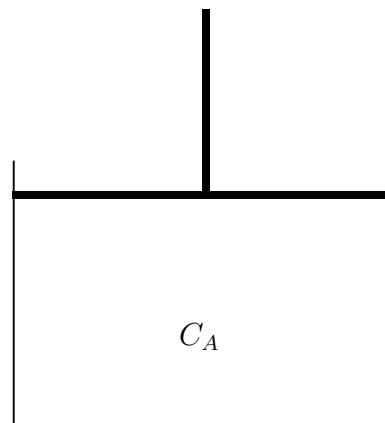


Design of Ideal Batch Reactors operated under Isothermal Conditions

(It is important to have this note set with you during all lecture classes.)

A batch reactor is such that a batch of reactants is fed to the reactor at the beginning, the reactants are allowed to react for a certain period of time, and the products are removed from the reactor at the end. While the reaction is progressing, nothing is fed to the batch reactor and nothing is taken away from the batch reactor. In an ideal batch reactor, the reacting mixture is assumed to be well mixed and therefore the properties of the reacting mixture are uniformly distributed through out the reactor.



C_A is the uniform concentration of the reactant A within the reacting mixture at time t

Design equation for reactant A in the batch reactor is obtained by writing the mass balance for reactant A over the volume of the reacting mixture V during time dt as follows:

$$\begin{aligned} & \text{mass of } A \text{ entering the reactor volume during time } dt \\ &= \text{mass of } A \text{ leaving the reactor volume during time } dt \\ & \quad + \text{mass of } A \text{ accumulated within the reactor volume during time } dt \\ & \quad + \text{mass of } A \text{ disappearing by the reaction during time } dt \end{aligned}$$

which becomes

$$0 = 0 + d(N_A M_A) + (-r_A) M_A V dt \quad (2.1)$$

where N_A is the number of moles of A within the reactor at time t , M_A is the molar mass of A , $d(M_A N_A)$ is the mass of A accumulated within the reactor during time dt , and $(-r_A)$ is the molar rate at which A is disappearing because of the progression of the reaction. Note that (r_A) is a negative quantity and therefore we have used the positive quantity $(-r_A)$ in the above mass balance. Also, note that the unit of r_A is in general moles per volume per time, and therefore r_A is multiplied by the molar mass of A to get the reaction rate in compatible unit for the mass balance given by (2.1).

Removing M_A from (2.1) and rearranging it, we get the design equation for reactant A in an ideal batch reactor as follows:

$$\frac{dN_A}{dt} = r_A V \quad (2.2)$$

Working out in terms of the number of moles of A, N_A :

The time t_f required to reduce the number of moles of A present in the batch reactor from N_{Ao} moles at the commencement of the reaction to N_{Af} moles at time t_f can be evaluated by integrating (2.2) as follows:

$$t_f = \int_{N_{Ao}}^{N_{Af}} \frac{1}{r_A V} dN_A = \int_{N_{Af}}^{N_{Ao}} \frac{1}{(-r_A) V} dN_A \quad (2.3)$$

where $(-r_A)$ should be expressed as a function of N_A in order to be able to perform the above integration.

Working out in terms of the concentration of A, C_A :

The concentration of A in the batch reactor is defined as

$$C_A \equiv \frac{\text{Number of moles of } A \text{ in the reacting mixture at time } t}{\text{Total volume of the reacting mixture at time } t} = \frac{N_A}{V} \quad (2.4)$$

Equation (2.4) gives $N_A = C_A V$. Substituting this in (2.2), we get

$$\frac{d(C_A V)}{dt} = r_A V \quad (2.5)$$

When the volume V of the reacting mixture remains a constant, (2.5) yields

$$t_f = \int_{C_{Ao}}^{C_{Af}} \frac{1}{r_A} dC_A = \int_{C_{Af}}^{C_{Ao}} \frac{1}{(-r_A)} dC_A \quad (2.6)$$

where C_{Ao} and C_{Af} are the respective concentrations of A at the beginning and at the end of the reaction, and $(-r_A)$ should be expressed as a function of C_A in order to perform the above integration.

If volume V does not remain constant during the reaction, the solution procedure gets slightly more complicated which will be discussed later in this note set.

Working out in terms of the conversion of A, x_A :

Conversion of A is defined by

$$x_A \equiv \frac{N_{Ao} - N_A}{N_{Ao}} \quad (2.7)$$

which gives $N_A = N_{Ao}(1 - x_A)$. Substituting it in (2.2), we get

$$\frac{-N_{Ao} dx_A}{dt} = r_A V \quad (2.8)$$

Upon integration of (2.8), we get

$$t_f = \int_0^{x_{Af}} \frac{N_{Ao}}{(-r_A) V} dx_A \quad (2.9)$$

where x_{Af} is the final conversion of A , and $(-r_A)$ should be expressed as a function of x_A in order to perform the above integration. If the volume of the reacting mixture V does not remain a constant during the reaction then V should also be expressed as a function of x_A , which will be worked out in Example 2.3 of this note set.

Example 2.1: Consider the elementary liquid-phase reaction $A \longrightarrow \text{products}$ taking place in an ideal batch reactor at constant temperature. Determine the time taken for the concentration of A to become half of its initial concentration.

Solution:

Since the given reaction is elementary, the reaction rate equation can be written as

$$r_A = -k C_A \quad (2.10)$$

where k , which is a function of temperature, remains constant since the reaction is said to take place at constant temperature.

Substituting r_A given by (2.10) in the design equation for A in an ideal batch reactor, given by (2.2), we get

$$\frac{dN_A}{dt} = -k C_A V \quad (2.11)$$

Since the concentration C_A in the batch reactor is defined as $C_A \equiv N_A/V$, see (2.4), we could rewrite (2.11) in terms of C_A as

$$\frac{d(C_A V)}{dt} = -k C_A V$$

The given reaction is a liquid phase-reaction, and therefore it is acceptable to assume that the density of the reacting mixture remains a constant. As far as there is no nuclear reaction taking place, the total mass of the reacting mixture remains a constant. Since the mass and the density of the reacting mixture are constants, the volume of the reacting mixture V is also a constant, which helps to simplify the above equation to

$$\frac{dC_A}{dt} = -k C_A \quad (2.12)$$

Integrating (2.12) with the initial condition $C_A = C_{A0}$ at $t = 0$, we get

$$C_A = C_{A0} \exp^{-kt}$$

which gives

$$t_f = \frac{-\ln(C_{Af}/C_{A0})}{k} \quad (2.13)$$

where t_f is the time taken to reach the final concentration of A and C_{Af} is the final concentration of A .

Therefore, the time taken to halve the initial concentration could be calculated as follows:

$$t_f = \frac{-\ln(0.5C_{A0}/C_{A0})}{k} = \frac{-\ln(0.5)}{k} \quad (2.14)$$

Note: Since r_A takes the unit mole per volume per time and C_A takes the unit mole per volume, (2.10) gives the unit of k as per time. (For example, if r_A is in moles/(litre.sec) and C_A is in moles/litre then k is in sec^{-1} .) Therefore, t_f in (2.14) would take the unit of time, as it should be. But, the unit of k is not always per time, and it depends on the form of the rate equation. Suppose the rate equation were given by $r_A = k C_A^2$ then the unit of k would be volume per mole per time so that r_A could take the unit mole per volume per time since C_A^2 takes the unit (mole/volume)².

Example 2.2: Determine the time taken to reach 90% conversion of A in the reaction of Example 2.1.

Solution:

Using $C_A = N_A/V$, we could rewrite (2.11) in terms of N_A as

$$\frac{dN_A}{dt} = -k N_A$$

From the definition of conversion, see (2.7), we get $N_A = N_{A0}(1 - x_A)$. Substituting this in the above equation, we get

$$-N_{A0} \frac{dx_A}{dt} = -k N_{A0}(1 - x_A)$$

which gets simplified to

$$\frac{dx_A}{dt} = k(1 - x_A) \quad (2.15)$$

Equation (2.15), when integrated with the conditions $x_A = 0$ at $t = 0$ and $x_A = x_{Af}$ at $t = t_f$, gives

$$t_f = \frac{1}{k} \int_0^{x_{Af}} \frac{dx_A}{(1 - x_A)} = \frac{1}{k} \left[-\ln(1 - x_A) \right]_0^{x_{Af}} = \frac{-\ln(1 - x_{Af})}{k} \quad (2.16)$$

Since $x_{Af} = 0.9$ we get

$$t_f = \frac{-\ln(0.1)}{k} \quad (2.17)$$

Example 2.3: Consider the gas-phase reaction $2A \rightarrow B + 2C$, for which the rate equation is given by

$$r_A = -k C_A^2 \quad (2.18)$$

Conversion of A required is expected to be 90%. Determine the time required to carry out the above reaction in an ideal batch reactor operated at constant temperature and constant pressure.

Solution:

Substituting r_A given by (2.18) in the design equation for reactant A in an ideal batch reactor, given by (2.2), we get

$$\frac{dN_A}{dt} = -k C_A^2 V \quad (2.19)$$

Since the reaction considered in this example is a gas-phase reaction, it is convenient to work it out in terms of conversion of A . In order to do that, we must first write the above differential equation in terms of N_A , which is done as follows:

Substituting $C_A = N_A/V$ in (2.19), we get a differential equation in terms of N_A as

$$\frac{dN_A}{dt} = -k \left(\frac{N_A}{V} \right)^2 V = -k \left(\frac{N_A^2}{V} \right) \quad (2.20)$$

From the definition of x_A given by (2.7), we get

$$N_A = N_{A_0}(1 - x_A) \quad (2.21)$$

Combining (2.20) and (2.21), we get

$$\frac{dx_A}{dt} = \frac{k N_{A_0}}{V} (1 - x_A)^2 \quad (2.22)$$

which is the differential equation in terms of conversion of A .

If the volume V remains a constant then (2.22) shall be integrated to obtain the time required to achieve 90% conversion of A as

$$t_f = \frac{1}{k C_{A_0}} \int_0^{0.9} \frac{1}{(1 - x_A)^2} dx_A \quad (2.23)$$

where $C_{A_0} = N_{A_0}/V$ for a constant-volume batch reactor.

But, the given reaction is a gas-phase reaction in which 2 moles of reactant give 3 moles of product. Besides, the temperature and the pressure remain constants. Therefore, the volume of the reacting mixture V would change with time. Let us use the ideal gas equation of state to describe the behaviour of the given gas mixture. We then get

$$P V = N_T R T \quad (2.24)$$

where N_T denotes the total number of moles of the reacting mixture at time t , and is given by

$$N_T = N_A + N_B + N_C + N_I \quad (2.25)$$

where N_A , N_B , N_C and N_I are the respective number of moles of A , B , C , and inert gas I present in the reactor at time t .

Stoichiometry gives

$$\frac{N_{A_0} - N_A}{2} = \frac{N_B - N_{B_0}}{1} = \frac{N_C - N_{C_0}}{2} \quad (2.26)$$

Equation (2.26) combined with (2.21) gives

$$N_B = N_{B_0} + N_{A_0}(x_A/2) \quad \text{and} \quad N_C = N_{C_0} + N_{A_0}(x_A) \quad (2.27)$$

The inert gas does not react, and therefore

$$N_I = N_{I_0} \quad (2.28)$$

Using (2.27) and (2.28) in (2.25), we get

$$N_T = N_{T_0} \left(1 + \frac{N_{A_0} x_A}{N_{T_0} 2} \right) \quad (2.29)$$

where $N_{T_0} = N_{A_0} + N_{B_0} + N_{C_0} + N_{I_0}$, denotes the total number of moles of the reacting mixture at the commencement of the reaction.

Substituting N_T from (2.29) in (2.24), we get

$$V = \frac{N_{T_o} R T}{P} \left(1 + \frac{N_{A_o} x_A}{N_{T_o} 2} \right). \quad (2.30)$$

Since the initial volume of the reacting mixture V_o also satisfies the ideal gas equation of state, given by $P_o V_o = N_{T_o} R T_o$, (2.30) can be rewritten as

$$= \frac{P_o}{P} \frac{T}{T_o} V_o \left(1 + \frac{N_{A_o} x_A}{N_{T_o} 2} \right). \quad (2.31)$$

Since the reactor is operated at constant pressure and constant temperature, (2.31) becomes

$$V = V_o \left(1 + \frac{N_{A_o} x_A}{N_{T_o} 2} \right). \quad (2.32)$$

Substituting V from (2.32) in (2.22), we get

$$\frac{dx_A}{dt} = \frac{k N_{A_o}}{V_o} \frac{(1 - x_A)^2}{1 + \frac{N_{A_o} x_A}{N_{T_o} 2}} = k C_{A_o} \frac{(1 - x_A)^2}{1 + \frac{N_{A_o} x_A}{N_{T_o} 2}} \quad (2.33)$$

where C_{A_o} is the initial concentration of A given by (N_{A_o}/V_o) .

Equation (2.33) shall be integrated to obtain the time required to achieve 90% conversion of A as

$$t_f = \frac{1}{k C_{A_o}} \int_0^{0.9} \frac{1 + \frac{N_{A_o} x_A}{N_{T_o} 2}}{(1 - x_A)^2} dx_A \quad (2.34)$$

If only pure A is present at the commencement of the reaction, then (2.34) reduces to

$$t_f = \frac{1}{k C_{A_o}} \int_0^{0.9} \frac{1 + 0.5 x_A}{(1 - x_A)^2} dx_A \quad (2.35)$$

For a general gas-phase reaction,



V is related to x_A by

$$V = \frac{P_o}{P} \frac{T}{T_o} V_o (1 + \epsilon_A x_A). \quad (2.37)$$

where

$$\epsilon_A = \frac{N_{A_o}}{N_{T_o}} \left[\frac{(p + q + s + \dots) - (a + b + c + \dots)}{a} \right] \quad (2.38)$$

and $N_{T_o} = (N_{A_o} + N_{B_o} + N_{C_o} + \dots) + (N_{P_o} + N_{Q_o} + N_{R_o} + \dots) + N_{I_o}$ is the total number of moles of the reacting mixture at the commencement of the reaction.

Self-study 3: Determine the numerical values of the integrations in (2.23) and (2.35).