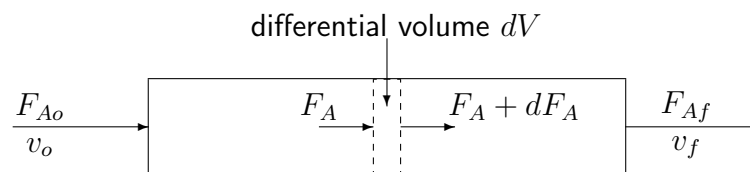


Design of Ideal Plug Flow Reactors (PFRs) operated at Steady State under Isothermal Conditions

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

In a plug flow reactor (abbreviated PFR), reactants are fed to the reactor at the inlet and the products are removed from the reactor at the outlet. The reaction takes place within the reactor as the reacting mixture moves through the pipe. In an ideal plug flow reactor, the reacting mixture is assumed to move as a plug and its properties are assumed to be uniformly distributed across the cross-section of the reactor.



F_A is the molar flow rate of A in moles per time

F_{Ao} is the molar flow rate of A at the inlet in moles per time

F_{Af} is the molar flow rate of A at the exit in moles per time

v_o is the volumetric flow rate at the inlet in volume per time

v_f is the volumetric flow rate at the exit in volume per time

Design equation for reactant A in the PFR is obtained by writing the mass balance for reactant A over a differential volume of the reacting mixture dV as follows:

$$\begin{aligned} & \text{mass of } A \text{ entering the volume } dV \text{ per unit time} \\ &= \text{mass of } A \text{ leaving the volume } dV \text{ per unit time} \\ &+ \text{mass of } A \text{ accumulated within the volume } dV \text{ per unit time} \\ &+ \text{mass of } A \text{ disappearing by the reaction within the volume } dV \text{ per unit time} \end{aligned}$$

At steady state, no accumulation takes place. Therefore, at steady state, the above reduces to

$$F_A M_A = (F_A + dF_A) M_A + (-r_A) M_A dV \quad (4.1)$$

where F_A is the number of moles of A per unit time entering the differential volume dV , $(F_A + dF_A)$ is the number of moles of A per unit time leaving the differential volume dV , M_A is the molar mass of A , and $(-r_A)$ is the molar rate at which A is disappearing because of the progression of the reaction. 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 (4.1).

Removing M_A from (4.1) and rearranging it, we get the design equation for reactant A in an ideal PFR operated at steady-state as follows:

$$\frac{dF_A}{dV} = r_A \quad (4.2)$$

Working out in terms of the molar flow rate of A, F_A :

The volume V_{PFR} required to reduce the molar flow rate of A in the PFR from F_{Ao} mol/sec at the entrance of the reactor to F_{Af} mol/sec at the exit of the reactor can be evaluated by integrating (4.2) as follows:

$$V_{PFR} = \int_{F_{Ao}}^{F_{Af}} \frac{1}{r_A} dF_A = \int_{F_{Af}}^{F_{Ao}} \frac{1}{(-r_A)} dF_A \quad (4.3)$$

where $(-r_A)$ should be expressed as a function of F_A .

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

Concentration C_A in an ideal PFR is defined as follows:

$$C_A \equiv \frac{\text{Molar flow rate of } A \text{ at a certain cross-section}}{\text{Volumetric flow rate of the reacting mixture at the cross-section}} = \frac{F_A}{v} \quad (4.4)$$

Equation (4.4) gives $F_A = C_A v$. Substituting which in (4.2), we get

$$\frac{d(C_A v)}{dV} = r_A \quad (4.5)$$

If the volumetric flow rate v is a constant then (4.5) yields

$$V_{PFR} = \int_{C_{Ao}}^{C_{Af}} \frac{v}{r_A} dC_A = \int_{C_{Af}}^{C_{Ao}} \frac{v}{(-r_A)} dC_A \quad (4.6)$$

where C_{Ao} and C_{Af} are the respective concentrations of A at the entrance and at the exit of the reactor, respectively, and $(-r_A)$ should be expressed as a function of C_A .

If the volumetric flow rate v is not a constant then the solution procedure gets slightly more complicated which will be discussed in Example 4.3 of this note set.

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

Conversion of A in a PFR is defined by

$$x_A \equiv \frac{F_{Ao} - F_A}{F_{Ao}} \quad (4.7)$$

which gives $F_A = F_{Ao}(1 - x_A)$. Substituting which in (4.2), we get

$$\frac{-F_{Ao} dx_A}{dV} = r_A \quad (4.8)$$

Equation (4.8), when integrated with the conditions $x_A = 0$ at the entrance (where $V = 0$) and $x_A = x_{Af}$ at the exit (where $V = V_{PFR}$), gives

$$V_{PFR} = \int_0^{x_{Af}} \frac{F_{Ao}}{(-r_A)} dx_A \quad (4.9)$$

where x_{Af} is the conversion of A at the exit of the reactor, and $(-r_A)$ should be expressed as a function of x_A .

Example 4.1: Consider the elementary liquid-phase reaction $A \rightarrow \text{products}$ taking place in an ideal PFR operated at steady state at constant temperature. Determine the space-time required for the concentration of A to become half of its inlet concentration.

Solution:

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

$$r_A = -k C_A \quad (4.10)$$

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 (4.10) in the design equation for A in an ideal PFR operated at steady state, given by (4.2), we get

$$\frac{dF_A}{dV} = -k C_A \quad (4.11)$$

Substituting $F_A = C_A v$ in (4.11), we get a differential equation in terms of C_A as

$$\frac{d(C_A v)}{dV} = -k C_A$$

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. At steady flow, the mass flow rate of the reacting mixture remains a constant. Thus, the volumetric flow rate of the reacting mixture v remains a constant, which helps to simplify the above equation to

$$v \frac{dC_A}{dV} = -k C_A \quad (4.12)$$

The space-time for an ideal PFR is defined as

$$\tau \equiv \frac{\text{Volume of the reactor}}{\text{Volumetric flow rate of the reacting mixture}} = \frac{V}{v} \quad (4.13)$$

where v is taken as a constant.

From (4.13), we get $dV = v d\tau$. Using which (4.12) can be rewritten as

$$\frac{dC_A}{d\tau} = -k C_A \quad (4.14)$$

Note that (4.14) is very similar to (2.12) describing the batch reactor (see Set #2), except for the fact time t for the batch reactor is replaced by space-time τ for the PFR.

The differential equation describing the liquid-phase reaction in an ideal PFR operated at steady-state and the differential equation describing the liquid-phase reaction in a batch reactor are very similar in nature.

At the entrance of the reactor, τ takes the value zero and $C_A = C_{A_0}$. Integrating (4.14) with this condition, we get

$$C_A = C_{A_0} \exp^{-k\tau}$$

which gives

$$\tau_f = \frac{-\ln(C_{Af}/C_{Ao})}{k} \quad (4.15)$$

where τ_f is the space-time required to obtain the final concentration of A and C_{Af} is the final concentration of A .

Therefore, the space-time required to halve the initial concentration could be calculated as follows:

$$\tau_f = \frac{-\ln(0.5C_{Ao}/C_{Ao})}{k} = \frac{-\ln(0.5)}{k} \quad (4.16)$$

Example 4.2: Determine the space-time taken to reach 90% conversion of A in the reaction considered in Example 4.1.

Solution:

Using $C_A = F_A/v$ and $dV = v d\tau$ for constant v in (4.11), we get a differential equation in terms of F_A as

$$\frac{dF_A}{d\tau} = -k F_A$$

Substituting $F_A = F_{Ao}(1 - x_A)$ in the above equation, we get

$$-F_{Ao} \frac{dx_A}{d\tau} = -k F_{Ao}(1 - x_A)$$

which gets simplified to

$$\frac{dx_A}{d\tau} = k(1 - x_A) \quad (4.17)$$

which is similar to (2.15) describing the batch reactor (see Set #2).

Equation (4.17), when integrated with the conditions $x_A = 0$ at the entrance (where $V = 0$) and $x_A = x_{Af}$ at the exit (where $V = V_{PFR}$), gives

$$\tau_f = \frac{1}{k} \int_0^{x_{Af}} \frac{dx_A}{(1 - x_A)} = \frac{1}{k} \left[-\ln(1 - x_A) \right]_0^{x_{Af}} = \frac{-\ln(1 - x_{Af})}{k} \quad (4.18)$$

Since $x_{Af} = 0.9$ we get

$$\tau_f = \frac{-\ln(0.1)}{k} \quad (4.19)$$

Example 4.3: Consider the gas-phase reaction $2A \rightarrow B + 2C$, for which the rate equation is given by

$$r_A = -k C_A^2 \quad (4.20)$$

Conversion of A required is expected to be 90%. Determine the space-time required to carry out the above reaction in an ideal PFR operated at steady state under constant temperature and constant pressure conditions.

Solution:

Substituting r_A given by (4.20) in the design equation of an ideal PFR operated at steady state, given by (4.2), we get

$$\frac{dF_A}{dV} = -k C_A^2 \quad (4.21)$$

Since the problem 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 F_A , which is done as follows:

Substituting $C_A = F_A/v$ in (4.21), we get a differential equation in terms of F_A as

$$\frac{dF_A}{dV} = -k \left(\frac{F_A^2}{v^2} \right) \quad (4.22)$$

Conversion of A at distance l from the entrance of a PFR is denoted by x_A and is defined as $x_A \equiv \frac{F_{A0} - F_A}{F_{A0}}$ which gives

$$F_A = F_{A0}(1 - x_A) \quad (4.23)$$

Combining (4.21) and (4.23), we get

$$\frac{dx_A}{dV} = \frac{k F_{A0}}{v^2} (1 - x_A)^2 \quad (4.24)$$

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

If the volumetric flow rate v remains a constant then (4.24) can be integrated to obtain the volume V required to achieve 90% conversion of A .

$$V = \frac{v}{k C_{A0}} \int_0^{0.9} \frac{1}{(1 - x_A)^2} dx_A \quad (4.25)$$

where $C_{A0} = F_{A0}/v$ for an ideal PFR with constant volumetric flow rate.

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 volumetric flow rate v would change with the distance l from the entrance of the reactor. Let us use the ideal gas equation of state to describe the behaviour of the given gas mixture. We then get

$$Pv = F_T RT \quad (4.26)$$

where F_T denotes the total molar flow rate of the reacting mixture at distance l from the entrance of the reactor, and is given by

$$F_T = F_A + F_B + F_C + F_I \quad (4.27)$$

where F_A , F_B , F_C and F_I are the respective molar flow rates of A , B , C , and inert gas I at distance l from the entrance of the reactor.

Stoichiometry gives

$$\frac{F_{A0} - F_A}{2} = \frac{F_B - F_{B0}}{1} = \frac{F_C - F_{C0}}{2} \quad (4.28)$$

Equation (4.28) combined with (4.23) gives

$$F_B = F_{B0} + F_{A0}(x_A/2) \quad \text{and} \quad F_C = F_{C0} + F_{A0}(x_A) \quad (4.29)$$

The inert gas does not react, and therefore

$$F_I = F_{I_o} \quad (4.30)$$

Using (4.29) and (4.30) in (4.27), we get

$$F_T = F_{T_o} \left(1 + \frac{F_{A_o}}{F_{T_o}} \frac{x_A}{2} \right) \quad (4.31)$$

where $F_{T_o} = F_{A_o} + F_{B_o} + F_{C_o} + F_{I_o}$, denotes the total molar flow rate of the reacting mixture at the entrance of the reactor.

Substituting F_T from (4.31) in (4.26), we get

$$v = \frac{F_{T_o} R T}{P} \left(1 + \frac{F_{A_o}}{F_{T_o}} \frac{x_A}{2} \right) \quad (4.32)$$

Since the volumetric flow rate of the feed v_o also satisfies the ideal gas equation of state, as $P_o v_o = F_{T_o} R T_o$, (4.32) can be rewritten as

$$v = \frac{P_o}{P} \frac{T}{T_o} v_o \left(1 + \frac{F_{A_o}}{F_{T_o}} \frac{x_A}{2} \right) \quad (4.33)$$

Since the reactor is maintained at constant pressure and temperature, (4.33) becomes

$$v = v_o \left(1 + \frac{F_{A_o}}{F_{T_o}} \frac{x_A}{2} \right) \quad (4.34)$$

Substituting v from (4.34) in (4.24), we get

$$\frac{dx_A}{dV} = \frac{k F_{A_o}}{v_o^2} \frac{(1 - x_A)^2}{\left(1 + \frac{F_{A_o}}{F_{T_o}} \frac{x_A}{2} \right)^2} = \frac{k C_{A_o}}{v_o} \frac{(1 - x_A)^2}{\left(1 + \frac{F_{A_o}}{F_{T_o}} \frac{x_A}{2} \right)^2} \quad (4.35)$$

where C_{A_o} is the concentration of A at the entrance of the reactor given by (F_{A_o}/v_o) .

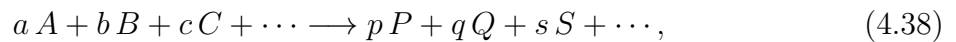
Equation (4.35) shall be integrated to obtain the space-time of an ideal PFR required to achieve 90% conversion of A as

$$\tau \equiv \frac{V}{v_o} = \frac{1}{k C_{A_o}} \int_0^{0.9} \frac{\left(1 + \frac{F_{A_o}}{F_{T_o}} \frac{x_A}{2} \right)^2}{(1 - x_A)^2} dx_A \quad (4.36)$$

Let us suppose that only pure A is fed to the reactor. Then (4.36) reduces to

$$\tau = \frac{1}{k C_{A_o}} \int_0^{0.9} \frac{(1 + 0.5 x_A)^2}{(1 - x_A)^2} dx_A \quad (4.37)$$

For a general gas-phase reaction,



the volumetric flow rate v is related to x_A by

$$v = \frac{P_o}{P} \frac{T}{T_o} v_o (1 + \epsilon_A x_A). \quad (4.39)$$

where

$$\epsilon = \frac{F_{A_o}}{F_{T_o}} \left[\frac{(p + q + s + \dots) - (a + b + c + \dots)}{a} \right] \quad (4.40)$$

and $F_{T_o} = (F_{A_o} + F_{B_o} + F_{C_o} + \dots) + (F_{P_o} + F_{Q_o} + F_{R_o} + \dots) + F_{I_o}$ is the total number of moles of the reacting mixture entering the reactor.