal{E}}{\mathcal{R}}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)\right] \tag{7}$$

Therefore, the reaction rate constant at 65 °C (338 K) is

$$k = 8.4 \times 10^{-6} \exp\left[-\frac{50{,}000}{8.314}\left(\frac{1}{338} - \frac{1}{298}\right)\right] = 9.15 \times 10^{-5} \text{ m}^3/\text{mol·min} \tag{8}$$

Substitution of numerical values into Eq. (2) gives

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

b) The reactor volume, V, is given by

$$V = \tau \mathcal{Q}$$

The volumetric flow rate can be determined from the production rate of species $\mathcal{C}$, i.e.,

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

Hence, the reactor volume is

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