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Chemical Reaction Engineering

Rate Laws and Stoichiometry

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Content

- Reversible Reaction
- Reaction Rate Constant
- Activation Energy
- Stoichiometry

Reversible Reactions

- All rate laws for reversible reactions *must* reduce to the thermodynamic relationship relating the reacting species concentrations at equilibrium.
- At equilibrium, the rate of reaction is identically zero for all species

for the general reaction

$$aA + bB \rightleftarrows cC + dD$$

- The concentrations ax equilibrium are related by the thermodynamic relationship for the equilibrium constant K_c

$$K_C = \frac{C_{Ce}^{c} C_{De}^{d}}{C_{Ae}^{a} C_{Be}^{b}}$$

The units of the thermodynamic equilibrium constant, K_C, are $(\text{mol/dm}^3)^{d+c-b-a}$

Reversible Reactions

Rate laws for reversible reactions

For the reaction

$$2C_6H_6 \underset{k_{-B}}{\overset{k_B}{\rightleftarrows}} C_{12}H_{10} + H_2 \quad \text{or,} \quad 2B \underset{k_{-B}}{\overset{k_B}{\rightleftarrows}} D + H_2$$

Benzene diphenyl hydrogen

k_B and k_{-B}, are the forward and reverse specific reaction rate constants respectively and defined with respect to benzene.

The rate of disappearance of benzene $-r_{B,\text{forward}} = k_B C_B^2$

Or the rate of disappearance of benzene for the forward reaction

$$r_{B,\text{forward}} = -k_B C_B^2$$

- For the reverse reaction

$$C_{12}H_{10} + H_2 \xrightarrow{k_{-B}} 2C_6H_6$$

Reversible Reactions

The rate of formation of benzene $r_{B,\,reverse} = k_{-B} C_D C_{H_2}$

- ➢ The net rate of formation of benzene

$$r_B \equiv r_{B,\,net} = r_{B,\,forward} + r_{B,\,reverse}$$

➡

$$r_B = -k_B C_B^2 + k_{-B} C_D C_{H_2}$$

the rate of disappearance of benzene, $-r_B$:

$$-r_B = k_B C_B^2 - k_{-B} C_D C_{H_2} = k_B \left(C_B^2 - \frac{k_{-B}}{k_B} C_D C_{H_2} \right)$$

➡

$$-r_B = k_B \left(C_B^2 - \frac{C_D C_{H_2}}{K_C} \right)$$

Reversible Reactions

where

$$\frac{k_B}{k_{-B}} = K_C = \text{Concentration equilibrium constant}$$

- ➢ The equilibrium constant
  - ➢ Decreases with increasing temperature for exothermic reactions and
  - ➢ Increases **with** increasing temperature for endothermic reactions
- ➢ The rate of formation of diphenyl is:

$$r_D = k_D \left[C_B^2 - \frac{C_D C_{H_2}}{K_C} \right]$$

- ➢ Also, from stoichiometry

$$\frac{r_D}{1} = \frac{r_B}{-2} = \frac{k_B}{2} \left[C_B^2 - \frac{C_D C_{H_2}}{K_C} \right]$$

Reversible Reactions

Comparing

$$-r_B = k_B\left(C_B^2 - \frac{C_D C_{H_2}}{K_C}\right)$$

And

$$r_D = k_D\left[C_B^2 - \frac{C_D C_{H_2}}{K_C}\right]$$

And utilizing stoichiornetry

$$\frac{r_D}{1} = \frac{r_B}{-2} = \frac{k_B}{2}\left[C_B^2 - \frac{C_D C_{H_2}}{K_C}\right]$$

➡ $\boxed{k_D = \frac{k_B}{2}}$

At equilibrium, $-r_B \equiv 0$,

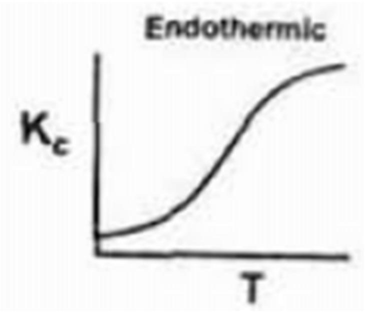
$$-r_B \equiv 0 = k_B\left[C_{Be}^2 - \frac{C_{De} C_{H_2e}}{K_C}\right]$$

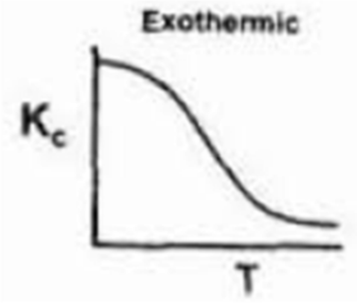
➡ $K_C = \dfrac{C_{De} C_{H_2e}}{C_{Be}^2}$

Reversible Reactions

- When there is no change in the total number of moles and the beat capacity term, $\Delta C_P = 0$

$$K_C(T) = K_C(T_1)\exp\left[\frac{\Delta H_{Rx}}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$$



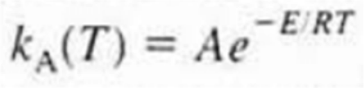


The Reaction Rate Constant

The specific reaction rate or the rate constant

- Is merely independent of the concentrations of the species involved in the reaction.
- Is almost always strongly dependent on temperature.
- Depends on whether or not a catalyst is present,
- In gas-phase reactions, it may be a function of total pressure
- In liquid systems it can also be a function of other parameters, such as ionic strength and choice of solvent

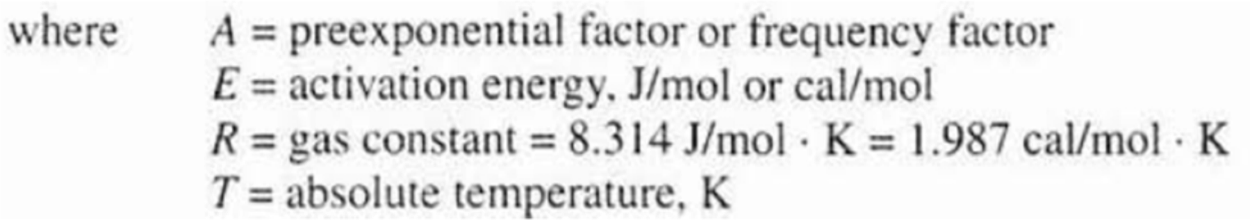
- The temperature dependence of the specific reaction rate, k_A could be correlated by



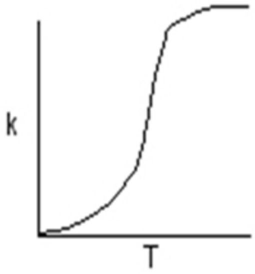
$$k_A(T) = Ae^{-E/RT}$$

Arrhenius Equation

The Reaction Rate Constant



where A = preexponential factor or frequency factor
E = activation energy, J/mol or cal/mol
R = gas constant = 8.314 J/mol · K = 1.987 cal/mol · K
T = absolute temperature, K



$$T \rightarrow \infty \quad k \rightarrow A$$

$$T \rightarrow 0 \quad k \rightarrow 0$$

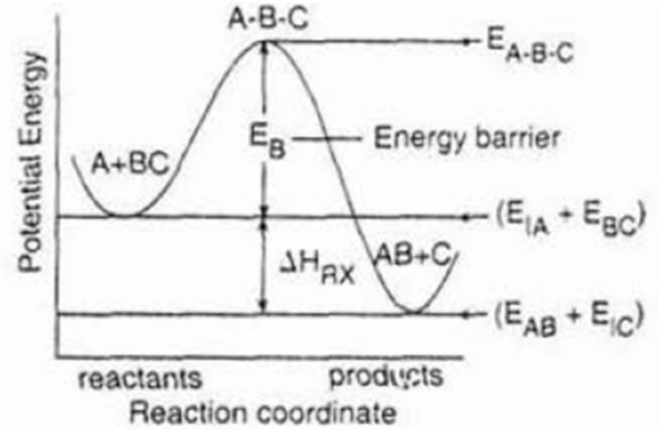
$$A \approx 10^{13}$$

The Activation Energy

- The activation energy can be thought of as a barrier to energy transfer (from **the** kinetic energy to the potential energy) between reacting molecule that must be overcome.

$$A + BC \rightleftarrows A-B-C \longrightarrow AB + C$$

reactants intermediate products



the potential energy of the system as a function of the progress along the reaction path

- The distance between A and B decreases, and the AB bond begins to form.
- As we proceed further, the distance between AB and C increases and
- The energy of the reacting pair decreases to that of the AB bond energy.

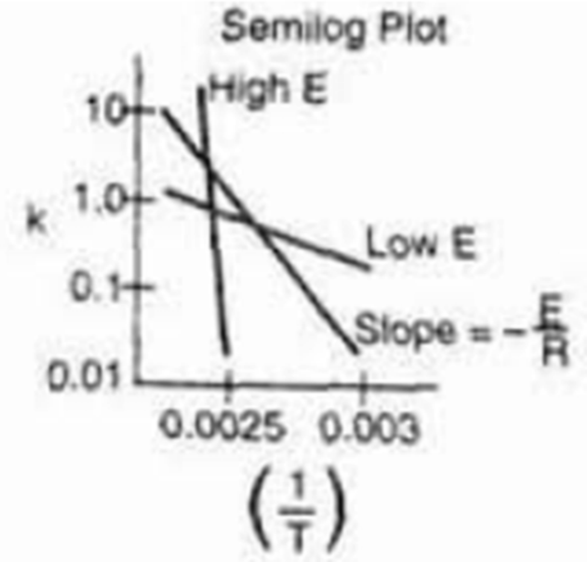
$$E_B = E^{\circ}_{fA-B-C} - (E^{\circ}_{fA} + E^{\circ}_{fB-C})$$

$E^{\circ}_{f_i}$: Energies of formation

The Activation Energy

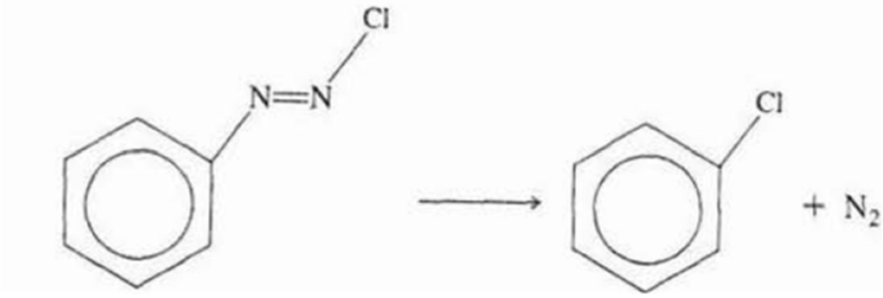
$$\ln k_A = \ln A - \frac{E}{R}\left(\frac{1}{T}\right)$$

- The larger the activation energy, the more temperature-sensitive is the rate of reaction.



Example

Calculate the activation energy for the decomposition of benzene diazonium chloride to give chlorobenzene and nitrogen:



using the information

k (s^{-1})	0.00043	0.00103	0.00180	0.00355	0.00717
T (K)	313.0	319.0	323.0	328.0	333.0

Example Cont.

Example Cont.

- If the specific reaction rate $k_o(T_o)$ at a temperature, T_o, and we know the activation energy, E. we can find the specific reaction rate $k(T)$ at any other temperature, T. for that reaction

$$k(T) = k(T_0)e^{\frac{E}{R}\left(\frac{1}{T_0}-\frac{1}{T}\right)} \quad \text{where} \quad k(T_0) = Ae^{-E/RT_0}$$

Review: Reactor Sizing and Design

- The rate of disappearance of A, $-r_A$, might be
  - Known **as** a function of conversion, X

$$-r_A = g(X)$$

  - Expressed in terms of the concentration of the reacting species

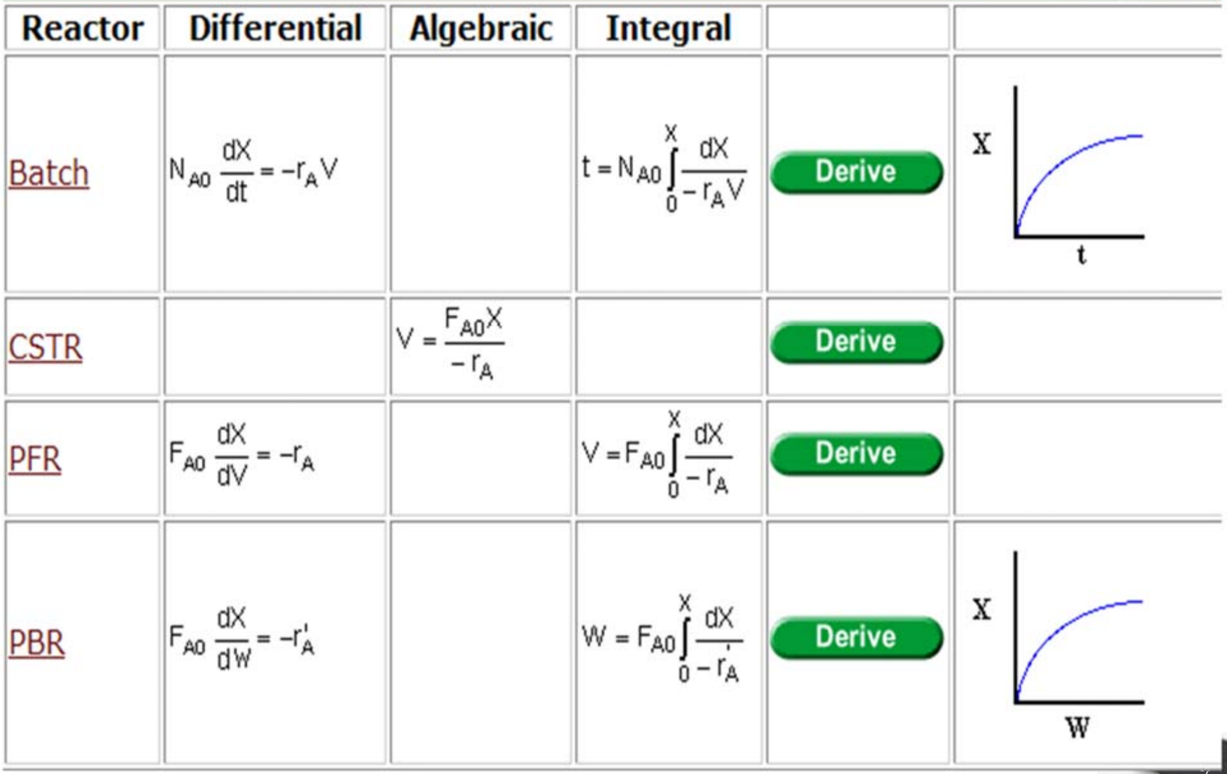
$$-r_A = [k_A(T)][\text{fn}(C_A, C_B, \ldots)]$$

- The concentration of the reacting species may he written in terms of the conversion X

$$C_j = h_j(X)$$

- If the rate law depends on more than one species, it is necessary to relate the concentrations of the different species to each other

Review: Reactor Sizing and Design



Reactor	Differential	Algebraic	Integral		
Batch	$N_{A0}\frac{dX}{dt} = -r_A V$		$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$	Derive	
CSTR		$V = \frac{F_{A0}X}{-r_A}$		Derive	
PFR	$F_{A0}\frac{dX}{dV} = -r_A$		$V = F_{A0}\int_0^X \frac{dX}{-r_A}$	Derive	
PBR	$F_{A0}\frac{dX}{dW} = -r'_A$		$W = F_{A0}\int_0^X \frac{dX}{-r'_A}$	Derive	

Stoichiometry

- A stoichiometric table is a table that presents the stoichiometric relationships between reacting molecules for a single reaction.
- Such table make it easier to relate the concentrations of the different species to each other for the case when the rate law depends on more than one species.
- For the reaction

$$aA + bB \rightleftarrows cC + dD$$

$$\frac{r_A}{-a} = \frac{r_B}{-b} = \frac{r_C}{c} = \frac{r_D}{d}$$

- In formulating our stoichiometric table, we shall take species A (limiting reactant) as a basis of calculation

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

Stoichiometry

Batch Systems

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

$$N_A = N_{A0} - N_{A0}X = N_{A0}(1 - X)$$

N_{A0}	the number of moles of A initially present in the reactor
$N_{A0}X$	moles of A are consumed
N_A	the number of moles of A remaining in the reactor

- ➢ How to express the number of moles of B, C, and D in terms of conversion of A?.

$$\text{moles B reacted} = \frac{\text{moles B reacted}}{\text{moles A reacted}} \cdot \text{moles A reacted} \quad = \frac{b}{a}(N_{A0}X)$$

$$\Rightarrow \quad N_B = N_{B0} - \frac{b}{a}N_{A0}X$$

Batch Systems

Species	Initially (mol)	Change (mol)	Remaining (mol)
A	N_{A0}	$-(N_{A0}X)$	$N_A = N_{A0} - N_{A0}X$
B	N_{B0}	$-\frac{b}{a}(N_{A0}X)$	$N_B = N_{B0} - \frac{b}{a}N_{A0}X$
C	N_{C0}	$\frac{c}{a}(N_{A0}X)$	$N_C = N_{C0} + \frac{c}{a}N_{A0}X$
D	N_{D0}	$\frac{d}{a}(N_{A0}X)$	$N_D = N_{D0} + \frac{d}{a}N_{A0}X$
I (inerts)	N_{I0}		$N_I = N_{I0}$
Totals	N_{T0}		$N_T = N_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)N_{A0}X$

Batch Systems

Let $$\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$$

Then $$N_T = N_{T0} + \delta N_{A0} X$$

The concentration of A is the number of moles of A per unit volume:

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

$$C_B = \frac{N_B}{V} = \frac{N_{B0} - (b/a)N_{A0}X}{V} \qquad C_C = \frac{N_C}{V} = \frac{N_{C0} + (c/a)N_{A0}X}{V}$$

$$C_D = \frac{N_D}{V} = \frac{N_{D0} + (d/a)N_{A0}X}{V}$$

Batch Systems

defining the parameter Θ_i,

$$\Theta_i = \frac{N_{i0}}{N_{A0}} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}}$$

Then

$$C_B = \frac{N_{A0}[N_{B0}/N_{A0} - (b/a)X]}{V} = \frac{N_{A0}[\Theta_B - (b/a)X]}{V}$$

with $\Theta_B = \dfrac{N_{B0}}{N_{A0}}$

$$C_C = \frac{N_{A0}[\Theta_C + (c/a)X]}{V}, \quad \text{with } \Theta_C = \frac{N_{C0}}{N_{A0}}$$

$$C_D = \frac{N_{A0}[\Theta_D + (d/a)X]}{V}, \quad \text{with } \Theta_D = \frac{N_{D0}}{N_{A0}}$$

Constant-Volume Batch Reaction Systems

- For the constant-volume systems

$$V = V_0$$

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

$$C_B = N_{A0}\frac{[(N_{B0}/N_{A0})-(b/a)X]}{V_0} = \frac{N_{A0}[\Theta_B-(b/a)X]}{V_0} = C_{A0}\left(\Theta_B - \frac{b}{a}X\right)$$

$$C_C = N_{A0}\frac{[(N_{C0}/N_{A0})+(c/a)X]}{V_0} = C_{A0}\left(\Theta_C + \frac{c}{a}X\right)$$

$$C_D = N_{A0}\frac{[(N_{D0}/N_{A0})+(d/a)X]}{V_0} = C_{A0}\left(\Theta_D + \frac{d}{a}X\right)$$

Batch Systems

- For liquid-phase reactions (or as we will soon see for isothermal and isobaric gas-phase reactions with no change in the total number of moles,

For $$-r_A = k_A C_A C_B$$

Then $$-r_A = kC_AC_B = kC_{A0}^2(1-X)\left(\Theta_B - \frac{b}{a}X\right) = f(X)$$

Example

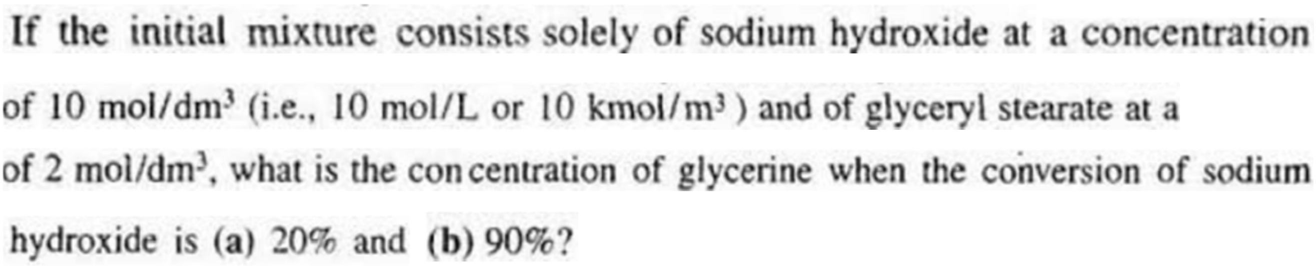
For the reaction

$$3NaOH(aq) + (C_{17}H_{35}COO)_3C_3H_5 \longrightarrow 3C_{17}H_{35}COONa + C_3H_5(OH)_3$$

Express the concentrations of the different species as function *X*.

Example Cont.

Example



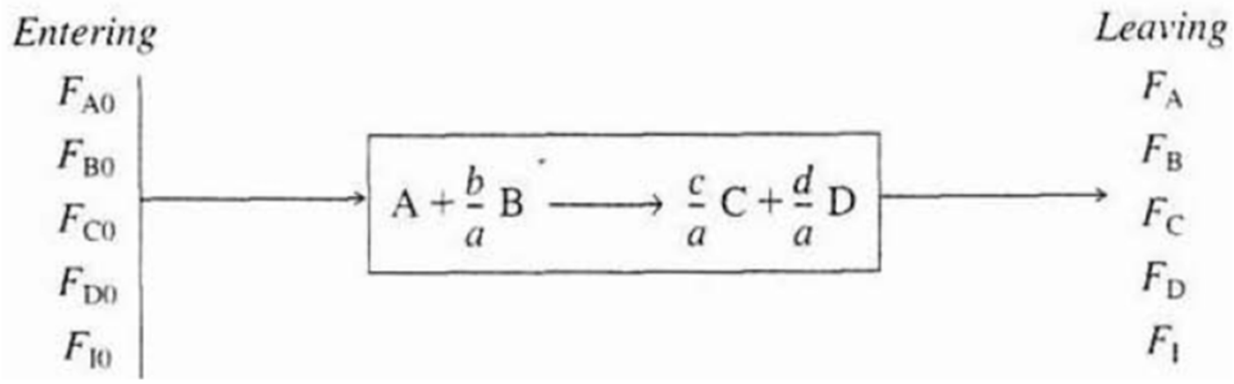
If the initial mixture consists solely of sodium hydroxide at a concentration of 10 mol/dm^3 (i.e., 10 mol/L or 10 kmol/m^3) and of glyceryl stearate at a of 2 mol/dm^3, what is the concentration of glycerine when the conversion of sodium hydroxide is (a) 20% and **(b)** 90%?

Example Cont.

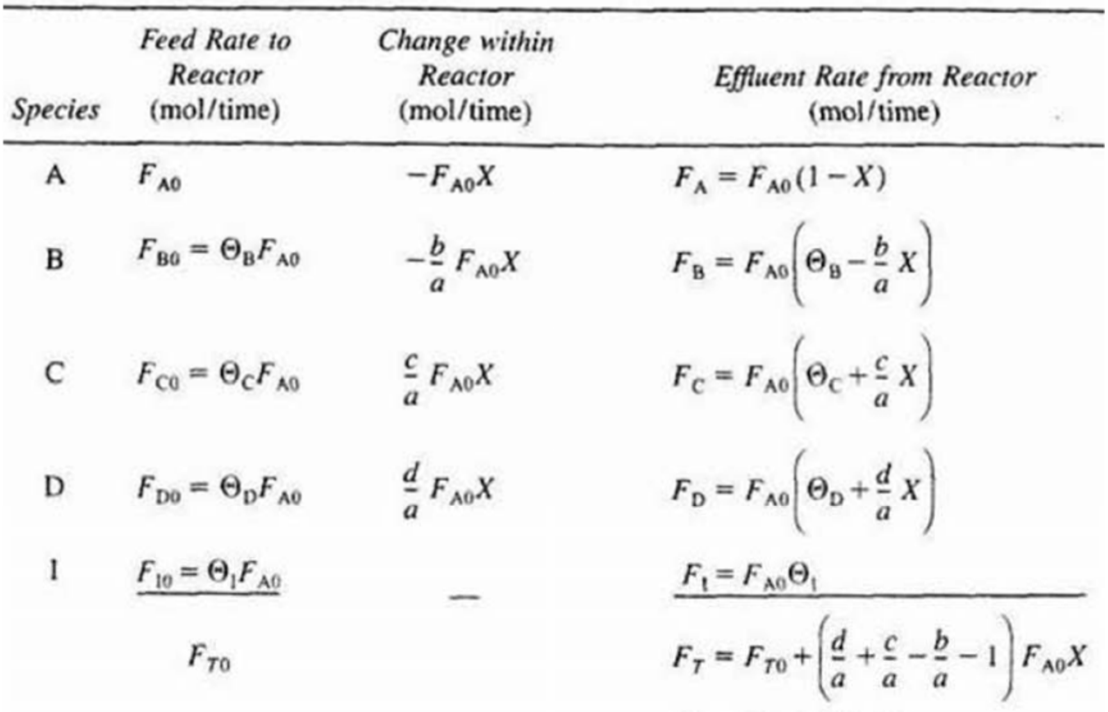
Stoichiometry

Flow Systems

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



Flow Systems



Species	Feed Rate to Reactor (mol/time)	Change within Reactor (mol/time)	Effluent Rate from Reactor (mol/time)
A	F_{A0}	$-F_{A0}X$	$F_A = F_{A0}(1-X)$
B	$F_{B0} = \Theta_B F_{A0}$	$-\frac{b}{a}F_{A0}X$	$F_B = F_{A0}\left(\Theta_B - \frac{b}{a}X\right)$
C	$F_{C0} = \Theta_C F_{A0}$	$\frac{c}{a}F_{A0}X$	$F_C = F_{A0}\left(\Theta_C + \frac{c}{a}X\right)$
D	$F_{D0} = \Theta_D F_{A0}$	$\frac{d}{a}F_{A0}X$	$F_D = F_{A0}\left(\Theta_D + \frac{d}{a}X\right)$
I	$F_{I0} = \Theta_I F_{A0}$	—	$F_I = F_{A0}\Theta_I$
	F_{T0}		$F_T = F_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)F_{A0}X$
			$F_T = F_{T0} + \delta F_{A0}X$

Concentrations in Flow Systems

where

$$\Theta_B = \frac{F_{B0}}{F_{A0}} = \frac{C_{B0}v_0}{C_{A0}v_0} = \frac{C_{B0}}{C_{A0}} = \frac{y_{B0}}{y_{A0}}$$

and Θ_C, Θ_D, and Θ_I are defined similarly.

Equations for Concentrations in Flow Systems

For a flow system,

$$C_A = \frac{F_A}{v} = \frac{\text{moles/time}}{\text{liters/time}} = \frac{\text{moles}}{\text{liter}}$$

Concentrations in Flow Systems

$$C_A = \frac{F_A}{v} = \frac{F_{A0}}{v}(1-X)$$

$$C_B = \frac{F_B}{v} = \frac{F_{B0}-(b/a)F_{A0}X}{v}$$

$$C_C = \frac{F_C}{v} = \frac{F_{C0}+(c/a)F_{A0}X}{v}$$

$$C_D = \frac{F_D}{v} = \frac{F_{D0}+(d/a)F_{A0}X}{v}$$

Liquid-Phase Concentrations

- For liquids, volume change with reaction is negligible when no phase change are taking place

$$v = v_0$$

Liquid-Phase Concentrations

$$C_A = \frac{F_{A0}}{v_0}(1-X) = C_{A0}(1-X)$$

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

➡ $-r_A = f(X)$

Change in the Total Number of Moles with Reaction in the Gas Phase

- Variation on the flow rate occurs quite frequently in gas-phase reactions that do not have an equal number of product and reactant moles

$$N_2 + 3H_2 \rightleftarrows 2NH_3$$

4 mol of reactants gives 2 mol of product.

Variable Volume

- Variable-volume situation could occur in batch reactors where volume changes with time as in internal-combustion engine

Batch Reactors with Variable Volume

$$PV = ZN_TRT$$

where

V = volume and N_T = total number of moles

T = temperature, K

P = total pressure, atm (kPa; 1 atm = 101.3 kPa)

Z = compressibility factor

R = gas constant = 0.08206 $dm^3 \cdot atm/mol \cdot K$

Batch Reactors with Variable Volume

This equation is valid at any point in the system at any time t.

At $t = 0$

$$P_0 V_0 = Z_0 N_{T0} R T_0$$

$$\Rightarrow \quad V = V_0 \left(\frac{P_0}{P}\right) \frac{T}{T_0} \left(\frac{Z}{Z_0}\right) \frac{N_T}{N_{T0}}$$

But $N_T = N_{T0} + \delta N_{A0} X$

where $\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$ $\quad \delta = \frac{\text{Change in total number of moles}}{\text{Mole of A reacted}}$

Batch Reactors with Variable Volume

divide by N_{T0}:

$$\frac{N_T}{N_{T0}} = 1 + \frac{N_{A0}}{N_{T0}} \delta X = 1 + \overbrace{\delta y_{A0}}^{\varepsilon} X$$

where y_{A0} is the mole fraction of A initially present,

$$\Rightarrow \quad \frac{N_T}{N_{T0}} = 1 + \varepsilon X$$

where

$$\varepsilon = \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right) \frac{N_{A0}}{N_{T0}} = y_{A0} \delta$$

For both batch and flow systems

Batch Reactors with Variable Volume

Also

$$\varepsilon = \frac{N_T - N_{T0}}{N_{T0} X}$$

at complete conversion, (i.e., $X = 1$ and $N_T = N_{Tf}$)

$$\varepsilon = \frac{N_{Tf} - N_{T0}}{N_{T0}}$$

$$= \frac{\text{Change in total number of moles for complete conversion}}{\text{Total moles fed}}$$

If all species are in the gas phase,

$$V = V_0 \left(\frac{P_0}{P}\right) \frac{T}{T_0} \left(\frac{Z}{Z_0}\right) (1 + \varepsilon X)$$

Batch Reactors with Variable Volume

- If the temperatures and pressures are changed such that the compressibility factor will not change significantly during the course of the reaction

$$Z_0 \cong Z$$

Then, for a variable volume batch system, the volume of gas at any time t is

$$V = V_0 \left(\frac{P_0}{P}\right) (1 + \varepsilon X) \frac{T}{T_0}$$

Flow Reactors with Variable Volumetric Flow Rate

- The total concentration can be defined as

$$C_T = \frac{F_T}{\upsilon} = \frac{P}{ZRT}$$

Flow Reactors with Variable Volumetric Flow Rate

At the entrance to the reactor,

$$C_{T0} = \frac{F_{T0}}{v_0} = \frac{P_0}{Z_0 R T_0}$$

Taking the ratio

$$\Rightarrow \quad v = v_0 \left(\frac{F_T}{F_{T0}}\right) \frac{P_0}{P} \left(\frac{T}{T_0}\right)$$

⇒ the concentration of species *j* for a flow system

$$C_j = \frac{F_j}{v} = \frac{F_j}{v_0 \left(\frac{F_T}{F_{T0}} \frac{P_0}{P} \frac{T}{T_0}\right)} = \left(\frac{F_{T0}}{v_0}\right)\left(\frac{F_j}{F_T}\right)\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right)$$

Flow Reactors with Variable Volumetric Flow Rate

$$\Rightarrow \quad C_j = C_{T0} \left(\frac{F_j}{F_T}\right)\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right)$$

And $\quad F_T = F_A + F_B + F_C + F_D + F_I + \cdots = \sum_{j=1}^{n} F_j$

But $\quad F_T = F_{T0} + F_{A0}\,\delta X$

Then

$$v = v_0 \frac{F_{T0} + F_{A0}\,\delta X}{F_{T0}} \left(\frac{P_0}{P}\right) \frac{T}{T_0}$$

$$= v_0 \left(1 + \frac{F_{A0}}{F_{T0}}\,\delta X\right) \frac{P_0}{P} \left(\frac{T}{T_0}\right) = v_0 (1 + y_{A0}\,\delta X)\, \frac{P_0}{P} \left(\frac{T}{T_0}\right)$$

Flow Reactors with Variable Volumetric Flow Rate

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

The concentration of species *j* is $C_j = \dfrac{F_j}{v}$

The molar flow rate of species *j* is $F_j = F_{j0} + \nu_j(F_{A0}X) = F_{A0}(\Theta_j + \nu_j X)$

where ν_i is the stoichiometric coefficient, negative for reactants
positive for products.

- For the reaction $\mathrm{A} + \frac{b}{a}\mathrm{B} \longrightarrow \frac{c}{a}\mathrm{C} + \frac{d}{a}\mathrm{D}$

$\nu_A = -1$, $\nu_B = -b/a$, $\nu_C = c/a$, $\nu_D = d/a$, and $\Theta_j = F_{j0}/F_{A0}$.

Flow Reactors with Variable Volumetric Flow Rate

➡ $$C_j = \frac{F_{A0}(\Theta_j + \nu_j X)}{v_0\left((1+\varepsilon X)\dfrac{P_0}{P}\dfrac{T}{T_0}\right)}$$

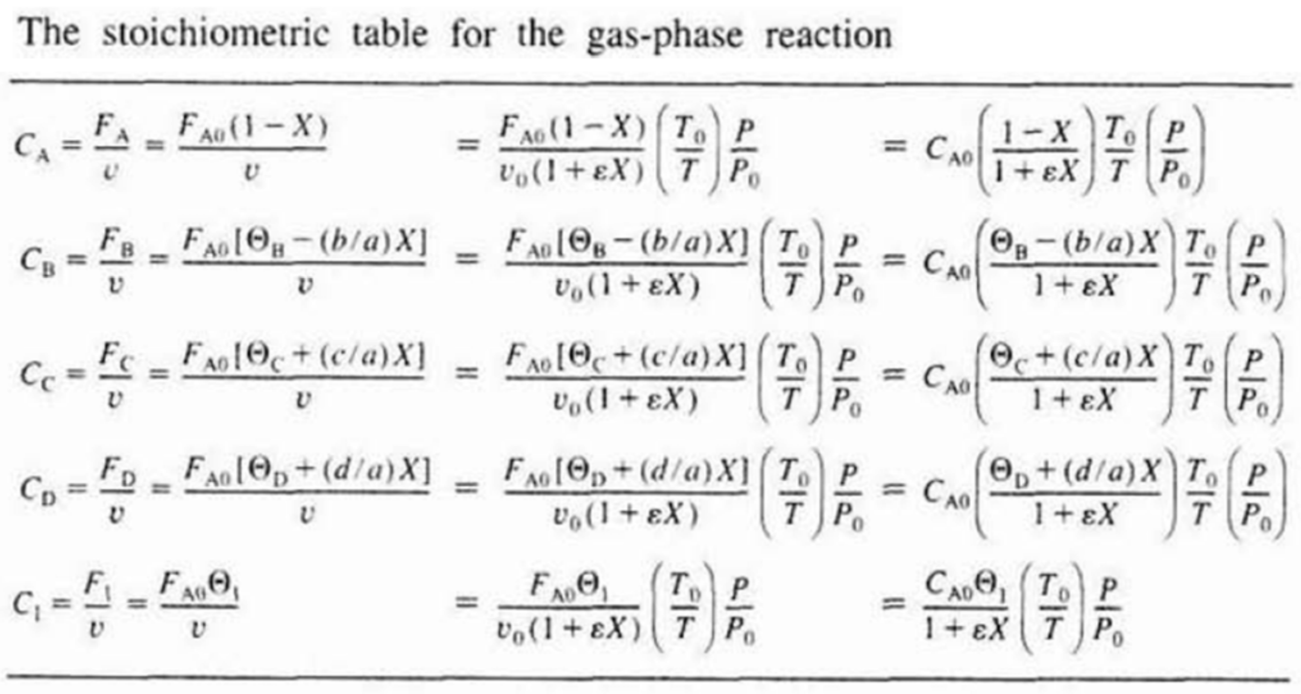
Rearranging

$$C_j = \frac{C_{A0}(\Theta_j + \nu_j X)}{1+\varepsilon X}\left(\frac{P}{P_0}\right)\frac{T_0}{T}$$

Recall that

$$y_{A0} = F_{A0}/F_{T0},\ C_{A0} = y_{A0}C_{T0},\ \varepsilon = y_{A0}\delta$$

Flow Reactors with Variable Volumetric Flow Rate



The stoichiometric table for the gas-phase reaction

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v} = \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{1-X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

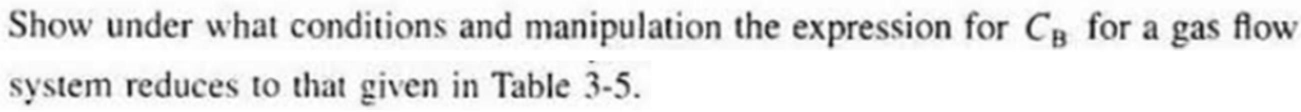
$$C_B = \frac{F_B}{v} = \frac{F_{A0}[\Theta_B-(b/a)X]}{v} = \frac{F_{A0}[\Theta_B-(b/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{\Theta_B-(b/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_C = \frac{F_C}{v} = \frac{F_{A0}[\Theta_C+(c/a)X]}{v} = \frac{F_{A0}[\Theta_C+(c/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{\Theta_C+(c/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_D = \frac{F_D}{v} = \frac{F_{A0}[\Theta_D+(d/a)X]}{v} = \frac{F_{A0}[\Theta_D+(d/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{\Theta_D+(d/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_I = \frac{F_I}{v} = \frac{F_{A0}\Theta_I}{v} = \frac{F_{A0}\Theta_I}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = \frac{C_{A0}\Theta_I}{1+\varepsilon X}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$$

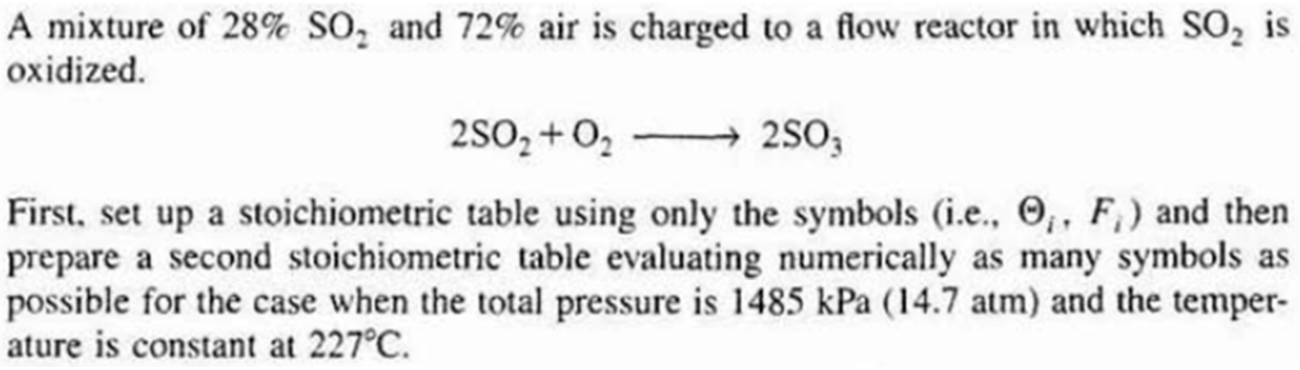
Example



Show under what conditions and manipulation the expression for C_B for a gas flow system reduces to that given in Table 3-5.

Example Cont.

Example



A mixture of 28% SO_2 and 72% air is charged to a flow reactor in which SO_2 is oxidized.

$$2SO_2 + O_2 \longrightarrow 2SO_3$$

First, set up a stoichiometric table using only the symbols (i.e., Θ_i, F_i) and then prepare a second stoichiometric table evaluating numerically as many symbols as possible for the case when the total pressure is 1485 kPa (14.7 atm) and the temperature is constant at 227°C.

Example Cont.

Example Cont.

Example Cont.

Example Cont.

Example Cont.

Example Cont.

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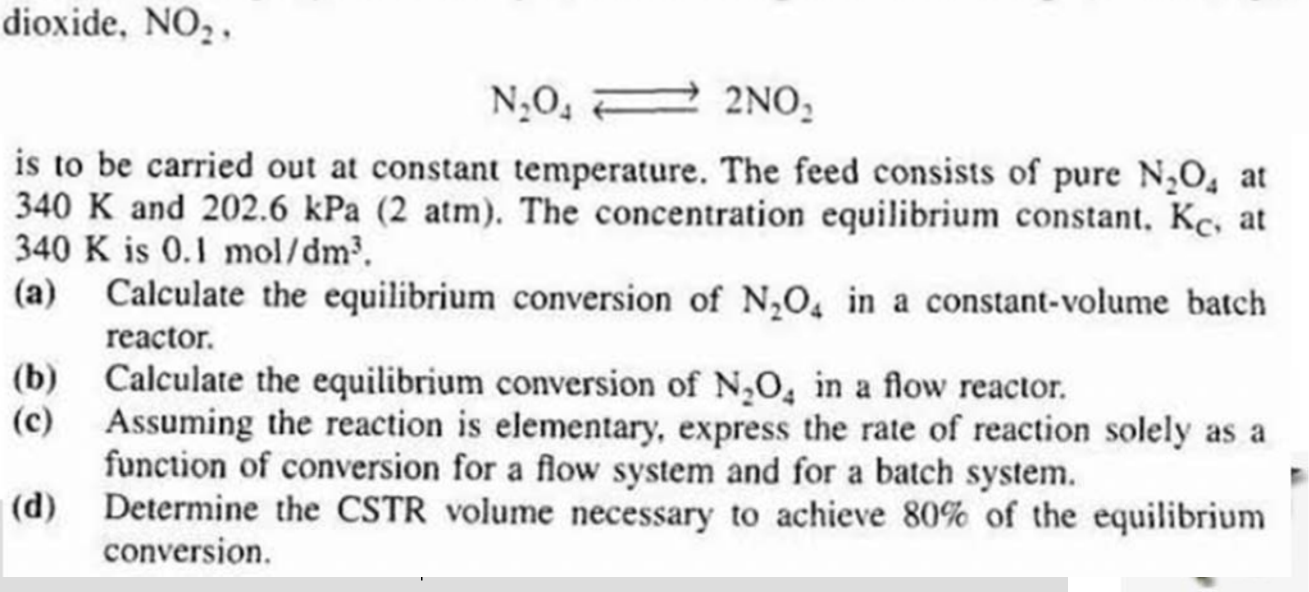
Example Cont.

Example



The reversible gas-phase decomposition of nitrogen tetroxide, N_2O_4, to nitrogen dioxide, NO_2,

$$N_2O_4 \rightleftarrows 2NO_2$$

is to be carried out at constant temperature. The feed consists of pure N_2O_4 at 340 K and 202.6 kPa (2 atm). The concentration equilibrium constant, K_C, at 340 K is 0.1 mol/dm^3.

(a) Calculate the equilibrium conversion of N_2O_4 in a constant-volume batch reactor.

(b) Calculate the equilibrium conversion of N_2O_4 in a flow reactor.

(c) Assuming the reaction is elementary, express the rate of reaction solely as a function of conversion for a flow system and for a batch system.

(d) Determine the CSTR volume necessary to achieve 80% of the equilibrium conversion.

Example Cont.

Example Cont.

Example Cont.

Example Cont.

Example Cont.

Example Cont.

Example Cont.