# Reactor Design

Teacher :Suha Mahdi

References

Chemical Reaction Engineering
Octave Levenspiel

Chemical reaction engineering is the branch of chemical engineering which deals with chemical reactors and their design, especially by application of chemical kinetics to industrial systems.

A **chemical reactor** is an enclosed volume in which a chemical reaction takes place. In chemical engineering, it is generally understood to be a process vessel used to carry out a chemical reaction, which is one of the classic unit operations in chemical process analysis. The design of a chemical reactor deals with multiple aspects of chemical engineering. Chemical engineers design reactors to maximize net present value for the given reaction. Designers ensure that the reaction proceeds with the highest efficiency towards the desired output product, producing the highest yield of product while requiring the least amount of money to purchase and operate. Normal operating expenses include energy input, energy removal, raw material costs, labor, etc. Energy changes can come in the form of heating or cooling, pumping to increase pressure, frictional pressure loss or agitation.

Types of reactor
1-Batch reactor
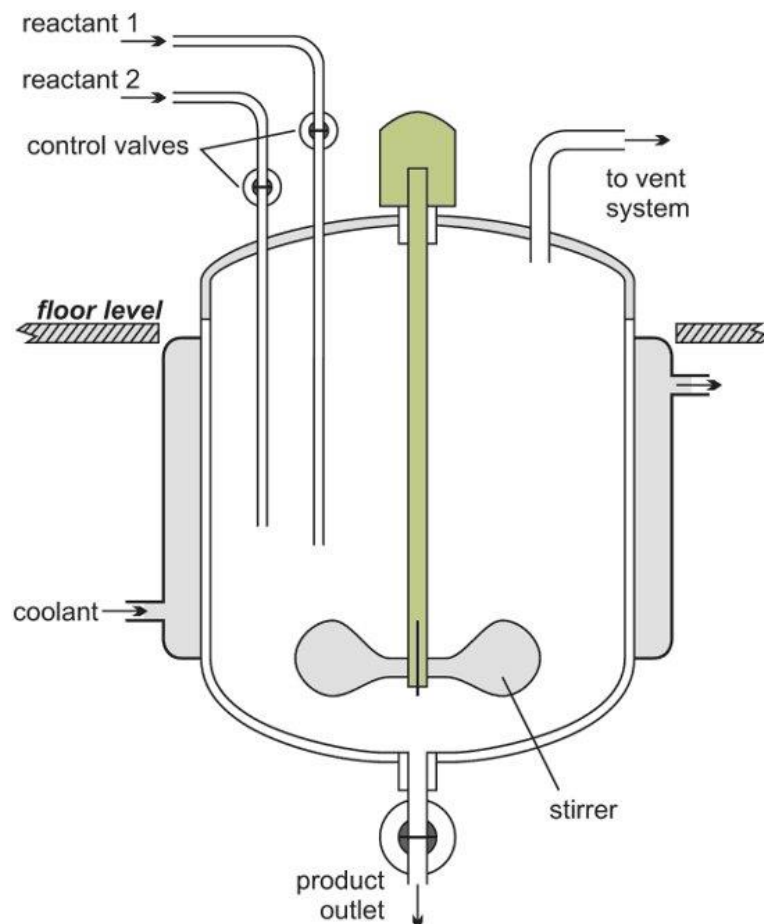
The simplest type of reactor is a batch reactor. Materials are loaded into a batch reactor, and the reaction proceeds with time. A batch reactor does not reach a steady state, and control of temperature, pressure and volume is often necessary. Many batch reactors therefore have ports for sensors and material input and output. Batch reactors are typically used in small-scale production and reactions with biological materials, such as in brewing, pulping, and production of enzymes. One example of a batch reactor is a pressure reactor.

2-CSTR (continuous stirred-tank reactor
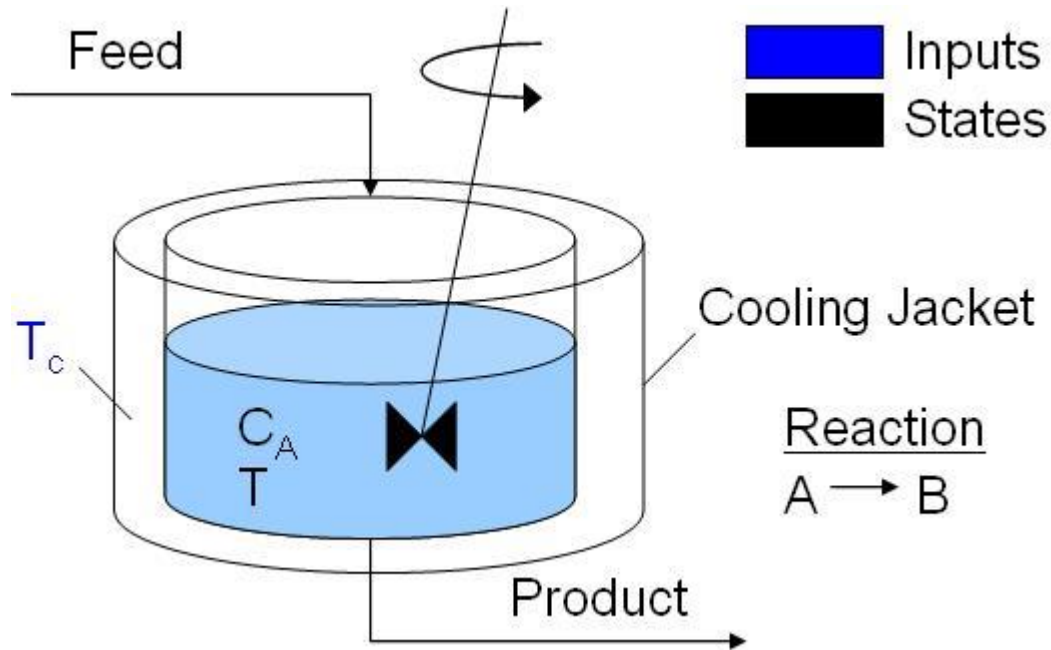
In a CSTR, one or more fluid reagents are introduced into a tank reactor which is typically stirred with an impeller to ensure proper mixing of the reagents while the reactor effluent is removed. Dividing the volume of the tank by the average volumetric flow rate through the tank gives the space time, or the time required to process one reactor volume of fluid. Using chemical kinetics, the reaction's expected percent completion can be calculated. Some important aspects of the CSTR:

- At steady-state, the mass flow rate in must equal the mass flow rate out, otherwise the tank will overflow or go empty (transient state). While the reactor is in a transient state the model equation must be derived from the differential mass and energy balances.
- The reaction proceeds at the reaction rate associated with the final (output) concentration, since the concentration is assumed to be homogenous throughout the reactor.
- Often, it is economically beneficial to operate several CSTRs in series. This allows, for example, the first CSTR to operate at a higher

reagent concentration and therefore a higher reaction rate. In these cases, the sizes of the reactors may be varied in order to minimize the total capital investment required to implement the process.

- It can be demonstrated that an infinite number of infinitely small CSTRs operating in series would be equivalent to a PFR.[9]

The behavior of a CSTR is often approximated or modeled by that of a Continuous Ideally Stirred-Tank Reactor (CISTR). All calculations performed with CISTRs assume perfect mixing. If the residence time is 5-10 times the mixing time, this approximation is considered valid for engineering purposes. The CISTR model is often used to simplify engineering calculations and can be used to describe research reactors. In practice it can only be approached, particularly in industrial size reactors in which the mixing time may be very large.

3-PFR (plug flow reactor)
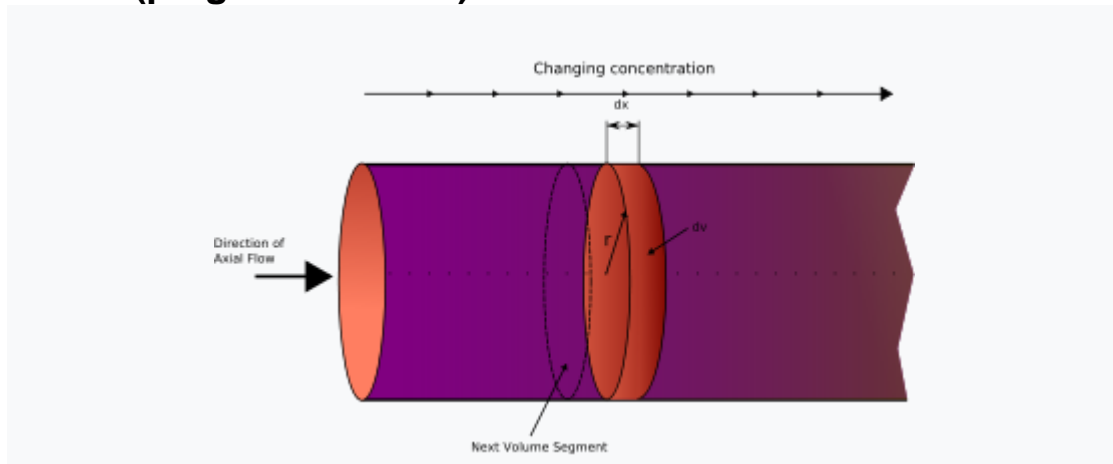
In a PFR, sometimes called continuous tubular reactor (CTR),[10] one or more fluid reagents are pumped through a pipe or tube. The chemical reaction proceeds as the reagents travel through the PFR. In this type of reactor, the changing reaction rate creates a gradient with respect to distance traversed; at the inlet to the PFR the rate is very high, but as the concentrations of the reagents decrease and the concentration of the product(s) increases the reaction rate slows. Some important aspects of the PFR:

- The idealized PFR model assumes no axial mixing: any element of fluid traveling through the reactor doesn't mix with fluid upstream or downstream from it, as implied by the term "plug flow".
- Reagents may be introduced into the PFR at locations in the reactor other than the inlet. In this way, a higher efficiency may be obtained, or the size and cost of the PFR may be reduced.

- A PFR has a higher theoretical efficiency than a CSTR of the same volume. That is, given the same space-time (or residence time), a reaction will proceed to a higher percentage completion in a PFR than in a CSTR. This is not always true for reversible reactions.

For most chemical reactions of industrial interest, it is impossible for the reaction to proceed to 100% completion. The rate of reaction decreases as the reactants are consumed until the point where the system reaches dynamic equilibrium (no net reaction, or change in chemical species occurs). The equilibrium point for most systems is less than 100% complete. For this reason a separation process, such as distillation, often follows a chemical reactor in order to separate any remaining reagents or byproducts from the desired product. These reagents may sometimes be reused at the beginning of the process, such as in the Haber process. In some cases, very large reactors would be necessary to approach equilibrium, and chemical engineers may choose to separate the partially reacted mixture and recycle the leftover reactants.

Under laminar flow conditions, the assumption of plug flow is highly inaccurate, as the fluid traveling through the center of the tube moves much faster than the fluid at the wall. The continuous oscillatory baffled reactor (COBR) achieves thorough mixing by the combination of fluid oscillation and orifice baffles, allowing plug flow to be approximated under laminar flow conditions.

4-Semibatch reactor
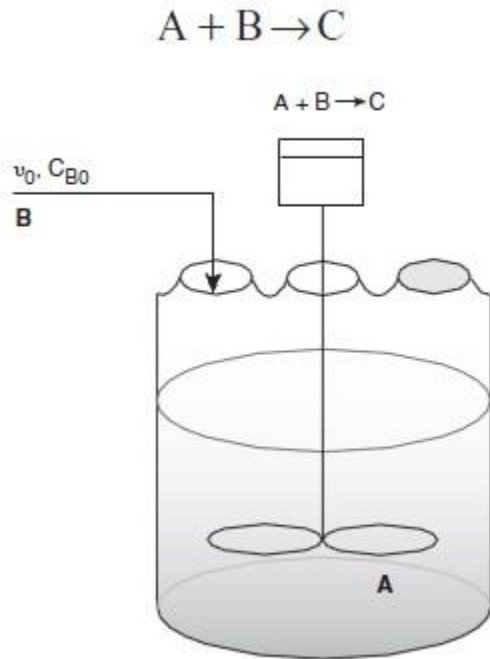
$$A + B \rightarrow C$$

Figure 4-15   Semibatch reactor.

A semibatch reactor is operated with both continuous and batch inputs and outputs. A fermenter, for example, is loaded with a batch of medium and microbes which constantly produces carbon dioxide that must be removed continuously. Similarly, reacting a gas with a liquid is usually difficult, because a large volume of gas is required to react with an equal mass of liquid. To overcome this problem, a continuous feed of gas can be bubbled through a batch of a liquid. In general, in semibatch operation, one chemical reactant is loaded into the reactor and a second chemical is added slowly (for instance, to prevent side reactions), or a product which results from a phase change is continuously removed, for example a gas formed by the reaction, a solid that precipitates out, or a hydrophobic product that forms in an aqueous solution.

5-Catalytic reactor
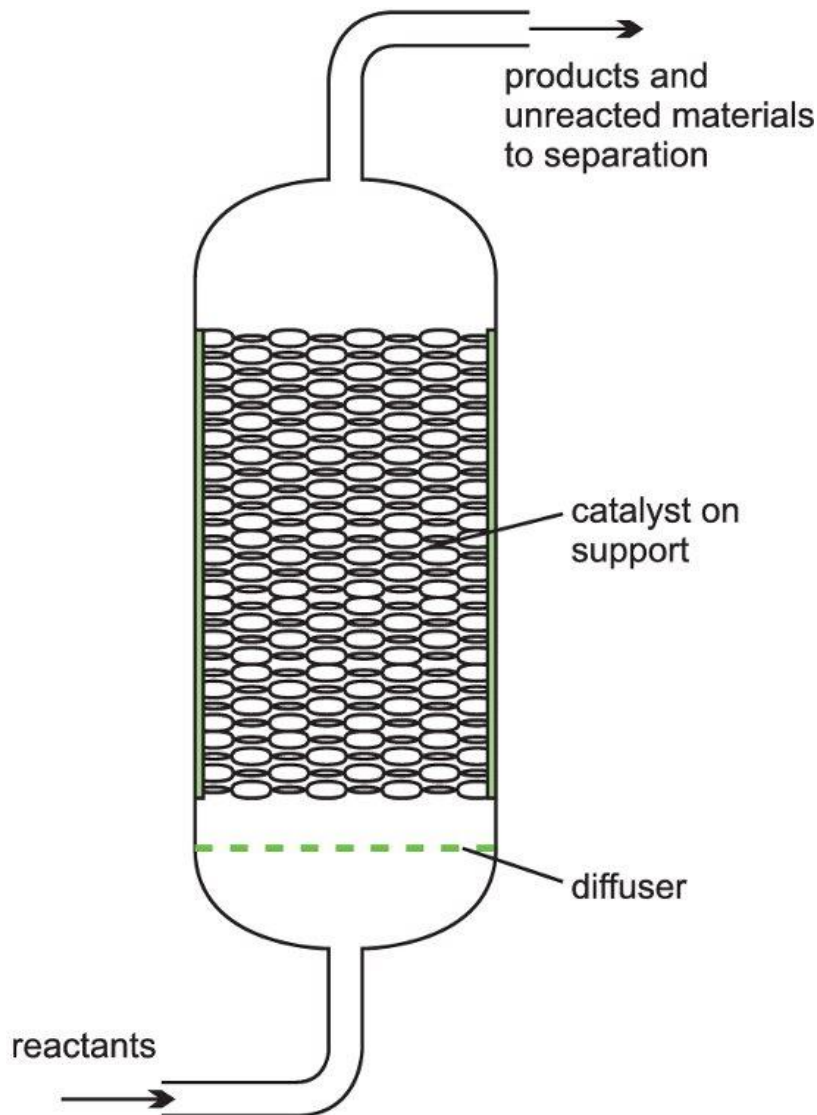
Although catalytic reactors are often implemented as plug flow reactors, their analysis requires more complicated treatment. The rate of a catalytic reaction is proportional to the amount of catalyst the reagents contact, as well as the concentration of the reactants. With a solid phase catalyst and fluid phase reagents, this is proportional to the exposed area, efficiency of diffusion of reagents in and products out, and efficacy of mixing. Perfect mixing usually cannot be assumed. Furthermore, a catalytic reaction pathway often occurs in multiple steps with intermediates that are chemically bound to the catalyst; and as the chemical binding to the catalyst is also a chemical reaction, it may affect the kinetics. Catalytic reactions often display so-called *falsified kinetics*, when the apparent kinetics differ from the actual chemical kinetics due to physical transport effects.

The behavior of the catalyst is also a consideration. Particularly in high-temperature petrochemical processes, catalysts are deactivated by processes such as sintering, coking, and poisoning.

A common example of a catalytic reactor is the catalytic converter that processes toxic components of automobile exhausts. However, most petrochemical reactors are catalytic, and are responsible for most industrial chemical production, with extremely high-volume examples including sulfuric acid, ammonia, reformate/BTEX (benzene, toluene, ethylbenzene and xylene), and fluid catalytic cracking. Various configurations are possible, see Heterogeneous catalytic reactor.

Design equations

Firstly to understand the design equation we must know what is the definition of conversion the general reaction aA+bB=cC+dD

The capital letters represent chemical species and lower case letters represent stoichiometric coefficients

$$A+\frac{b}{a}B=\frac{c}{a}C+\frac{d}{a}D$$
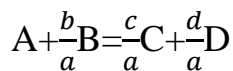
Batch system

$$X_A = \frac{moles\ of\ A\ reacted}{moles\ of\ A\ fed}$$

X=X_A

$$\begin{bmatrix} mole\ of\ A \\ consumed \end{bmatrix} = \begin{bmatrix} mole\ of\ A \\ fed \end{bmatrix} . \begin{bmatrix} \frac{mole\ of\ A\ reacted}{mole\ of\ A\ fed} \end{bmatrix}$$

$$\begin{bmatrix} mole\ of\ A\ reacted \\ consumed \end{bmatrix} = [NA_o].[X]$$

$$\begin{bmatrix} mole\ of\ A\ in\ the \\ reactor\ at\ time\ t \end{bmatrix} = \begin{bmatrix} mole\ of\ inially \\ fed \\ to\ the\ reactor\ at\ t=0 \end{bmatrix} - $$
$$\begin{bmatrix} moles\ of\ A \\ that\ have\ been\ consumed\ by\ chemical\ reaction \end{bmatrix}$$

$$NA = [NA_o] - [NA_oX]$$

NA=$NA_o - NA_oX$=$NA_o(1-X)$

$$\frac{dNA}{dt} = r_A V$$

Reactant A is disappearing therefore we multiplying both sides of equation by -1

$$-\frac{dNA}{dt} = -r_A V$$

Rate equation $-r_A = K C_A C_B$

$$NA = NA_o - NA_o X \dots \dots 1$$

$$\frac{dNA}{dt} = 0 - NA_o \frac{dX}{dt} \dots \dots 2$$

$$-NA_o \frac{dX}{dt} = r_A V \dots \dots 3$$

$$NA_o \frac{dX}{dt} = -r_A V \dots \dots 4$$

$$-\frac{1}{V} \frac{dNA}{dt} = -\frac{d(NA/V)}{dt} = -\frac{dCA}{dt} = -r_A \dots \dots 5$$

$$Vdt = NA_o \frac{dX}{-r_A} \dots \dots 6$$

$$dt = NA_o \frac{dX}{-r_A V}$$

$$\int_0^t Vdt = NA_o \int_0^x \frac{dX}{-r_A}$$

$$t = NA_o \int_0^x \frac{dX}{-r_A V}$$

Flow system

FA_o is the molar flow rate of species A

$$[FA_o].[X] = \frac{moles\ of\ A\ fed}{time} * \frac{moles\ of\ A reacted}{moles\ of\ A\ fed}$$

$$FA_o X = \frac{moles \ of \ A reacted}{time}$$

$$\begin{bmatrix} molar \ flow \ rate \\ at \ which \ A \ is \ fed \ to \ the \ system \end{bmatrix} -$$
$$\begin{bmatrix} molar \ rate \ at \ which \\ A \ is \ consumed \ with \ in \ the \ system \end{bmatrix} =$$
$$\begin{bmatrix} molar \ rate \ at \ which \\ A \ is \ leave \ with \ in \ the \ system \end{bmatrix}$$

$$FA_o - FA_o X = FA$$

$$FA = FA_o(1 - x)$$

CSTR or back mix reactor

$$A + \frac{b}{a}B = \frac{c}{a}C + \frac{d}{a}D$$

Input −output=generation

$$FA_o - FA = -r_A V$$

$$FA_o x = -r_A V$$

$$V = \frac{FA_o x}{-r_A} \text{ for CSTR}$$

$$-r_A = \frac{-dFA}{dV}$$

$$FA = FA_o - FA_o x$$

$$FA_o \cdot \frac{dx}{dV} = -r_A$$

$$V = FA_o \int_0^x \frac{dx}{-r_A} \text{for plug flow reactor}$$

Reactors in series

$$FA_1 = FA_o - FA_o x_1$$

$$FA_2 = FA_o - FA_o x_2$$
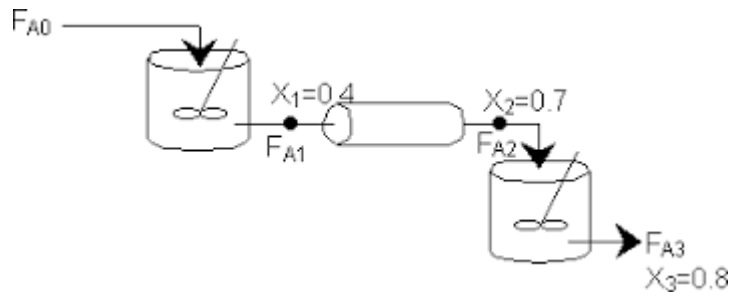
$$FA_3 = FA_o - FA_o x_3$$

$$x_2 = \frac{total\ moles\ of\ A\ reacted\ up\ to\ point\ 2}{mole\ of\ A\ fed\ to\ first\ order}$$

IN-OUT+GENERATION=0

$$FA_1 - FA_2 + r_{A2} v_2 = 0$$

$$v_2 = \frac{FA_1 - FA_2}{-r_A}$$

$$v_2 = \frac{FA_o(x_2 - x_1)}{-r_{A2}} \quad \text{for CSTR}$$

CSTR in parallel
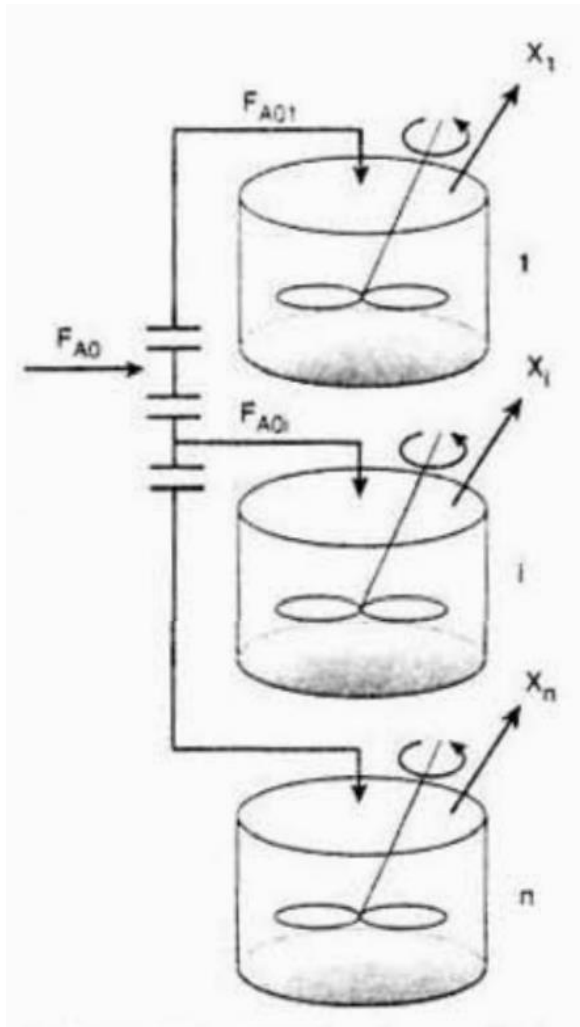
For i reactors in parallel (see diagram),

$$V_i = F_{Aoi}\left(\frac{x_i}{-r_{Ai}}\right)$$

The volume of each individual reactor is related to the total volume of all reactors by $V_i = \frac{V}{n}$ similarly $F_{Aoi} = \frac{F_{Ao}}{n}$

$V = \frac{F_{Ao}X}{-r_A}$ The conversion in any one reactor in parallel is identical to what would be achieved if the reactant was fed to one large reactor of volume V

The space time for plug flow reactor

$$\tau=\frac{v}{v_o} \quad ,\tau = CA_o \int_0^x \frac{dx}{-r_A} \quad ,v= FA_o \int_0^x \frac{dx}{-r_A}$$

$$FA_o = v_o CA_o$$

$$X=\frac{FA_o-FA}{FA_o}=\frac{CA_o v_o-CA\,v}{CA_o v_o}$$

$$X=\frac{CA_o-CA}{CA_o} \text{ where x=0,CA=}CA_o\text{,x=x,CA=CA}$$

$$dx=\frac{-dCA}{CA_o}, V=v_o \int_{CA}^{CA_o} \frac{dCA}{-r_A}$$

$$\tau=\int_{CA}^{CA_o} \frac{dCA}{-r_A}$$

A Second-Order Reaction in a CSTR

_ Using the algorithm discussed earlier in this section a second-order liquid-phase reaction in a CSTR

Has $\tau=\frac{C_{Ao}X}{k\,C_{Ao}^2(1-X)^2}$ When solved, this yield X=$\frac{(1+2D_a)-\sqrt{1+4D_a}}{2D_a}$

Tubular Reactors

_ Using the algorithm discussed earlier in this section, a second-order reaction in a PFR in the liquid phase yields **X**=$\frac{\tau k C_{Ao}}{1+\tau k C_{Ao}}$

, $D_a = \tau k C_{Ao}$

For a second-order reaction in a PFR in the gas-phase at constant pressure and temperature2

V=$\frac{v_o}{k C_{Ao}}\left[\mathbf{2}\varepsilon(1 + \varepsilon)in\,(1 - X) + \varepsilon^2 X + \frac{(1+\varepsilon)^2 X}{1-X}\right]$

The Reaction Order and the Rate Law

_ A reaction rate is described as (using the reaction defined earlier),

$$-r_A = k_A C_A^\alpha C_B^\alpha$$

where the order with respect to A is _, the order with respect to B is _, and the total order is _ + _

_ For a zero-order reaction, the units of k are mol/L_s

_ For a first-order reaction, the units of k are 1/s

_ For a second-order reaction, the units of k are L/mol_s

_ For an elementary reaction, the rate law order is identical to the stoichiometric coefficients

_ For heterogeneous reactions, partial pressures are used instead of concentrations

– To convert between partial pressure and concentration, one can use the ideal gas law

– The reaction rate per unit volume is related to the rate of reaction per unit weight of catalyst via

$$-r_A = \rho - r_A{}'$$

_ The equilibrium constant is defined (for the general reaction) as

$$k_c = \frac{forword}{reverse}$$

_ The net rate of formation of substance A is the sum of the rates of formation from the forward reaction
and reverse reaction for a system at equilibrium

– For instance, if we have the elementary, reversible reaction of 2A B + C, we can state that

$$-r_A for\ word = k_A C_A^2, r_A reverse = K - AC_B C_c$$

Therefore $-r_A for\ word + r_A reverse = k_A C_A^2 -$

$k_{-A} C_B C_c = k_A (C_A^2 - \frac{k_{-A}}{k_A} C_B C_c) using\ k_c = \frac{C_B C_c}{C_A^2}$

$= k_A (C_A^2 - \frac{C_B C_c}{k_c})$

The temperature dependence of the concentration equilibrium constant is the following when there is no change in the total number of moles and the heat capacity does not change

$$k_c(T) = k_c(T_1) \exp\left[\frac{\Delta H_{rxn}^o}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$$

The Reaction Rate Constant

_ The Arrhenius equation states that

$$k_A(T) = A\exp - \frac{E}{RT}$$

Plotting lnk vs $\frac{1}{T}$ yields a line with slope$-\frac{E}{R}$

and y-intercept is lnA
_ Equivalently,

K(T)=k(T_o)exp$\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$

3. Reversible Reaction To determine the conversion or reactor volume for reversible reactions, one must first calculate the maximum conversion that can be achieved at the isothermal reaction temperature, which is the equilibrium conversion. (See Example 3-8 in the text for additional coverage of equilibrium conversion in isothermal reactor design.) Equilibrium Conversion, Xe

Stoichiometric Tables

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$
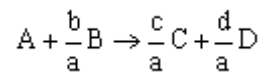
Using stoichiometry, we set up all of our equations with the amount of reactant A as our basis.

Batch System Stoichiometric Table :

Species	**Symbol**	**Initial**	**Change**	**Remaining**
A	A	N_{A0}	$-N_{A0}X$	$N_A = N_{A0}(1-X)$
B	B	$N_{B0} = N_{A0}\Theta_B$	$-\dfrac{b}{a}N_{A0}X$	$N_B = N_{A0}\left(\Theta_B - \dfrac{b}{a}X\right)$
C	C	$N_{C0} = N_{A0}\Theta_C$	$+\dfrac{c}{a}N_{A0}X$	$N_C = N_{A0}\left(\Theta_C + \dfrac{c}{a}X\right)$
D	D	$N_{D0} = N_{A0}\Theta_D$	$+\dfrac{d}{a}N_{A0}X$	$N_D = N_{A0}\left(\Theta_D + \dfrac{d}{a}X\right)$
Inert	I	$N_I = N_{A0}\Theta_I$	-------	$N_I = N_{A0}\Theta_I$
		$\overline{}$		$\overline{}$
		N_{T0}		$N_T = N_{T0} + \delta N_{A0}X$

Where:

$$\Theta_i = \frac{N_{i0}}{N_{A0}} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}} \quad \text{and} \quad \delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$$

Concentration -- Batch System: $\quad C_A = \dfrac{N_A}{V}$

Constant Volume Batch:

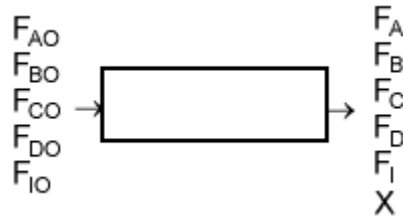[a liquid phase reaction, or a gas phase reaction in a rigid (e.g., steel) reactor]

$$V = V_0$$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V_0} = C_{A0}(1-X)$$

$$C_B = \frac{N_B}{V} = \frac{N_{A0}}{V_0}\left(\Theta_B - \frac{b}{a}X\right) = C_{A0}\left(\Theta_B - \frac{b}{a}X\right)$$

etc.

Writing -r$_A$ only as a function of X

Flow System Stoichiometric Table :

$$F_{AO}, F_{BO}, F_{CO}, F_{DO}, F_{IO} \rightarrow \boxed{} \rightarrow F_A, F_B, F_C, F_D, F_I, X$$

Species	**Symbol**	**Reactor Feed**	**Change**	**Reactor Effluent**
A	A	F_{A0}	$-F_{A0}X$	$F_A = F_{A0}(1-X)$
B	B	$F_{B0} = F_{A0}\Theta_B$	$-\dfrac{b}{a}F_{A0}X$	$F_B = F_{A0}\left(\Theta_B - \dfrac{b}{a}X\right)$
C	C	$F_{C0} = F_{A0}\Theta_C$	$+\dfrac{c}{a}F_{A0}X$	$F_C = F_{A0}\left(\Theta_C + \dfrac{c}{a}X\right)$
D	D	$F_{D0} = F_{A0}\Theta_D$	$+\dfrac{d}{a}F_{A0}X$	$F_D = F_{A0}\left(\Theta_D + \dfrac{d}{a}X\right)$
Inert	I	$F_{I0} = F_{A0}\Theta_I$	-------	$F_I = F_{A0}\Theta_I$
		$\overline{}$		$\overline{}$
		F_{T0}		$F_T = F_{T0} + \delta F_{A0}X$

Where:

$$\Theta_i = \frac{F_{i0}}{F_{A0}} = \frac{C_{i0}\upsilon_0}{C_{A0}\upsilon_0} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}} \quad \text{and} \quad \delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$$

Concentration -- Flow System:

$$C_A = \frac{F_A}{\upsilon}$$

Liquid Phase Flow System:

$$\upsilon = \upsilon_0$$

$$C_A = \frac{F_A}{\upsilon} = \frac{F_{A0}(1-X)}{\upsilon_0} = C_{A0}(1-X)$$

$$C_B = \frac{F_B}{\upsilon} = \frac{F_{A0}}{\upsilon_0}\left(\Theta_B - \frac{b}{a}X\right) = C_{A0}\left(\Theta_B - \frac{b}{a}X\right)$$

etc.

If the rate of reaction were
$$-r_A = kC_A C_B$$
then we would have
$$-r_A = kC_{A0}^2(1-X)\left(\theta_B - \frac{b}{a}X\right)$$
This gives us $-r_A = f(X)$. Consequently, we can use the methods discussed in Chapter 2 to size a large number of reactors, either alone or in series.

Gas Phase Flow System:

$$\upsilon = \upsilon_0 (1+\varepsilon X)\frac{T}{T_0}\frac{P_0}{P}$$

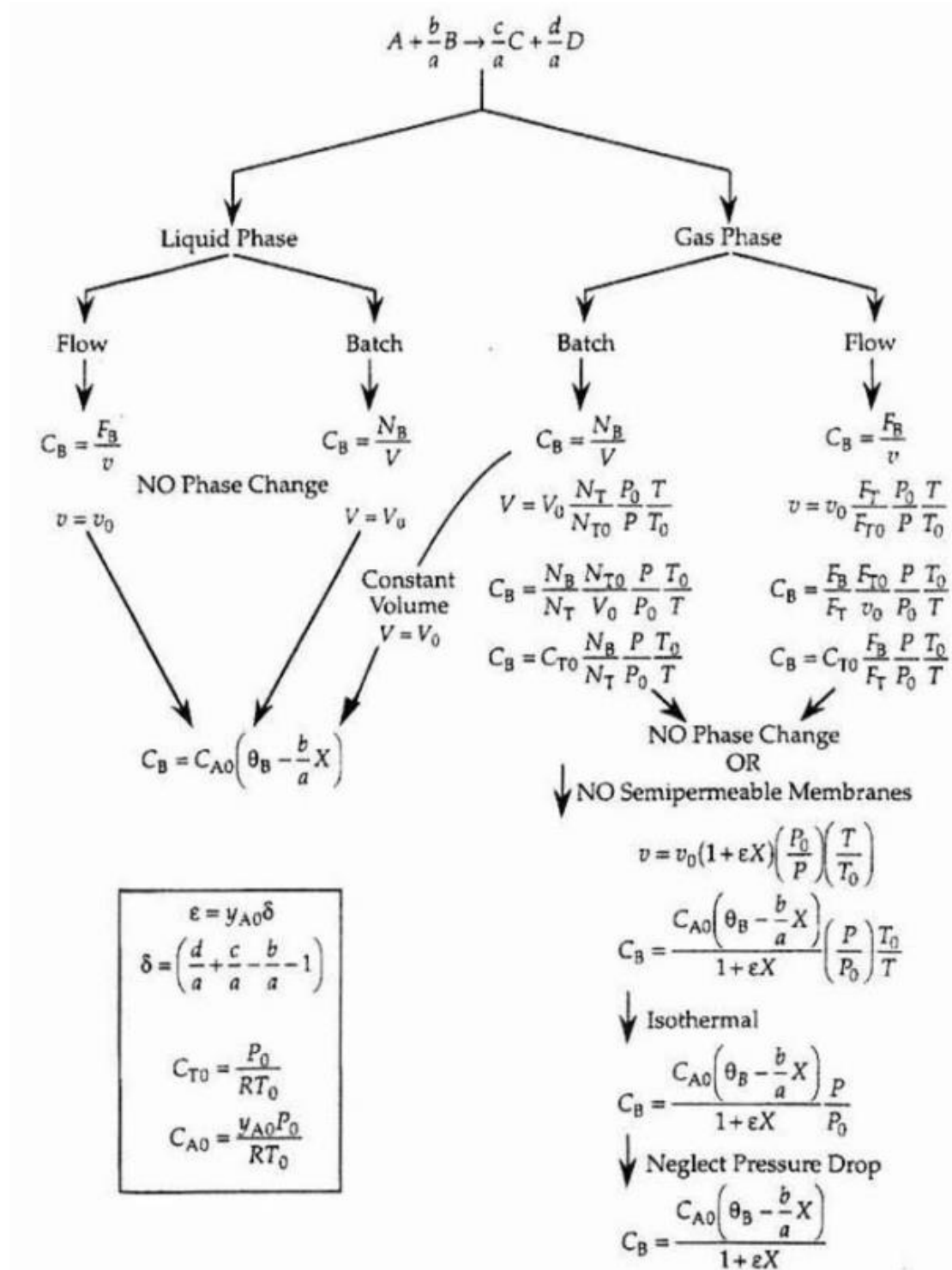$$C_A = \frac{F_A}{\upsilon} = \frac{F_{A0}(1-X)}{\upsilon_0(1+\varepsilon X)}\frac{T_0}{T}\frac{P}{P_0} = C_{A0}\frac{(1-X)}{(1+\varepsilon X)}\frac{T_0}{T}\frac{P}{P_0}$$

$$C_B = \frac{F_B}{\upsilon} = \frac{F_{A0}\left(\Theta_B - \frac{b}{a}X\right)}{\upsilon_0(1+\varepsilon X)}\frac{T_0}{T}\frac{P}{P_0} = C_{A0}\frac{\left(\Theta_B - \frac{b}{a}X\right)}{(1+\varepsilon X)}\frac{T_0}{T}\frac{P}{P_0}$$

etc.

Again, these equations give us information about $-r_A = f(X)$, which we can use to size reactors.

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$

Liquid Phase

Flow

$$C_B = \frac{F_B}{v}$$

Batch

$$C_B = \frac{N_B}{V}$$

NO Phase Change

$$v = v_0 \qquad\qquad V = V_0$$

Constant Volume $V = V_0$

$$C_B = C_{A0}\left(\theta_B - \frac{b}{a}X\right)$$

Gas Phase

Batch

$$C_B = \frac{N_B}{V}$$

$$V = V_0 \frac{N_T}{N_{T0}} \frac{P_0}{P} \frac{T}{T_0}$$

$$C_B = \frac{N_B}{N_T} \frac{N_{T0}}{V_0} \frac{P}{P_0} \frac{T_0}{T}$$

$$C_B = C_{T0} \frac{N_B}{N_T} \frac{P}{P_0} \frac{T_0}{T}$$

Flow

$$C_B = \frac{F_B}{v}$$

$$v = v_0 \frac{F_T}{F_{T0}} \frac{P_0}{P} \frac{T}{T_0}$$

$$C_B = \frac{F_B}{F_T} \frac{F_{T0}}{v_0} \frac{P}{P_0} \frac{T_0}{T}$$

$$C_B = C_{T0} \frac{F_B}{F_T} \frac{P}{P_0} \frac{T_0}{T}$$

NO Phase Change
OR
NO Semipermeable Membranes

$$v = v_0(1 + \varepsilon X)\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)$$

$$C_B = \frac{C_{A0}\left(\theta_B - \frac{b}{a}X\right)}{1 + \varepsilon X}\left(\frac{P}{P_0}\right)\frac{T_0}{T}$$

Isothermal

$$C_B = \frac{C_{A0}\left(\theta_B - \frac{b}{a}X\right)}{1 + \varepsilon X}\frac{P}{P_0}$$

Neglect Pressure Drop

$$C_B = \frac{C_{A0}\left(\theta_B - \frac{b}{a}X\right)}{1 + \varepsilon X}$$

$$\varepsilon = y_{A0}\delta$$

$$\delta = \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)$$

$$C_{T0} = \frac{P_0}{RT_0}$$

$$C_{A0} = \frac{y_{A0}P_0}{RT_0}$$

CHAPTER 2 EXAMPLE

Reactors in Series: CSTR-PFR-CSTR

Using either the data in Table E2-W.1, calculate the reactor volumes V_1, V_2, and V_3 for the CSTR/PFR/CSTR reactors in series sequence shown in Figure E2-W.1 along with the corresponding conversion.
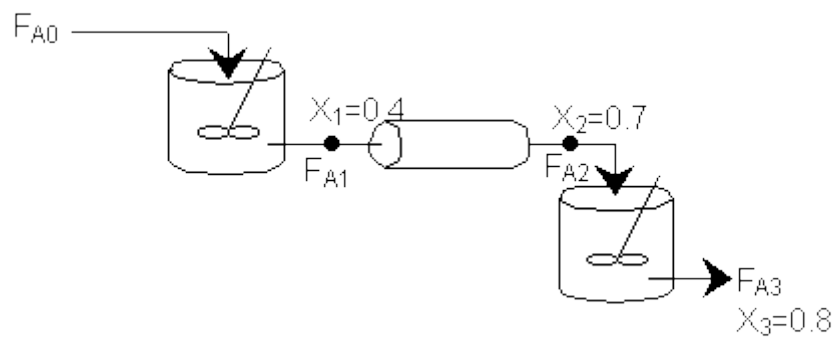

Figure E2-W.1 CSTR/PFR reactor in series.

Table E2-W.1 Processed Data

X	0	0.2	0.4	0.6	0.8
$-r_A \left(\dfrac{mol}{dm^3 \bullet s} \right)$	0.010	0.0091	0.008	0.005	0.002
$(1/-r_A) \left(\dfrac{dm^3 \bullet s}{mol} \right)$	100	110	125	200	500
$F_{A0}/-r_A \ (dm^3)$	200	220	250	400	1000

Solution

SOLUTION

We again use the plot of $\left(\dfrac{F_{A0}}{-r_A}\right)$ vs. X
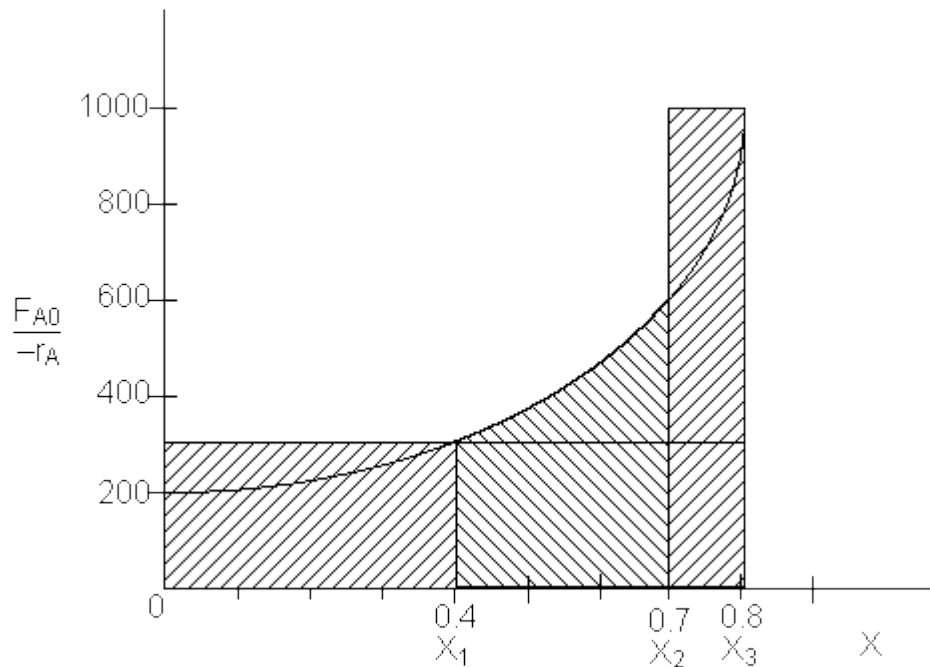

Figure E2-W.2 Levenspiel plot for CSTR/PFR/CSTR sequence.

(a) The CSTR design equation for Reactor 1 is

$$V_1 = \left(\frac{F_{A0}\,X}{-r_{A1}}\right)$$

(E2-W.1)

at $X = X_1 = 0.4$ the $(F_{A0}/-r_{A1}) = 300$ dm^3

$V_1 = (300$ dm^3) $(0.4) = 120$ dm^3

The volume of the first CSTR is 120 dm^3.

(b)Reactor 2: PFR The differential form of the PFR design is

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}}$$

(E2-W.2)

Rearranging and integrating with limits

when $V = 0$ $X = X_1 = 0.4$

when $V = V_2$ $X = X_2 = 0.7$

$$V = \int_{X_1}^{X_2} \left(\frac{F_{A0}}{-r_A}\right) dX = \int_{0.4}^{0.7} \left(\frac{F_{A0}}{-r_A}\right) dX$$

(E2-W.3)

Choose three point quadrature formula with $\quad \Delta X = \dfrac{X_2 - X_1}{2} = \dfrac{0.7 - 0.4}{2} = 0.15$

$$V_2 = \frac{\Delta X}{3}\left[\frac{F_{A0}}{-r_A(0.4)} + \frac{4F_{A0}}{-r_A(0.55)} + \frac{F_{A0}}{-r_A(0.7)}\right]$$

(E2-W.4)

Interpreting for $(F_{A0}/-r_A)$ at $X = 0.55$ we obtain

$$\left(\frac{F_{A0}}{-r_A}\right)_{X=0.55} = 370 \ dm^3$$

$$V_2 = \frac{0.15}{3}\left[300 \ dm^3 + 4\left(370 \ dm^3\right) + 600 \ dm^3\right] = 119 \ dm^3$$

The volume of the PFR is $\boxed{V_2 = 119 \ dm^3}$

(c) Reactor 3: CSTR

    Balance

$$in \ - \ out \ + \ generation$$
$$F_{A2} \ - \ F_{A3} \ + \quad r_{A3}V_3 \quad = \ 0$$

(E2-W.5)

    Rearranging

$$\boxed{V_3 = \frac{F_{A2} - F_{A3}}{-r_{A3}}}$$

(E2-W.6)

$$F_{A2} = F_{A0}\left(1 - X_2\right)$$

(E2-W.7)

$$F_{A3} = F_{A0}\left(1 - X_3\right)$$

(E2-W.8)

$$V_3 = \frac{F_{A0}}{-r_{A3}}\left(X_3 - X_2\right)$$

(E2-W.9)

$$V_3 = 600 \ dm^3 \ \left(0.7 - 0.4\right) = 180 \ dm^3$$

The volume of the last CSTR is 180 dm^3.

Summary		
CSTR	$X_1 = 0.4$	$V_1 = 120 \ dm^3$
PFR	$X_2 = 0.7$	$V_2 = 119 \ dm^3$
CSTR	$X_3 = 0.8$	$V_3 = 180 \ dm^3$

$$V_3 = \frac{F_{A0}}{-r_{A3}}\left(X_3 - X_2\right)$$