

and pressure

$$\frac{dX}{dW} = F_1(X, P) \quad \dots (4-26)$$

We now need to relate the pressure drop to the catalyst weight in order to determine the conversion as a function of catalyst weight.

4.4.2 Flow Through a Packed Bed

The majority of gas-phase reactions are catalyzed by passing the reactants through a packed bed of catalyst particles. The equation used most to calculate pressure drop in a packed porous bed is the Ergun Equation.

$$\frac{dP}{dL} = - \frac{G}{\rho g_c D_p} \left(\frac{1-\Phi}{\Phi^3} \right) \left[\frac{150(1-\Phi)\mu}{D_p} + 1.75 G \right] \dots (4-27)$$

where: P = Pressure, lb/ft²

Φ = porosity = $\frac{\text{volume of void}}{\text{total bed volume}}$

$1-\Phi$ = $\frac{\text{volume of solid}}{\text{total bed volume}}$

$g_c = 3.2.174 \frac{\text{lbm} \cdot \text{ft}}{\text{s}^2 \cdot \text{lb}_f}$ (conversion factor)
 $= 4.17 \times 10^8 \frac{\text{lbm} \cdot \text{ft}}{\text{h}^2 \cdot \text{lb}_f}$

D_p = diameter of particle in bed, ft

μ = viscosity of gas passing through the bed, $\frac{\text{lbm}}{\text{ft} \cdot \text{h}}$

L = length down the pipe, ft

u = superficial velocity = volumetric flow ÷ cross-sectional area of pipe, ft/h

ρ = gas density, lb/ft³

$G = \rho u$ = superficial mass velocity, g/cm².s or lbm/ft².h

For packed-bed reactors, we are usually more interested in the relationships between pressure and catalyst weight rather than pressure and reactor volume. The reactor volume and catalyst weight W are related through the eqn.:

$$W = (1 - \Phi) A_c L * \rho_c \quad \text{--- (4-28)}$$

$$\left[\text{Weight of catalyst} \right] = \left[\text{Volume of solid} \right] * \left[\text{density of solid catalyst} \right]$$

Where A_c is the cross-sectional area. Changing variables to write eqn (4-27) in terms of weight

$$\frac{dP}{dW} = \frac{G}{\rho g_c D_p} \left(\frac{1}{\Phi_3} \right) \left[\frac{150(1-\Phi)\mu}{D_p} + 1.75 G \right] \frac{1}{A_c \rho_c} \quad \text{--- (4-29)}$$

In calculating the pressure drop using the Ergun equation, the only parameter that varies with pressure on the R.H.S of eqn. (4-27) is the gas density, ρ . We are now going to calculate the pressure through the bed for two cases.

Case 1: Constant Density : If we assume that the gas density is constant at a mean value,

$\bar{\rho}$, then :

$$\frac{dP}{dL} = -\bar{\beta}$$

where

$$\bar{\beta} = \frac{G(1-\Phi)}{\bar{\rho} g_c D_p \Phi^3} \left[\frac{150(1-\Phi)\mu}{D_p} + 1.75G \right] \quad \dots (4-30)$$

Integrating with limits $P = P_0$ at $L = 0$ and $P = P$ at $L = L$, the pressure P at a distance L down the reactor is

$$P = P_0 - \bar{\beta} L$$

Dividing by P_0 gives

$$\frac{P}{P_0} = 1 - \frac{\bar{\beta} L}{P_0}$$

We can also relate pressure to volume :

$$V = A_c L$$

$$\frac{P}{P_0} = 1 - \frac{\bar{\beta} V}{P_0 A_c} \quad \dots (4-31)$$

Equation (4-31) gives the pressure as a function of volume of the reactor through which the gas has passed. To relate the pressure to catalyst weight, we recall Equation (4-28) :

$$W = (1-\Phi) \bar{\rho}_c V, \text{ therefore}$$

Pressure ratio for constant gas density

$$\frac{P}{P_0} = 1 - \frac{\bar{\beta}}{A_c P_0 (1-\Phi)/c} W = 1 - \bar{\alpha} W \quad \text{--- (4-32)}$$

where $\bar{\alpha} = \frac{\bar{\beta}}{A_c P_0 (1-\Phi)/c}$

Now that we have expressed pressure as a function of catalyst weight for the case of constant density, i.e.,

$$\boxed{\frac{P}{P_0} = 1 - \bar{\alpha} W} \quad \text{--- (4-32)}$$

We can return to the first order isothermal reaction $A \rightarrow B$, to relate conversion and catalyst weight.

Combining equations (4-24) and (4-32) and noting that $E=0$ for isomerization reactions, we obtain for isothermal operation

$$-r_A' = K C_{A0} (1-X) (1 - \bar{\alpha} W) \quad \text{--- (4-33)}$$

Substituting in the design equation yields

$$F_{A0} \frac{dX}{dW} = K C_{A0} (1-X) (1 - \bar{\alpha} W) \quad \text{--- (4-34)}$$

Separating variables gives

$$\frac{F_{A0}}{K C_{A0}} \int_0^X \frac{dX}{1-X} = \int_0^W (1 - \bar{\alpha} W) dW \quad \text{--- (4-35)}$$

and integrating with limits $x=0$ when $W=0$;
 $x=X$ when $W=W$

$$\frac{U_0}{K} \ln \frac{1}{1-x} = W \left(1 - \frac{\bar{\alpha} W}{2} \right) \quad \dots (4-36)$$

Solving for the catalyst weight,

$$\left(\begin{array}{l} \text{catalyst} \\ \text{weight for} \\ \text{1st order reaction} \\ \text{constant } \rho \end{array} \right) W = \frac{1 - \left\{ 1 - (2U_0 \bar{\alpha} / K) \ln [1/(1-x)] \right\}^{1/2}}{\bar{\alpha}} \quad \dots (4-37)$$

Case 2: Variable density

Because the reactor is operated at steady state, the mass flow rate at any point down the reactor, \dot{m} (kg/s), is equal to the entering mass flow rate, \dot{m}_0 (i.e., equation of continuity),

$$\dot{m}_0 = \dot{m}$$

$$\rho_0 U_0 = \rho U$$

Recalling eqn. (C-10), we have

$$U = U_0 (1 + \epsilon x) \left(\frac{\rho_0}{\rho} \right) \left(\frac{T}{T_0} \right) \quad \dots ()$$

$$\rho = \rho_0 \frac{U_0}{U} = \rho_0 \left[\left(\frac{T_0}{T} \right) \left(\frac{1}{1 + \epsilon x} \right) \right] \frac{\rho}{\rho_0} \quad \dots (4-38)$$

Combining equations (4-38) and (4-27) gives,

$$\frac{dP}{dL} = - \frac{G}{\rho_0 g_c D_p} \frac{(1-\Phi)}{\Phi^3} \left[\frac{150(1-\Phi) \mu}{D_p} + 1.75 G \right] \frac{\rho_0 T}{P T_0} \quad \dots (4-39)$$

$$\frac{dP}{dL} = - \beta_0 \left[\frac{T \rho_0}{T_0 P} (1 + \epsilon x) \right] \quad \dots (4-40)$$

where

$$\beta_0 = \frac{G(1-\Phi)}{\rho_0 g_c D_p \Phi^3} \left[\frac{150(1-\Phi)\mu}{D_p} + 1.75 G \right] \quad \dots (4-41)$$

with the aid of eqn. (4-28), eqn. (4-40) can be expressed in terms of catalyst weight.

$$\frac{dP}{dW} = - \frac{\beta_0}{A_c \rho_0 (1-\Phi)} \cdot \frac{T P_0}{T_0 P} (1 + \varepsilon x)$$

$$\boxed{\frac{dP}{dW} = - \frac{\alpha}{2} \frac{T}{T_0} \frac{P_0}{(P/P_0)} (1 + \varepsilon x)} \quad \dots (4-42)$$

where $\alpha = \frac{2\beta_0}{A_c \rho_0 (1-\Phi) P_0}$

For isothermal operation, eqn. (4-42) is only a function of conversion and pressure, i.e.,

$$\frac{dP}{dW} = F_2(X, P) \quad \dots (4-43)$$

Recalling eqn. (4-26)

$$\frac{dX}{dW} = F_1(X, P) \quad \dots (4-26)$$

We see that we have two coupled first-order differential equations (4-26), and (4-43) that must be solved simultaneously. A variety of numerical integration schemes are available for this purpose, some of which are given in Appendix A6.

However, if $\varepsilon = 0$, or if we can neglect (εx) w.r.t 1.0 (i.e., $1 \gg \varepsilon x$), we can obtain an analytical solution to eqn. (4-40) for isothermal operation. For isothermal operation, eqn. (4-40) becomes,

Isothermal
with $\varepsilon=0$

$$\frac{dP}{dL} = -\beta_0 \frac{P_0}{P}$$

Integrating with $P=P_0$ at $L=0$

$$\left(\frac{P}{P_0}\right)^2 = 1 - \frac{2\beta_0 L}{P_0}$$

$$\boxed{\frac{P}{P_0} = \left(1 - \frac{2\beta_0 L}{P_0}\right)^{1/2}} \quad \dots \dots (4-44)$$

In terms of catalyst weight

Pressure
ratio for
variable gas
density

$$\boxed{\frac{P}{P_0} = (1 - \alpha W)^{1/2}} \quad \dots \dots (4-45)$$

Where again $\alpha = \frac{2\beta_0}{A_c(1-\phi)\rho_c P_0}$

Equation (4-45) can be used to substitute for the pressure in the rate law, in which case the mole balance can be written solely as a function of conversion and catalyst weight. The resulting equation can be readily solved either analytically or numerically.

Example (4-5) : Calculating Pressure Drop in a Packed Bed

Calculate the pressure drop in a 60 ft length of $1\frac{1}{2}$ in. schedule 40 pipe packed with catalyst pellets $\frac{1}{4}$ in. in diameter where 104.4 lb/h of gas is passing through the bed. The temperature is constant along the length of pipe at 260°C . The void fraction is 45% and the properties of the gas

are similar to those of air at this temperature. The entering pressure is 10 atm. Assume variable density.

Solution

$$\frac{P}{P_0} = \left(1 - \frac{2\beta_0 L}{P_0}\right)^{1/2} \quad \text{--- (4-44)}$$

$$\beta_0 = \frac{G(1-\Phi)}{g_c \rho_0 D_p \Phi^3} \left[\frac{150(1-\Phi)\mu}{D_p} + 1.75G \right] \quad \text{--- (4-41)}$$

For $1\frac{1}{2}$ in, schedule 40 pipe, $A_c = 0.01414 \text{ ft}^2$

$$G = \frac{104.4}{0.01414} = 7383.3 \text{ lb/h. ft}^2$$

For air at 260°C and 10 atm

$$\mu = 0.0673 \text{ lbm/ft.h}$$

$$\rho_0 g_c = 0.413 \text{ lbm/ft}^3$$

From problem statements $D_p = \frac{1}{4} \text{ in} = 0.0208 \text{ ft}$
 $g_c = 4.17 \times 10^8 \text{ lbm.ft/lbf.h}^2$

Substituting the values above into Equation (4-41) to obtain:

$$\beta_0 = \left[\frac{7383.3}{0.0208 \times 4.17 \times 10^8 \times 0.413 \times (0.45)^3} \right] \times \left[\frac{150(1-0.45)0.0673}{0.0208} + 1.75(7383.3) \right]$$

$$= 0.0775 \frac{\text{atm}}{\text{ft}}$$

$$\frac{P}{P_0} = \left(1 - \frac{2\beta_0 L}{P_0}\right)^{1/2} = \left(1 - \frac{2 \times 0.0775 \times 60}{10}\right)^{1/2}$$

$$P = 0.265 P_0 = 2.65 \text{ atm}$$

$$\Delta P = P_0 - P = 10 - 2.65 = 7.35 \text{ atm.}$$

We now proceed (Example 4.6) to combine pressure drop with reaction in packed-bed for the case where we will assume $\varepsilon X \ll 1$ in the Ergun eqn. but not in the rate law in order to obtain an analytical solution.

Example (4.6) Calculating X in a Reactor with Pressure Drop

Approximately 5 billion pounds of ethylene oxide was produced in the USA in 1990. Over 60% of the ethylene oxide produced is used to make ethylene glycol. The end uses of ethylene oxide are antifreeze (30%), polyester (30%), surfactants (10%), and solvents (5%).

We want to calculate the catalyst weight necessary to achieve 60% conversion when ethylene oxide is to be made by the vapour-phase catalytic oxide of ethylene with air



Ethylene and Oxygen are fed in stoichiometric proportions to a packed-bed reactor operated isothermally at 260°C. Ethylene is fed at a rate of 0.30 lbmol/s at a

pressure of 10 atm. It is proposed to use 10 banks of $1\frac{1}{2}$ in.-diameter schedule 40 tubes packed with catalyst with 100 tubes per bank. Consequently, the molar flow rate to each tube is to be 3×10^{-4} lbmol/s. The properties of the reacting fluid are to be considered identical to those of air at this temperature and pressure. The density of the $\frac{1}{4}$ in.-catalyst particle is 120 lb/ft³ and the bed void is 0.45. The rate law is:

$$-r_A' = K P_A^{1/3} P_B^{2/3} \quad \text{lbmol/lb cat} \cdot \text{h}$$

with $K = 0.0141$
260°C.

lbmol/atm. lb cat. h at

Solution

1. Differential mole balance: $F_{A0} \frac{dX}{dW} = -r_A' \quad \dots (E4-6.1)$

2. Rate law: $-r_A' = K P_A^{1/3} P_B^{2/3} = K (C_A R T)^{1/3} (C_B R T)^{2/3} \dots (E4-6.2)$
 $= K R T_0 C_A^{1/3} C_B^{2/3} \dots (E4-6.3)$

3. Stoichiometry: Gas-phase, isothermal $V = V_0(1+EX)(P_0/P)$
 $C_A = \frac{F_A}{V} = \frac{C_{A0}(1-X)}{(1+EX)} \frac{P}{P_0} \dots (E4-6.4)$

$C_B = \frac{F_B}{V} = \frac{C_{A0}(\Theta_B - X/2)}{(1+EX)} \left(\frac{P}{P_0}\right) \dots (E4-6.5)$

4. Combining the rate law and concentrations:

$$-r_A' = K R T_0 \left[\frac{C_{A0}(1-X)}{1+EX} \left(\frac{P}{P_0}\right) \right]^{1/3} \left[\frac{C_{A0}(\Theta_B - X/2)}{1+EX} \left(\frac{P}{P_0}\right) \right]^{2/3} \dots (E4-6.6)$$

$$-r'_A = \frac{K C_{A_0} R T_0}{1 + \varepsilon X} \left(\frac{P}{P_0} \right) (1 - X)^{1/3} \left(\theta_B - \frac{X}{2} \right)^{2/3} \dots (E4-6.7)$$

For stoichiometric feed, $\theta_B = 1/2$;

$$\begin{aligned} -r'_A &= K P_{A_0} \frac{(1 - X)^{1/3} \left(\frac{1}{2} - \frac{X}{2} \right)^{2/3}}{1 + \varepsilon X} \left(\frac{P}{P_0} \right) \\ &= K' \left(\frac{1 - X}{1 + \varepsilon X} \right) \frac{P}{P_0} \dots (E4-6.8) \end{aligned}$$

where $K' = K P_{A_0} \left(\frac{1}{2} \right)^{2/3} = 0.63 P_{A_0}$

5. Developing the design equation: For a packed-bed reactor the relationship between P and W then $\varepsilon X \ll 1$ is,

$$\frac{P}{P_0} = (1 - \alpha W)^{1/2} \dots (4-32)$$

Combining equations (E4-6.8) and (4-32) gives us

$$-r'_A = K' \left(\frac{1 - X}{1 + \varepsilon X} \right) (1 - \alpha W)^{1/2} \dots (E4-6.9)$$

Combining equations (E4-6.9) and (E4-6.1), we have

$$F_{A_0} \frac{dX}{dW} = -r'_A = K' \left(\frac{1 - X}{1 + \varepsilon X} \right) (1 - \alpha W)^{1/2}$$

Separating variables to form the integrals yields

$$\int_0^X \frac{F_{A_0} (1 + \varepsilon X) dX}{K' (1 - X)} = \int_0^W (1 - \alpha W)^{1/2} dW$$

Integrating gives us

$$\frac{F_{A_0}}{K'} \left[(1 + \varepsilon) \ln \frac{1}{1 - X} - \varepsilon X \right] = \frac{2}{3\alpha} \left[1 - (1 - \alpha W)^{3/2} \right] \dots (E4-6.10)$$

Solving for W , we obtain

$$W = \frac{1 - \left[1 - (3\alpha F_{A_0} / 2K') \{ (1 + \varepsilon) \ln [1/(1 - X)] - \varepsilon X \} \right]^{2/3}}{\alpha} \dots (E4-6.11)$$

6. Parameter evaluation per tube (i.e., divide feed rates by 1000)

Ethylene: $F_{A_0} = 3 \times 10^{-4} \text{ lbmol/s} = 1.08 \text{ lbmol/h}$

Oxygen: $F_{B_0} = 1.5 \times 10^{-4} \text{ lbmol/s} = 0.54 \text{ lbmol/h}$

Inerts = N_2 : $F_I = 1.5 \times 10^{-4} \times \frac{0.79}{0.21} = 5.64 \times 10^{-4} \text{ lbmol/s}$
 $= 2.03 \text{ lbmol/h}$

Summing $F_{T_0} = 3.65 \text{ lbmol/h}$
 (59)

$$y_{A_0} = \frac{F_{A_0}}{F_{T_0}} = \frac{1.08}{3.65} = 0.3$$

$$\varepsilon = y_{A_0} \phi = 0.3 \left(1 - \frac{1}{2} - 1\right) = -0.15$$

$$P_{A_0} = y_{A_0} P_0 = 3.0 \text{ atm.}$$

$$K' = K P_{A_0} \left(\frac{1}{2}\right)^{2/3} = 0.0141 \times 3 \times 0.63 = 0.0266$$

$$W = \frac{1 - [1 - (3 \times F_{A_0} / 2K')] \left\{ (1 - 0.15) \ln[1 / (1 - 0.6)] - (-0.15)(0.6) \right\}}{\alpha} \quad \text{--- (E4-6.12)}$$

In order to evaluate α

$$\alpha = \frac{2/\beta_0}{A_c(1-\phi)/P_c P_0}$$

We need the superficial mass velocity, G . The mass flow rates of each entering species are:

$$\dot{m}_{A_0} = 1.08 \times 28 = 30.24 \text{ lb/h}$$

$$\dot{m}_{B_0} = 0.54 \times 32 = 17.28 \text{ lb/h}$$

$$\dot{m}_{I_0} = 2.03 \times 28 = 56.84 \text{ lb/h}$$

The total mass flow rate is

$$\dot{m}_{T_0} = 104.4 \text{ lb/h}$$

$$G = \frac{\dot{m}_{T_0}}{A_c} = \frac{104.4}{0.01414} = 7383.3 \text{ lb/h.ft}^2$$

This is essentially the same superficial mass velocity, temperature and pressure as in example (4.5). Consequently we can use the value of β_0 calculated in example (4.5).

$$\beta_0 = 0.0775 \text{ atm/ft}$$

$$\alpha = \frac{2/\beta_0}{A_c(1-\phi)/P_c P_0} = \frac{2(0.0775)}{0.01414(0.55)(120)(10)}$$

$$\alpha = 0.0166 \text{ lb cat}^{-1}$$

Substituting into equation (E4-6.12) yields

$$W = \frac{1 - \left[1 - \frac{1.303(0.0166)(1.08)}{0.0266} \right]^{2/3}}{0.0166} = 45.4 \text{ lb of catalyst tube}$$

or $45.4 \times 1000 = 45400$ lb of catalyst total

This catalyst weight corresponds to a pressure of approximately 5 atm. If we had neglected pressure drop, the result would have been.

$$W = \frac{F_{A0}}{K'} \left[(1 + \varepsilon) \ln \frac{1}{1-x} - \varepsilon x \right]$$
$$= \frac{1.08}{0.0266} \left[(1 - 0.15) \ln \frac{1}{1-0.6} - (-0.15)(0.6) \right]$$

$$W = \underline{35.3} \text{ lb of catalyst per tube}$$

and we would have had insufficient catalyst to achieve the desired conversion

4.5 Continuous Stirred Tank Reactor (CSTR)

Design of CSTRs

A continuous-stirred tank reactor (CSTR) is used when intense agitation is required. The CSTR can either be used itself or, in the manner as a part of a series or battery of CSTRs. It is relatively easy to maintain good temp. control with a CSTR. There is however, the disadvantage that the conversion of reactant per volume of reactor is the smallest of the flow reactors.

When a series of stirred-tanks is used as a chemical reactor and the reactants are fed at a constant rate, eventually the system reaches a steady state such that the concentrations in the individual tanks, although, do not vary with time

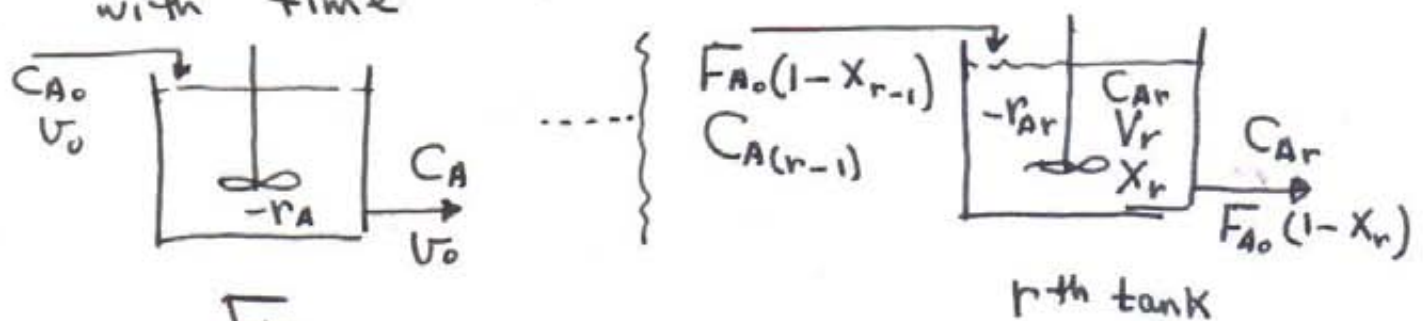


Fig.

$$\begin{array}{ccc} \text{In} & \text{Out} & \text{reaction} \\ F_{A0}(1-X_{r-1}) & - F_{A0}(1-X_r) & - (-r_A)V_r = 0 \quad \dots (4-46) \end{array}$$

X_{r-1} = the fractional conversion of A in the mixture leaving tank $r-1$ and entering tank r , and

X_r = the fractional conversion of A in the mixture leaving tank r

$$\frac{V_r}{F_{A0}} = \frac{X_r - X_{r-1}}{(-r_A)} \quad \dots (4-47)$$

For $r=1$ eqn. (4-47) becomes

$$\frac{V_1}{F_{A0}} = \frac{X - X_0}{(-r_A)_{\text{exit}}} \quad \dots (4-48)$$

In terms of concentration, eqn. 4-46 is given as:

$$V_0 C_{Ar-1} - V_0 C_{Ar} - V_r (-r_{Ar}) = 0 \quad \dots (4-49)$$

For $r=1$:

$$V_0 C_{A0} - V_0 C_{A1} - (-r_{A1}) V_1 = 0$$

$$V_1 = \frac{V_0 (C_{A0} - C_A)}{(-r_A)_{\text{exit}}} \quad \dots (4-50)$$

$$\tau = \frac{V_1}{V_0} = \frac{C_{A0} - C_A}{(-r_A)_{\text{exit}}} \quad \dots (4-51)$$

For a 1st order reaction $-r_A = KC_A$

We combine the rate law and mole balance to give

$$\tau = \frac{C_{A0} - C_A}{KC_A}$$

Solving for the effluent concentration of A, C_A

$$C_A = \frac{C_{A0}}{1 + \tau K} \quad \dots (4-52)$$

For the case we are considering, there is no volume change during the course of the reaction.

$$X = \frac{C_{A0} - C_A}{C_{A0}} \quad \dots (4-53)$$

Combining equations (4-52) and (4-53) gives us
 (Relationship between space time & conversion for 1st order liq. phase reaction) $\Rightarrow X = \frac{\tau K}{1 + \tau K} \quad \dots (4-54)$

The product τK is sometimes referred to as the reaction (Damkohler number).

The (Damkohler number) is a dimensionless number that give us a quick estimate of the degree of the conversion that can be achieved in continuous flow reactions. For first- and second-order irreversible reactions, the Damkohler number are $Da = \tau K$ and $Da = \tau K C_{A0}$ respectively.

It is important to know what values of the Da , give high and low conversion in continuous flow reactions. A value of $Da = 0.1$ or less will usually give less than 10% conversion and a value of $Da = 10.0$ or greater will usually give greater than 90% conversion.

4.5.2 CSTR in Series

A first order reaction with no volume change ($V:V_0$) is to be carried out in two (CSTRs) placed in series (Fig 4-).

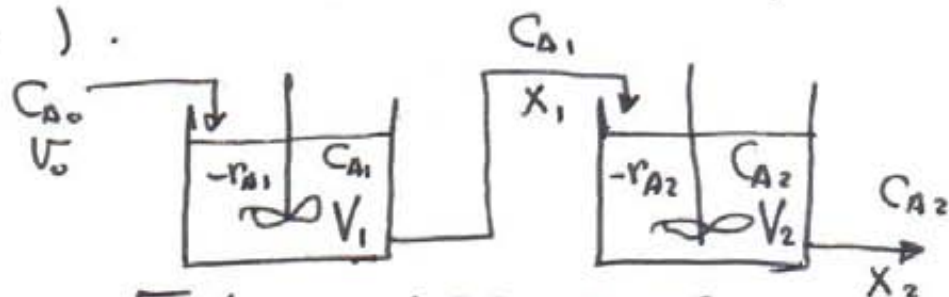


Fig. (4-) Two CSTRs in series

The effluent concentration of A from reactor 1 is

$$C_{A1} = \frac{C_{A0}}{1 + \tau_1 K_1} \quad \dots \quad (4-52)$$

From a material balance on reactor 2,

$$V_2 = \frac{F_{A1} - F_{A2}}{-r_{A2}} = \frac{V_0(C_{A1} - C_{A2})}{K_2 C_{A2}} \quad \dots (4-55)$$

Solving for C_{A2} , the concentration exiting the second reactor

$$C_{A2} = \frac{C_{A1}}{1 + \tau_2 K_2} = \frac{C_{A0}}{(1 + \tau_2 K_2)(1 + \tau_1 K_1)} \quad \dots (4-56)$$

If instead of two CSTRs in series, we had n equal sized CSTRs connected in series ($\tau_1 = \tau_2 = \dots = \tau_n = \tau$) operating at the same temperature ($K_1 = K_2 = \dots = K_n = K$)

Concentration leaving the last reactor would be:

$$C_{An} = \frac{C_{A0}}{(1 + \tau K)^n} = \frac{C_{A0}}{(1 + Da)^n} \quad \dots (4-57)$$

The conversion for these n tank reactors in series

Conversion as a function of the number of tanks in series

$$X = 1 - \frac{1}{(1 + \tau K)^n} \quad \dots (4-58)$$

The rate of disappearance of A in the n th reactor is

$$-r_{An} = K C_{An} = K \frac{C_{A0}}{(1 + \tau K)^n}$$

4.5.3 CSTRs in Parallel

We now consider the case in which equal-sized reactors are placed in parallel, rather than in series, and the feed is distributed equally among each of the reactors (Figure 4-). A balance on any reactor, say i , gives the individual reactor volume,

$$V_i = F_{A0i} \left(\frac{X_i}{-r_{Ai}} \right) \quad \dots (4-59)$$

Since the reactors are of equal size, operate at the same temperature, and have identical feed rates,

$$X_1 = X_2 = \dots = X_n = X$$

and

$$-r_{A1} = -r_{A2} = \dots = -r_{An} = -r_A$$

The volume of each individual reactor, V_i , is related to the total volume, V , of all the reactors by the equation,

$$V_i = \frac{V}{n}$$

A similar relationship exists for the total molar flow rates,

$$\bar{F}_{A0i} = \frac{\bar{F}_{A0}}{n}$$

Substituting these values into eqn. (4-59) yields

$$\frac{V}{n} = \frac{\bar{F}_{A0}}{n} \left(\frac{X_i}{-r_{Ai}} \right) \quad \dots (4-60)$$

or
Conversion for
tanks in Parallel

$$V = \frac{\bar{F}_{A0} X_i}{-r_{Ai}} = \frac{\bar{F}_{A0} X}{-r_A} \quad \dots (4-61)$$

This result shows that the conversion achieved in any one of the reactors in parallel is identical to what would be achieved if the reactant were fed in one stream to one large reactor of volume V .

Example (4-7) A Two-Stage CSTR

A solution of an ester $R\text{-COOR'}$ is to be hydrolysed with an excess of caustic soda solution. Two stirred tanks of equal size will be used. The ester and caustic soda solutions flow separately into the

first tank at rates of 0.004 and $0.001 \text{ m}^3/\text{s}$ and with concentrations of 0.02 and 1.0 kmol/m^3 respectively. The reaction :



is second order with a velocity constant of $0.033 \text{ m}^3/\text{kmol.s}$ of the temperature at which both tanks operate. Determine the volume of the tanks required to effect 95% conversion of the ester ($X_2 = 0.95$).

Solution :

A material balance on the ester over the 1st tank gives for steady state :

MB (1st Reactor)

$$\begin{array}{cccc} \text{In} & \text{Out} & \text{Reaction} & \text{Accum.} \\ V_0 C_{A0} & - V_0 C_{A1} & - V_1 K_1 C_{A1} C_{B1} & = 0 \end{array}$$

$$V_0 C_{A0} - V_0 (C_{A0} - X_1 C_{A0}) - V_1 K_1 (C_{A0} - X_1 C_{A0}) (C_{B0} - X_1 C_{A0}) = 0$$

$$X_1 V_0 C_{A0} = V_1 K_1 C_{A0}^2 (1 - X_1) \left(\frac{C_{B0}}{C_{A0}} - X_1 \right) \quad \text{--- (1)}$$

MB (2nd Reactor)

$$V_0 C_{A1} - V_0 C_{A2} - V_2 K_2 C_{A2} C_{B2} = 0$$

$$V_0 C_{A0} (X_2 - X_1) = V_2 K_2 C_{A0}^2 (1 - X_2) \left(\frac{C_{B0}}{C_{A0}} - X_2 \right)$$

$$V_2 = V_1 \quad (\text{The reactors are of equal size})$$

$$K_1 = K_2 \quad (T_1 = T_2)$$

$$\text{The total volumetric flow rate } (V_0) = 0.001 + 0.004 = 0.005 \text{ m}^3/\text{s}$$

$$C_{A0} = 0.02 \times \frac{0.004}{0.005} = 0.016 \text{ kmol/m}^3$$

$$C_{B0} = 1.0 \times \frac{0.001}{0.005} = 0.2 \text{ kmol/m}^3$$

Dividing eqn. (2) by (1) and substitute the known values to obtain:

$$\frac{X_2 - X_1}{X_1} = \frac{(1 - X_2) \left(\frac{C_{B0}}{C_{A0}} - X_2 \right)}{(1 - X_1) \left(\frac{C_{B0}}{C_{A0}} - X_1 \right)}$$

$$\frac{0.95 - X_1}{X_1} = \frac{(1 - 0.95) \left(\frac{0.2}{0.016} - 0.95 \right)}{(1 - X_1) \left(\frac{0.2}{0.016} - X_1 \right)}$$

$$X_1 = 0.1875$$

Substitute into eqn. (1), gives us

$$V_1 = \underline{\underline{2.8 \text{ m}^3}}$$

4.5-3 Graphical Methods

Provide a convenient method for dealing with sets of equal sized tanks of up to five in number all at the same temperature.

Graphical method arising from eqns (4.62) & (4.63).

$$-r_A = f(C_A) \quad \dots (4.62)$$

$$\frac{V_r}{V_0} = \frac{C_{Ar-1} - C_A}{-r_{Ar}} \quad \dots (4.63)$$

Combining the two eqns to obtain

$$-r_{Ar} = -\frac{V_0}{V_r} (C_{Ar} - C_{Ar-1}) \quad \dots (4.64)$$

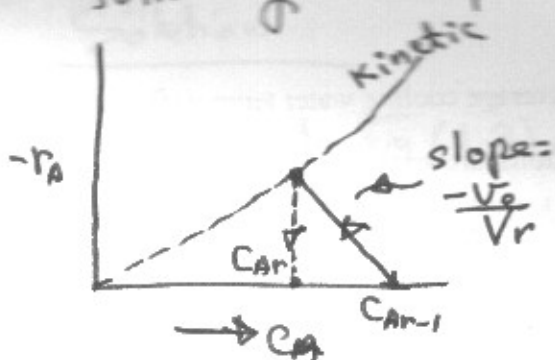
where the subscript r has been added to stress that $(-r_{Ar})$ is the value of $(-r_A)$ for the tank (r) . Consider now a graph of $-r_A$ versus C_A as shown in Fig. (4.2). From a point on the C_A -axis, $-r_A = 0$, $C_A = C_{Ar-1}$, we construct a line of slope =

$= \frac{-V_0}{V_r}$ and intercept with $-r_A$ (at $r_A = 0$, $C_A = C_{A-1}$) which therefore has the equation,
 $-r_A = -\frac{V}{V_r} (C_A - C_{A-1}) \dots (4.65)$ for any reactor.

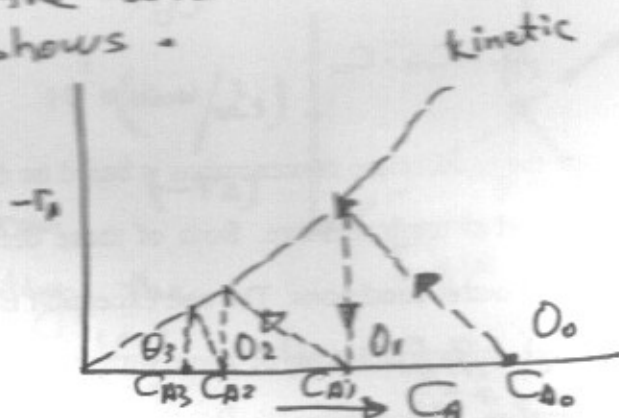
Equation (4.64) shows that the point $(-r_A, C_A)$ lies on this line, however $(-r_A)$ must also lie on the rate of reaction versus C_A curve, so that $(-r_A, C_A)$ is the point of intersection of the two as shown:

Kinetic $-r_A = f(C_A)$ (1st order $-r_A = k C_A$,
 zero order $-r_A = k$)

Thus starting with the 1st tank, we can draw the first line from the point $O_0(0, C_{A0})$ on Fig. (4.2) and locate C_{A1} , the concentration of the reactant leaving the 1st tank. Then from the point $O_1(0, C_{A1})$, we can draw a 2nd line to locate C_{A2} for the 2nd tank, and so on for the whole series as the following example shows.



(a)



(b)

Fig. (4.2) Graphical construction for CSTRs

(a) General method.

(b) Three equal tanks, outlet conc. C_{A3} unknown, V known.

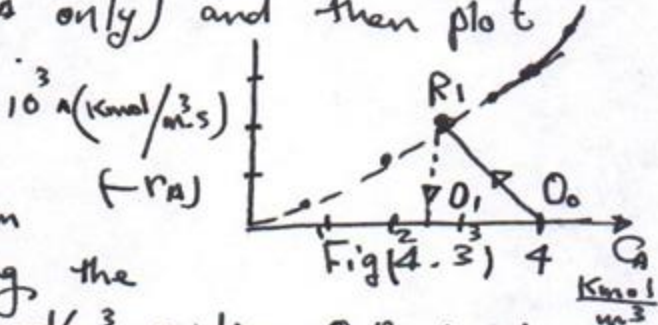
Example (4.8) Graphical Method for a 3-stage CSTR

- (a) A system of three stirred tanks is to be designed to treat a solution containing 4.0 kmol/m^3 of a reactant A. Experiments with a small reactor in the laboratory gave the kinetic data shown as a graph of rate of reaction versus C_A in Fig (4.3). If the feed rate to the reactor system (V_0) is $1.2 \times 10^{-4} \text{ m}^3/\text{s}$, what fractional conversion will be obtained if each of the tanks has a volume of 0.6 m^3 ?
- (b) Calculate the volumes of the tanks required for the same overall conversion if two equal tanks are used, and if only one tank is used.

Note: If $-r_A = f(C_A)$ is not given as graph, find the relationship between $-r_A$ and C_A (in terms of C_A only) and then plot $-r_A$ vs. C_A .

Solution

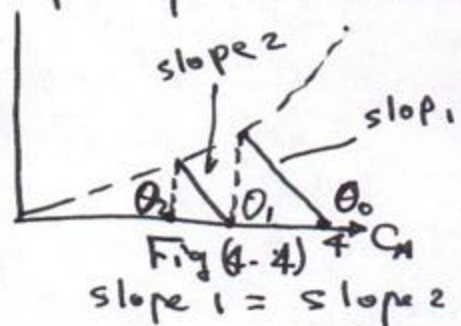
- (a) Referring to Fig (4.3), from the point O_0 representing the feed composition of 4.0 kmol/m^3 , a line $O_0 R_1$ is drawn of slope $(-V_0/V_r = -1.2 \times 10^{-4}/0.6 = -2 \times 10^{-4} \text{ s}^{-1})$ to intersect the rate curve at R_1 . This point of intersection gives the conc. of A in the 1st tank C_{A1} . A perpendicular $R_1 O_1$ is dropped from R_1 to the C_A axis, and from the point



0, a 2nd line also of slope $-2 \times 10^{-4} \text{ s}^{-1}$ is drawn. The construction is continued until O_3 is reached which gives the conc. of A leaving the last tank C_{A3} . Reading from the figure $C_{A3} = 1.23 \frac{\text{kmol}}{\text{m}^3}$. The fractional conversion is therefore:

$$\frac{4.0 - 1.23}{4.0} = \underline{\underline{0.69}}$$

- (b) When the volumes of the identical tanks are unknown the graphical construction must be carried out on a trial and error basis. The procedure for the case of two tanks; the points O_0 and O_2 are known, but the position of R_1 has to be adjusted to make O_0R_1 and O_1R_2 parallel because these lines must have the same slope if the tanks of equal size. From the figure this slope is $-r_A$ $1.13 \times 10^{-4} \text{ sec}^{-1}$. The volume of each tank must therefore be $1.2 \times 10^{-4} / 1.13 \times 10^{-4} = \underline{\underline{1.06 \text{ m}^3}}$.

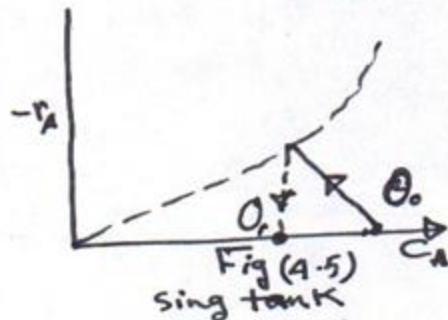


For a single tank the construction is straight forward as shown in Fig. (4-5) and the volume obtained is $\underline{\underline{3.16 \text{ m}^3}}$

It is interesting to compare the total volume required for the same duty in the three cases

$$\text{Total volume for 3 tanks} = 3 \times 0.6 = \underline{\underline{1.8 \text{ m}^3}}$$

$$\text{Total volume for 2 tanks} = 2 \times 1.06 = \underline{\underline{2.12 \text{ m}^3}}$$



$$\text{Total volume for } \underline{1 \text{ tank}} = \underline{3.16 \text{ m}^3}$$

These results illustrate the general conclusion that, as the number of tanks increased, the total volume required diminishes and tends to the limit to volume of the equivalent PFR. The only exception is in the case of a zero order reaction for which the total volume is constant and equal to that of the PFR for all configuration.

2.5 Semibatch Reactor

In a semibatch reactor, one of the reactants in the reaction:



(e.g., A) is slowly fed to the reactor

containing the other reactant (i.e., B),

which has already been charged to the reactor.

Fig. 5.1 illustrate this type of reactor which is usually used when unwanted side reactions occur at high concentrations of A, or the reaction is highly exothermic.

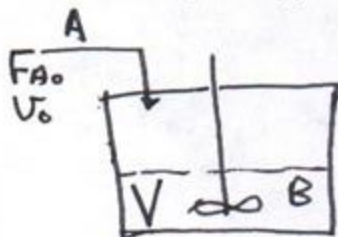


Fig. 5.1

In some reactions, the reactant A is a gas and is continuously bubbled through liquid reactant B.

To determine the conversion (or concentration) of reactant A as a function of time, a mole balance on species A is established:

$$\left[\text{rate} \right]_{\text{in}} - \left[\text{rate} \right]_{\text{out}} - \left[\text{rate of disappearance due to reaction} \right] = \left[\text{rate of accumulation} \right]$$