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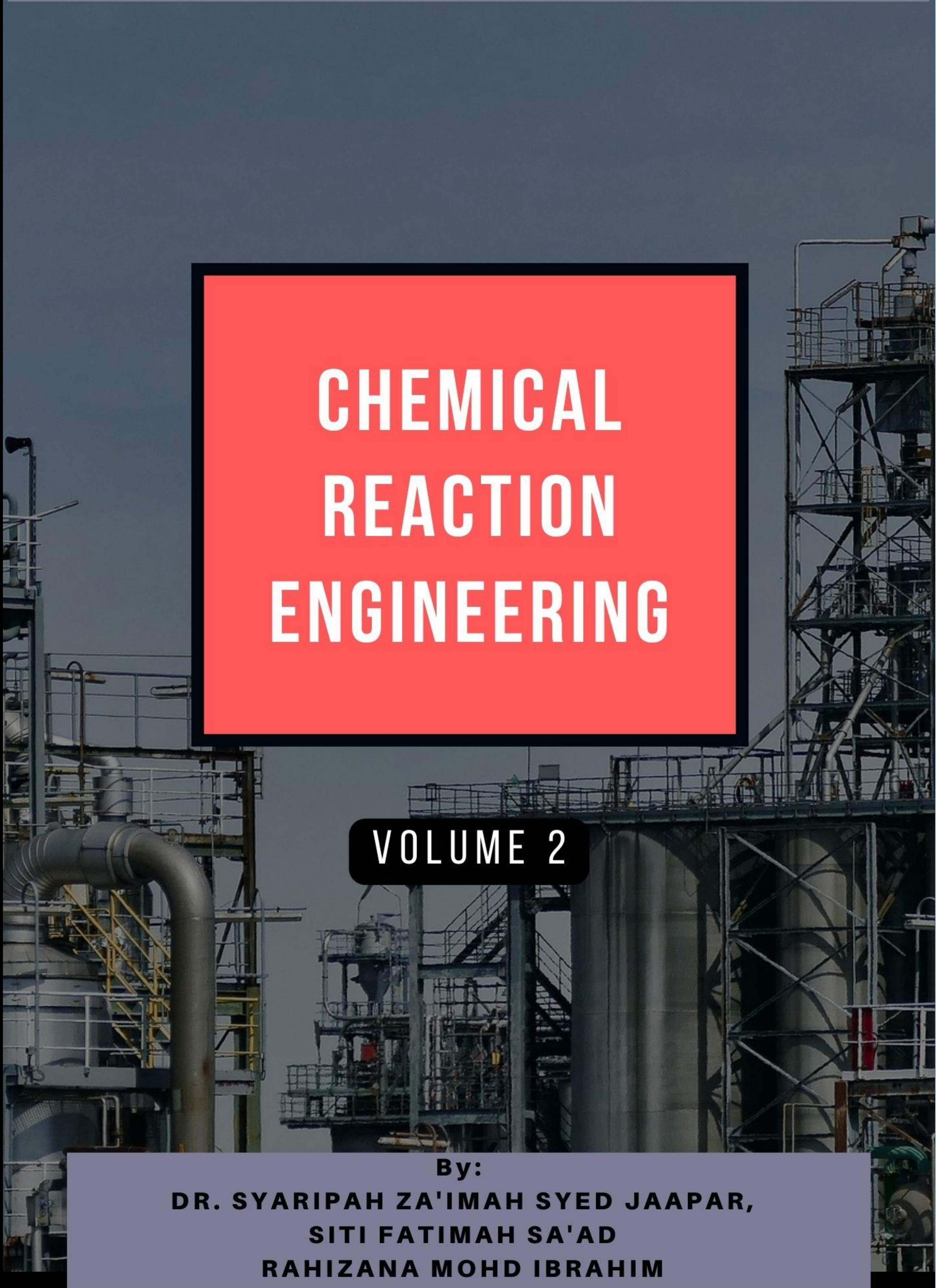

CHEMICAL REACTION ENGINEERING

VOLUME 2

By:
DR. SYARIPAH ZA'IMAH SYED JAAPAR,
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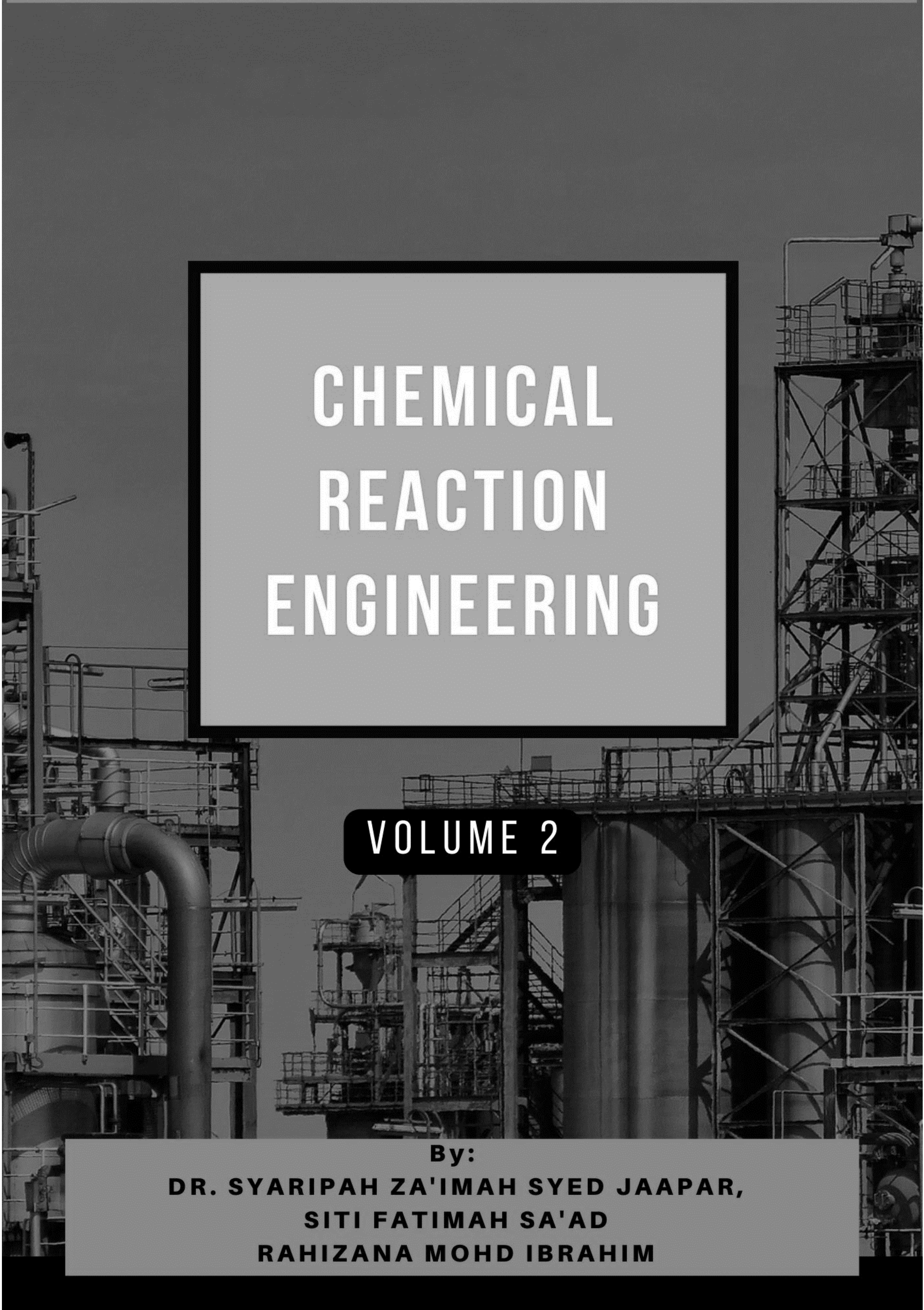

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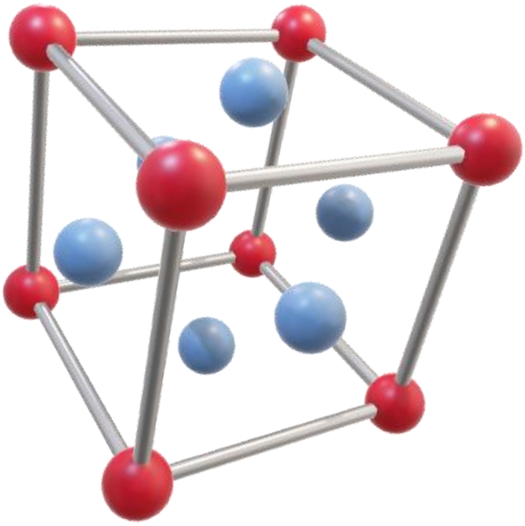
To all who love to learn and enjoy Chemical Reaction Engineering



PREFACE

CHEMICAL REACTION ENGINEERING (CRE) is a unique course to chemical engineering that separates the chemical engineer from other field of engineerings. CRE is a fun and great subject that is at the heart of chemical engineering. It contains fundamental theory on the design process for chemical engineering field.

Previous CRE ebook volume 1 gives exposure to basic principles of batch reactor, continuous stirred tank reactor (CSTR), plug flow reactor (PFR) and reactors in series. This course covers the fundamental of chemical kinetics principles and reactors design . It is including the conversion and sizing of chemical reactors such as CSTR, PFR and reactors in series. Meanwhile, this CRE ebook volume 2 covers rate laws and stoichiometric table. The course will discuss the design structure of isothermal batch, plug flow and continuous stirred tank reactors . The catalysis and catalytic reactors chapter will develop an understanding of catalysts, reaction mechanisms, and catalytic reactor design.

In this book, we as lecturers and authors for this Chemical Reaction Engineering eBook are presenting the theories and exercises in more engaging way. A lot of illustrated theories and tips have been done so as the students will be more enticed to use this book as the main references for them and aid in their understanding. The main objective of this ebook is to increase the student’s interest in this subject by presenting the theories and main point of the subject in the simplest and colourful way which highlighting the main points that need to be understood.

Last but not least, we also would like to express our gratitude to our families for their support, our colleagues who shared their tips and knowledge, eLearning unit for workshops, UIDM, the library , management of Politeknik Tun Syed Nasir Ismail (PTSN) and JPPKK for giving us the chance to publish this CHEMICAL REACTION ENGINEERING (CRE) eBook.

CONTENTS

“Success is not final, failure is not fatal; it is the courage to continue that counts.”

— WINSTON CHURCHILL

04

Rate Laws and Stoichiometry

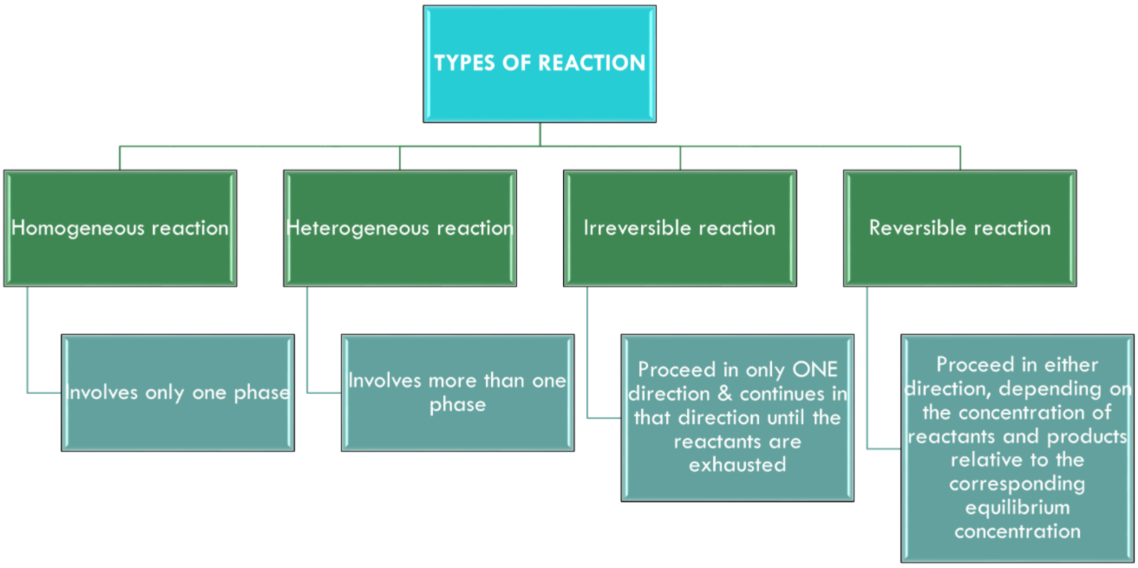
Chemical reaction engineering is the heart of every virtual chemical process. It separates the chemical engineer from others engineering's field.

CRE is the field that studies the rates and mechanisms of chemical reactions and the design of the reactors in which they take place.

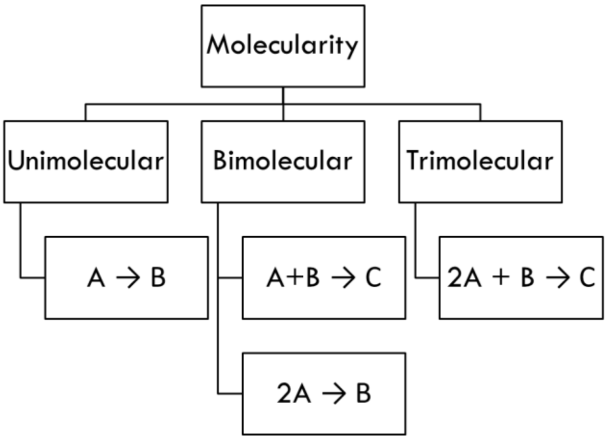
Reactor design uses information, knowledge, and experience from a variety of **areas-thermodynamics, chemical kinetics, fluid mechanics, heat transfer, mass transfer, and economics.** Chemical reaction engineering is the synthesis of all these factors with the aim of properly designing a chemical reactor.

4.1 APPLY THE REACTION ORDER AND RATE LAW

4.1.1. Define a rate law and reaction rate constant

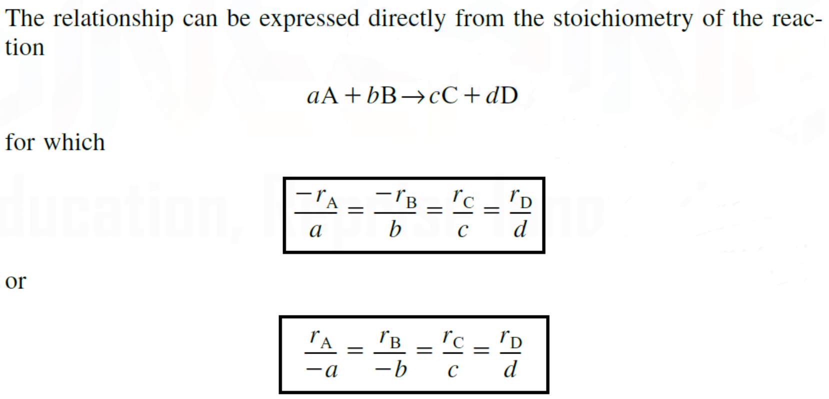


- **Molecularity of a reaction:** the number of atoms, ions, or molecules involved in a reaction step.
- The term unimolecular, bimolecular, and trimolecular refer to one, two, or three atoms, respectively, interacting in one reaction step.



4.1 APPLY THE REACTION ORDER AND RATE LAW

- **Relative rates:** how fast one species is disappearing or appearing relative to the other species in the given reaction.
- The relative rates of reaction of the various species involved in a reaction can be obtained from the ratio of stoichiometric coefficients.



The relationship can be expressed directly from the stoichiometry of the reaction

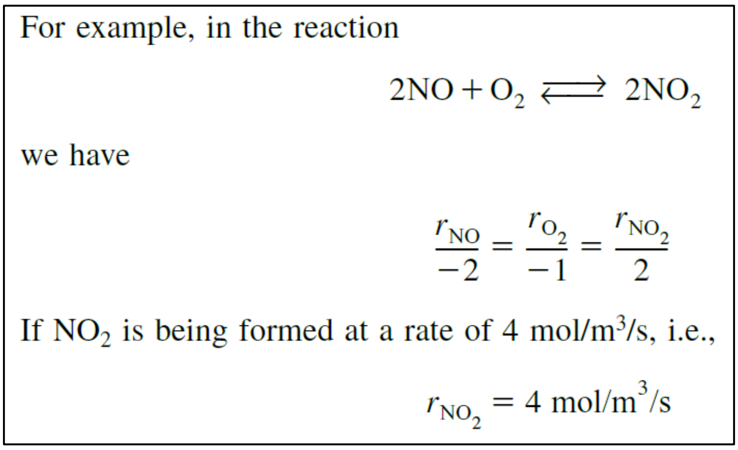
$$aA + bB \rightarrow cC + dD$$

for which

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

or

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



For example, in the reaction

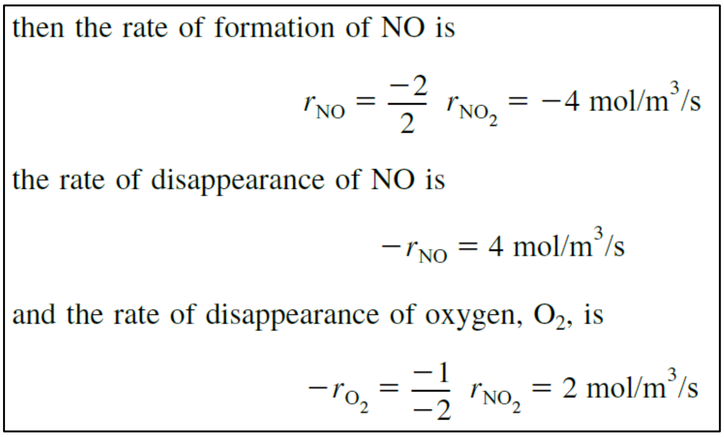
$$2NO + O_2 \rightleftarrows 2NO_2$$

we have

$$\frac{r_{NO}}{-2} = \frac{r_{O_2}}{-1} = \frac{r_{NO_2}}{2}$$

If NO_2 is being formed at a rate of 4 mol/m^3/s, i.e.,

$$r_{NO_2} = 4 \text{ mol/m}^3\text{/s}$$



then the rate of formation of NO is

$$r_{NO} = \frac{-2}{2} r_{NO_2} = -4 \text{ mol/m}^3\text{/s}$$

the rate of disappearance of NO is

$$-r_{NO} = 4 \text{ mol/m}^3\text{/s}$$

and the rate of disappearance of oxygen, O_2, is

$$-r_{O_2} = \frac{-1}{-2} r_{NO_2} = 2 \text{ mol/m}^3\text{/s}$$

4.1 APPLY THE REACTION ORDER AND RATE LAW

- **Rate law**: the algebraic equations that apply to a given reaction.
- **Rate law**: the algebraic equation that relates reaction rate to the species concentrations.
- It can be written as the **product of a reaction rate constant and a function of the concentrations** of the various species involved in the reaction.

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

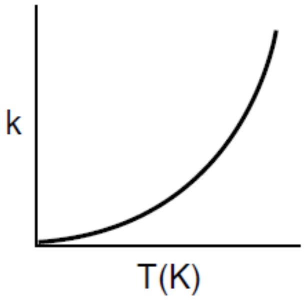
- $\boldsymbol{k_A}$ is the specific rate of reaction or rate constant & **subscript *A*** is referred to as a particular species.
- For the reaction in which the stoichiometric coefficient is 1 for all species involved in the reaction, the subscript can be deleted.

$$\boxed{1\ \text{NaOH} + 1\ \text{HC1} \rightarrow 1\ \text{NaC1} + 1\ \text{H}_2\text{O}}$$

⬇

$$\boxed{k = k_{\text{NaOH}} = k_{\text{HC1}} = k_{\text{NaC1}} = k_{\text{H}_2\text{O}}}$$

- The reaction rate constant is not truly constant; it is merely independent of the concentrations of the species involved in the reaction.
- It is dependent on temperature.



4.1.2. Define the Arrhenius Equation

- The temperature dependence of the specific reaction rate, k_A

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

A = pre-exponential 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

- **Activation energy**: A minimum energy that must be possessed by reacting molecules before the reaction will occur.
- **Activation energy**: A minimum increase in potential energy of the reactants that must be provided to transform the reactants into products.
- It also can be thought of as a barrier to energy transfer (from kinetic energy to potential energy) between reacting molecules that must be overcome.
- Determined experimentally by carrying out the reaction at several different temperatures.

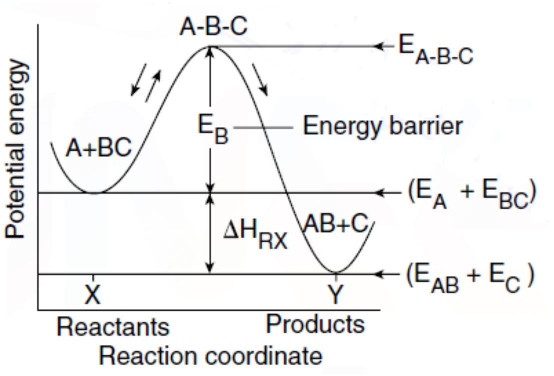
Why is there activation energy?

- The molecules need the energy to distort or stretch their bonds so that they break them and thus form new bonds.

- The steric and electron repulsion forces must be overcome as the reacting molecules come close together.

4.1 APPLY THE REACTION ORDER AND RATE LAW

Activation energy



- The figure shows the potential energy of the three atoms, A, B, and C, as well as the reaction progress.
- The reaction is from the reactant species A and BC to products AB and C.
- As the reaction moves along to the right, the reactant A and BC approach each other.
- The BC bond begins to break and the energy of the reaction pair increases.
- As a result, the potential energy of the initial three atoms is high.
- As the reaction proceeds, the AB bond begins to form.
- In conclusion, the reactants must overcome an energy barrier or activation energy.

4.1 APPLY THE REACTION ORDER AND RATE LAW

Activation energy from Arrhenius Equation

- Activation energy can be determined experimentally by carrying out the reaction at several different temperatures.
- Activation energy can be found from a plot of ln k_A as a function of (1/T)

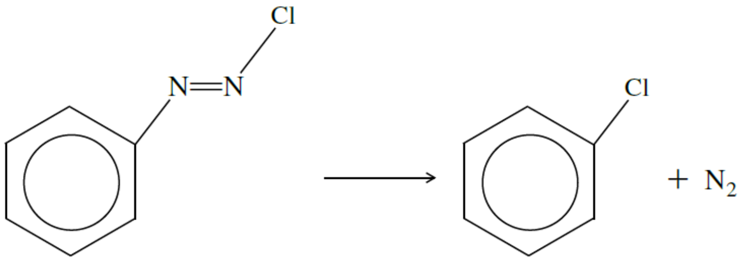
$$\boxed{k_A(T) = Ae^{-E/RT}}$$

$$\Downarrow$$

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

Example 3–1 Determination of the Activation Energy

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



using the information in Table E3-1.1 for this first-order reaction.

TABLE E3-1.1 DATA

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

4.1 APPLY THE REACTION ORDER AND RATE LAW

SOLUTION:

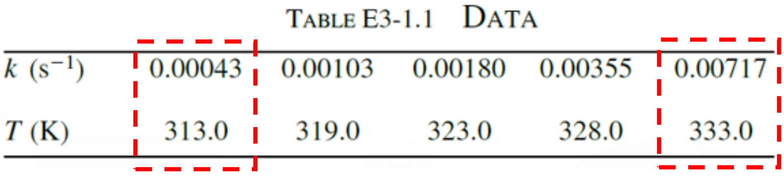


TABLE E3-1.1 DATA

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

$$\ln k_1 = \ln A - \frac{E}{R}\left(\frac{1}{T_1}\right) \quad \text{(Eq 1)}$$

$$\ln k_2 = \ln A - \frac{E}{R}\left(\frac{1}{T_2}\right) \quad \text{(Eq 2)}$$

Eq 1 − Eq 2

$$\ln k_1 - \ln k_2 = \frac{E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$E = \left(\ln \frac{k_1}{k_2}\right)(R)\left[\frac{1}{T_2} - \frac{1}{T_1}\right]^{-1}$$

$$E = \left(\ln \frac{0.00043}{0.00717}\right)\left(8.\frac{314J}{mol\,K}\right)\left[\frac{1}{333} - \frac{1}{313}\right]^{-1}$$

$$E = 121919 \frac{J}{mol\,K}.$$

Reaction rate constant at different temperature

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

$$\ln k = \ln A - \frac{E}{R}\left(\frac{1}{T}\right) \quad \text{Eq.1}$$

$$\ln k_0 = \ln A - \frac{E}{R}\left(\frac{1}{T_0}\right) \quad \text{Eq.2}$$

Eq. 1 – Eq. 2

$$\ln k - \ln k_0 = \frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)$$

$$\ln \frac{k}{k_0} = \frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)$$

4.1 APPLY THE REACTION ORDER AND RATE LAW

$$\boxed{k = k_0 \exp\left[\frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]}$$

⬇

$$\boxed{k(T) = k(T_0)e^{\frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)}}$$

4.1.3. Write the elementary rate laws and molecularity

Power Law Model

- Here, the rate law is the product of a reaction rate constant and a function of the concentrations of the individual species, **each concentration is raised to a power**.

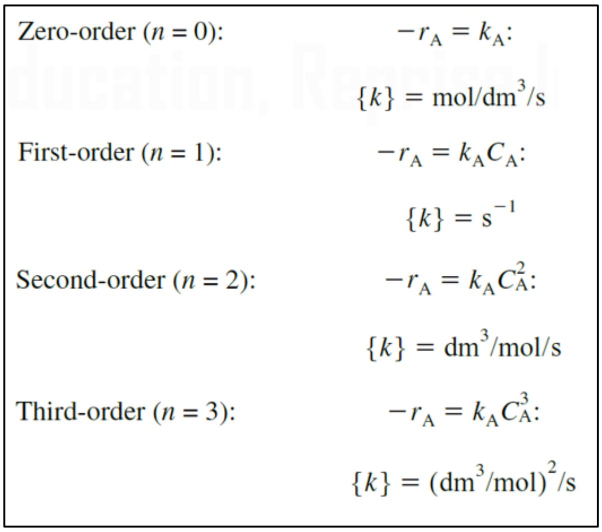
$$\boxed{-r_A = k_A C_A^{\alpha} C_B^{\beta}} \quad \rightarrow \text{Eq. 1}$$

- The **reaction order** is the powers to which the concentrations are raised in the kinetic rate law.
- From Eq. 1, **α order with respect to reactant A** and **β order with respect to reactant B**.
- The **overall order** of the reaction, *n* is

$$\boxed{n = \alpha + \beta}$$

4.1 APPLY THE REACTION ORDER AND RATE LAW

- The **units of the specific reaction rate constant** are;



Zero-order ($n = 0$): $-r_A = k_A$:

$\{k\} = \text{mol/dm}^3/\text{s}$

First-order ($n = 1$): $-r_A = k_A C_A$:

$\{k\} = \text{s}^{-1}$

Second-order ($n = 2$): $-r_A = k_A C_A^2$:

$\{k\} = \text{dm}^3/\text{mol/s}$

Third-order ($n = 3$): $-r_A = k_A C_A^3$:

$\{k\} = (\text{dm}^3/\text{mol})^2/\text{s}$

Elementary reaction

- **Elementary reaction**: involves a single step.
- For example; the bimolecular reaction between oxygen and methanol.
- In this reaction, the stoichiometric coefficients are **IDENTICAL** to the reaction order/power of the rate law.
- The reaction is first order in molecular oxygen & first order in methanol.

$$\boxed{\text{O}\bullet + \text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{O}\bullet + \text{OH}\bullet} \quad \Longrightarrow \quad \boxed{-r_{\text{O}\bullet} = kC_{\text{O}\bullet}\, C_{\text{CH}_3\text{OH}}}$$

4.1 APPLY THE REACTION ORDER AND RATE LAW

Nonelementary reaction

- **Nonelementary reaction**: involves multiple steps.
- For example; the oxidation of nitric oxide & gas-phase reaction between hydrogen and iodine.
- In these reactions, the stoichiometric coefficients are IDENTICAL to the reaction order/power of the rate law.
- Thus, it can be concluded that the reactions are not elementary but follow the elementary rate law.

$$\boxed{2\mathrm{NO} + \mathrm{O_2} \rightarrow 2\mathrm{NO_2}} \quad \Rightarrow \quad \boxed{-r_{\mathrm{NO}} = k_{\mathrm{NO}} C_{\mathrm{NO}}^2 C_{\mathrm{O_2}}}$$

$$\boxed{\mathrm{H_2} + \mathrm{I_2} \rightarrow 2\mathrm{HI}} \quad \Rightarrow \quad \boxed{-r_{\mathrm{H_2}} = k_{\mathrm{H_2}} C_{\mathrm{H_2}} C_{\mathrm{I_2}}}$$

4.1.4. Derive the reversible reactions rate law

- 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 ($-r_A = 0$).
- For elementary and reversible reaction, the rate law can be written as;

Elementary
reversible

$$\mathrm{A} \rightleftarrows \mathrm{B}$$

$$-r_{\mathrm{A}} = k\left(C_{\mathrm{A}} - \frac{C_{\mathrm{B}}}{K_{\mathrm{C}}}\right)$$

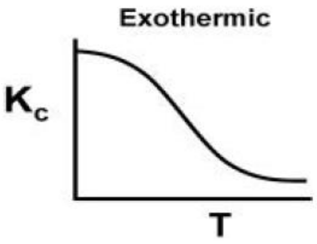
4.1 APPLY THE REACTION ORDER AND RATE LAW

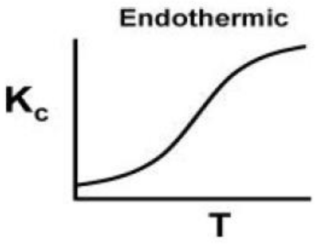
Equilibrium constant, K_C

$$aA + bB \rightleftharpoons cC + dD$$

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

- Unit of K_C is $(\frac{mol}{dm^3})^{d+c-b-a}$
- The equilibrium constant **decreases** with increasing temperature for an exothermic reaction.
- The equilibrium constant **increases** with increasing temperature for an endothermic reaction.





4.1 APPLY THE REACTION ORDER AND RATE LAW

Explanation on how to write reversible and elementary rate law

Let's consider the reaction of two benzene (B) molecules to form diphenyl (D) and hydrogen (H) is to be elementary and reversible.

$$2C_6H_6 \underset{k_{-B}}{\overset{k_B}{\rightleftarrows}} C_{12}H_{10} + H_2$$

or, symbolically,

$$2B \underset{k_{-B}}{\overset{k_B}{\rightleftarrows}} D + H_2$$

The forward and reverse specific reaction rate constants, k_B and k_{-B}, respectively, will ***be defined with respect to benzene***.

Benzene (B) is being depleted by the forward reaction

$$2C_6H_6 \xrightarrow{k_B} C_{12}H_{10} + H_2$$

in which the rate of disappearance of benzene is

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

For the reverse reaction between diphenyl (D) and hydrogen (H_2),

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

the rate of formation of benzene is given as

$$r_{B,\text{ reverse}} = k_{-B} C_D C_{H_2}$$

4.1 APPLY THE REACTION ORDER AND RATE LAW

The net rate of formation of benzene (B) is the sum of the rates of formation from the forward reaction and the reverse reaction.

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

$$r_{\mathrm{B}} = -k_{\mathrm{B}} C_{\mathrm{B}}^2 + k_{-\mathrm{B}} C_{\mathrm{D}} C_{\mathrm{H_2}}$$

Multiply both sides with (-1) to get the rate of disappearance of benzene

$$-r_{\mathrm{B}} = k_{\mathrm{B}} C_{\mathrm{B}}^2 - k_{-\mathrm{B}} C_{\mathrm{D}} C_{\mathrm{H_2}} = k_{\mathrm{B}} \left(C_{\mathrm{B}}^2 - \frac{k_{-\mathrm{B}}}{k_{\mathrm{B}}} C_{\mathrm{D}} C_{\mathrm{H_2}} \right)$$

$$\frac{k_{\mathrm{B}}}{k_{-\mathrm{B}}} = K_{\mathrm{C}} = \text{Concentration equilibrium constant}$$

$$-r_{\mathrm{B}} = k_{\mathrm{B}} \left(C_{\mathrm{B}}^2 - \frac{C_{\mathrm{D}} C_{\mathrm{H_2}}}{K_{\mathrm{C}}} \right)$$

Now, let's write the rate of formation of D by using the relationship of reaction rate between each species.

$$r_{\mathrm{D}} = k_{\mathrm{D}} \left(C_{\mathrm{B}}^2 - \frac{C_{\mathrm{D}} C_{\mathrm{H_2}}}{K_{\mathrm{C}}} \right)$$

$$k_{\mathrm{D}} = \frac{k_{\mathrm{B}}}{2}$$

$$\frac{r_{\mathrm{D}}}{1} = \frac{r_{\mathrm{B}}}{-2} = \frac{-k_{\mathrm{B}} \left[C_{\mathrm{B}}^2 - C_{\mathrm{D}} C_{\mathrm{H_2}} / K_{\mathrm{C}} \right]}{-2} = \frac{k_{\mathrm{B}}}{2} \left[C_{\mathrm{B}}^2 - \frac{C_{\mathrm{D}} C_{\mathrm{H_2}}}{K_{\mathrm{C}}} \right]$$

4.1 APPLY THE REACTION ORDER AND RATE LAW

If let’s say the reaction is at equilibrium thus, $-r_B$= 0.

$$\boxed{-r_{\mathrm{B}} \equiv 0 = k_{\mathrm{B}}\left[C_{\mathrm{Be}}^2 - \frac{C_{\mathrm{De}}C_{\mathrm{H_2e}}}{K_{\mathrm{C}}}\right]}$$

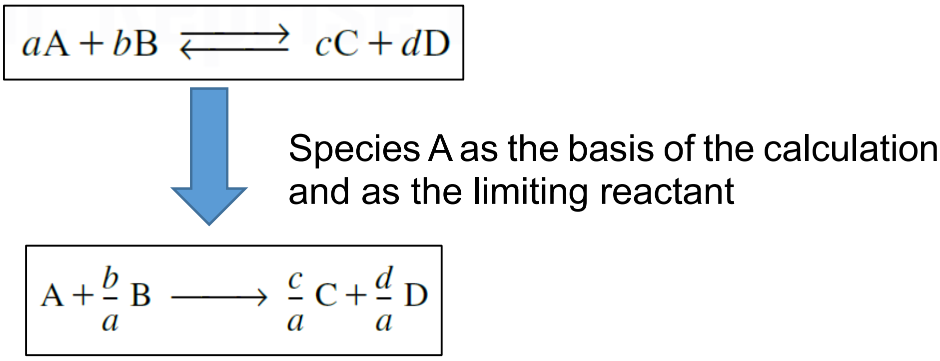
Rearrange

$$\boxed{K_{\mathrm{C}} = \frac{C_{\mathrm{De}}C_{\mathrm{H_2e}}}{C_{\mathrm{Be}}^2}}$$

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

4.2.1. Construct the stoichiometric table of a control volume batch system

Stoichiometry



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

Species A as the basis of the calculation and as the limiting reactant

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

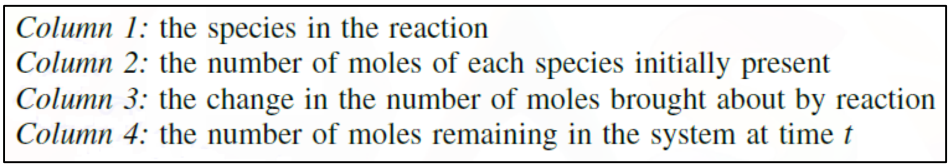
Batch system

- N_{A0} Is the number of moles of A initially present in the reactor.
- After a time of t, mole of A, $N_{A0}X$ are consumed in the system due to chemical reaction.
- Thus, the number of moles of A remaining in the reactor after a conversion of A is;

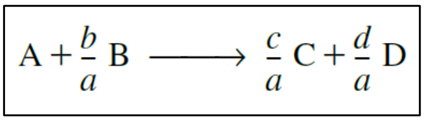
$$N_A = N_{A0} - N_{A0}X = N_{A0}(1 - X)$$

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

Components of the stoichiometric table



Column 1: the species in the reaction
Column 2: the number of moles of each species initially present
Column 3: the change in the number of moles brought about by reaction
Column 4: the number of moles remaining in the system at time *t*



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

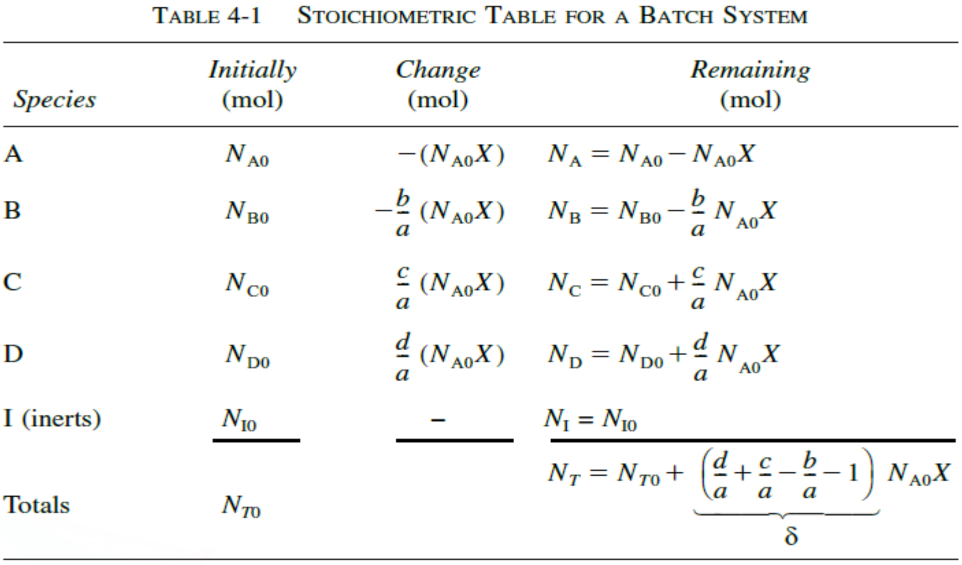
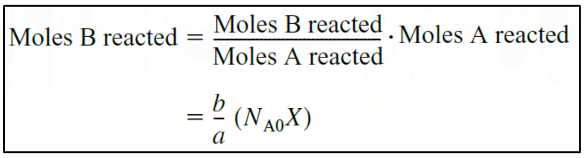


TABLE 4-1 STOICHIOMETRIC TABLE FOR A BATCH SYSTEM

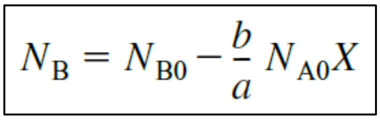
Species	*Initially* (mol)	*Change* (mol)	*Remaining* (mol)
A	N_{A0}	$-(N_{A0}X)$	$N_A = N_{A0} - N_{A0}X$
B	N_{B0}	$-\frac{b}{a}(N_{A0}X)$	$N_B = N_{B0} - \frac{b}{a}N_{A0}X$
C	N_{C0}	$\frac{c}{a}(N_{A0}X)$	$N_C = N_{C0} + \frac{c}{a}N_{A0}X$
D	N_{D0}	$\frac{d}{a}(N_{A0}X)$	$N_D = N_{D0} + \frac{d}{a}N_{A0}X$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

- For every mole of A that reacts, moles of B must react.
- Thus, the total number of moles of B that have reacted is;



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

- B is disappearing, the sign of the change is negative.
- Thus, the number of moles of B remaining in the system is;



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

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

Total number of moles

Symbol δ is the change in the total number of moles per mole of A reacted.

$$\boxed{\delta = \frac{\text{Change in the total number of moles}}{\text{Mole of A reacted}}}$$

$$\Downarrow$$

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

Thus, the total number of moles is;

$$\boxed{N_T = N_{T0} + \delta(N_{A0}X)}$$

Concentration in terms of conversion

In a batch system, the concentration is the number of moles per unit volume.

$$\boxed{\begin{aligned} C_A &= \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V} \\ C_B &= \frac{N_B}{V} = \frac{N_{B0} - (b/a)N_{A0}X}{V} \\ C_C &= \frac{N_C}{V} = \frac{N_{C0} + (c/a)N_{A0}X}{V} \\ C_D &= \frac{N_D}{V} = \frac{N_{D0} + (d/a)N_{A0}X}{V} \end{aligned}}$$

The reactor volume is constant, thus, $V = V_0$.

$$\boxed{\begin{aligned} C_A &= \frac{N_A}{V_0} = \frac{N_{A0}(1-X)}{V_0} \\ C_A &= C_{A0}(1-X) \end{aligned}}$$

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

Defining parameter Θ_i

$$\boxed{\Theta_i = \frac{\text{Moles of species "i" initially}}{\text{Moles of species A initially}}}$$

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

Example:

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

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

$$C_{\mathrm{B}} = C_{\mathrm{A0}}\left(\Theta_{\mathrm{B}} - \frac{b}{a}X\right)$$

$$\text{with } \Theta_{\mathrm{B}} = \frac{N_{\mathrm{B0}}}{N_{\mathrm{A0}}}$$

$$C_{\mathrm{C}} = \frac{N_{\mathrm{A0}}\left[\Theta_{\mathrm{C}} + (c/a)X\right]}{V_0}$$

$$C_{\mathrm{C}} = C_{\mathrm{A0}}\left(\Theta_{\mathrm{C}} + \frac{c}{a}X\right)$$

$$\text{with } \Theta_{\mathrm{C}} = \frac{N_{\mathrm{C0}}}{N_{\mathrm{A0}}}$$

$$C_{\mathrm{D}} = \frac{N_{\mathrm{A0}}\left[\Theta_{\mathrm{D}} + (d/a)X\right]}{V_0}$$

$$C_{\mathrm{D}} = C_{\mathrm{A0}}\left(\Theta_{\mathrm{D}} + \frac{d}{a}X\right)$$

$$\text{with } \Theta_{\mathrm{D}} = \frac{N_{\mathrm{D0}}}{N_{\mathrm{A0}}}$$

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

EXAMPLE 4.2.1

$$3A + B \rightarrow 3C + D$$

$$\Downarrow$$

$$A + \frac{1}{3}B \rightarrow C + \frac{1}{3}D$$

$$\boxed{\begin{array}{c} C_A = \dfrac{N_A}{V} = \dfrac{N_A}{V_0} = \dfrac{N_{A0}(1-X)}{V_0} = C_{A0}(1-X) \\ \Theta_B = \dfrac{C_{B0}}{C_{A0}} \quad \Theta_C = \dfrac{C_{C0}}{C_{A0}} \quad \Theta_D = \dfrac{C_{D0}}{C_{A0}} \end{array}}$$

Symbol	*Initially*	*Change*	*Remaining*	*Concentration*
A	N_{A0}	$-N_{A0}X$	$N_{A0}(1-X)$	$C_{A0}(1-X)$
B	N_{B0}	$-\frac{1}{3}N_{A0}X$	$N_{A0}\left(\Theta_B - \frac{X}{3}\right)$	$C_{A0}\left(\Theta_B - \frac{X}{3}\right)$
C	N_{C0}	$N_{A0}X$	$N_{A0}(\Theta_C + X)$	$C_{A0}(\Theta_C + X)$
D	N_{D0}	$\frac{1}{3}N_{A0}X$	$N_{A0}\left(\Theta_D + \frac{X}{3}\right)$	$C_{A0}\left(\Theta_D + \frac{X}{3}\right)$
I	N_{I0}	–	N_{I0}	C_{I0}
	N_{T0}	0	$N_T = N_{T0}$	

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

4.2.2. Calculate the concentration of limiting reactant

Based on Example 4.2.1, the initial concentration of A is 10 mol/dm^3 and the initial concentration of B is 2 mol/dm^3. What are the concentrations of B and D, when the conversion of A is (a) 20% and (b) 90%?

Initially, only A and B are present. Thus, $\boldsymbol{\Theta}_C$ and $\boldsymbol{\Theta}_D$ are 0.

(a) For 20% conversion of A

$$C_D = C_{A0}\left(\frac{X}{3}\right) = (10)\left(\frac{0.2}{3}\right) = 0.67 \text{ mol/L} = 0.67 \text{ mol/dm}^3$$

$$C_B = C_{A0}\left(\Theta_B - \frac{X}{3}\right) = 10\left(\frac{2}{10} - \frac{0.2}{3}\right) = 10(0.133) = 1.33 \text{ mol/dm}^3$$

(b) For 90% conversion of A

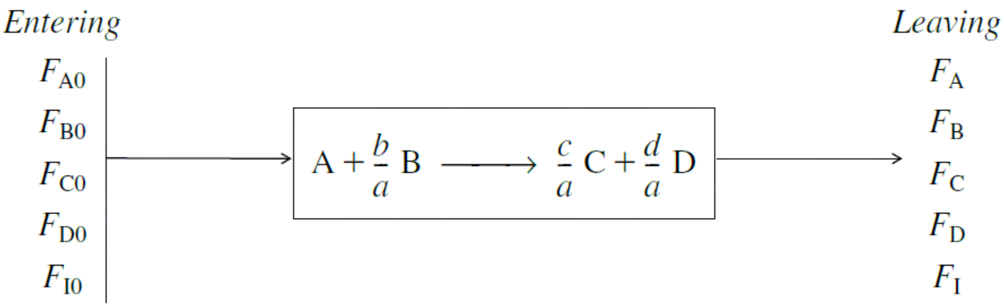
$$C_D = C_{A0}\left(\frac{X}{3}\right) = 10\left(\frac{0.9}{3}\right) = 3 \text{ mol/dm}^3$$

$$C_B = 10\left(\frac{2}{10} - \frac{0.9}{3}\right) = 10(0.2 - 0.3) = -1 \text{ mol/dm}^3$$

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

4.2.3. Form a stoichiometric table of a continuous flow system

In a flow system, we replace N_{j0} by F_{j0} & N_j by F_j.



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

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	$F_{I0} = \Theta_I F_{A0}$	–	$F_I = F_{A0}\Theta_I$
Totals	F_{T0}		$F_T = F_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right) F_{A0}X$ $F_T = F_{T0} + \delta F_{A0}X$

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

Total molar flow rate

The total molar flow rate is the sum of the molar flow rates of each species in the system.

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

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

Defining parameter ε

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

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

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

Thus,

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

We divide this equation through by F_{T0}

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

Then

$$\frac{F_T}{F_{T0}} = 1 + \varepsilon X$$

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

Concentration in terms of conversion

In a flow system, the concentration is the molar flow rate per volumetric flow rate.

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

⬇

$$C_A = \frac{F_A}{v} = \frac{F_{A0}}{v}(1-X) \qquad C_B = \frac{F_B}{v} = \frac{F_{B0}-(b/a)F_{A0}X}{v}$$

$$C_C = \frac{F_C}{v} = \frac{F_{C0}+(c/a)F_{A0}X}{v} \qquad C_D = \frac{F_D}{v} = \frac{F_{D0}+(d/a)F_{A0}X}{v}$$

Liquid phase concentration

For liquid phase, there is no change in the volumetric flow rate, thus, $v=v_0$.

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

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

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

Gas phase concentration

For gas phase, the volumetric flow rate most often changes during reaction because of a change in the temperature or pressure, thus, $v \neq v_0$.

$$\boxed{C_T = \frac{F_T}{v} = \frac{P}{ZRT}} \qquad \text{Eq. 1}$$

$$\boxed{C_{T0} = \frac{F_{T0}}{v_0} = \frac{P_0}{Z_0 R T_0}} \qquad \text{Eq. 2}$$

(Eq. 1) ÷ (Eq. 2)

Assume that the compressibility factor is constant, $Z = Z_0$, thus

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

$$\Big\downarrow \qquad \frac{F_T}{F_{T0}} = 1 + \varepsilon X$$

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

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

$$\boxed{C_j = \frac{F_j}{v}}$$

$$\boxed{F_j = F_{j0} + \nu_j(F_{A0}X) = F_{A0}(\Theta_j + \nu_j X)} \qquad \Downarrow \qquad \boxed{v = v_0(1+\varepsilon X)\frac{P_0}{P}\left(\frac{T}{T_0}\right)}$$

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

$$\Downarrow$$

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

$$
\begin{aligned}
C_A &= \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v} &&= \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} &&= C_{A0}\left(\frac{1-X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)\\
C_B &= \frac{F_B}{v} = \frac{F_{A0}[\Theta_B - (b/a)X]}{v} &&= \frac{F_{A0}[\Theta_B - (b/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} &&= C_{A0}\left(\frac{\Theta_B - (b/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)\\
C_C &= \frac{F_C}{v} = \frac{F_{A0}[\Theta_C + (c/a)X]}{v} &&= \frac{F_{A0}[\Theta_C + (c/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} &&= C_{A0}\left(\frac{\Theta_C + (c/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)\\
C_D &= \frac{F_D}{v} = \frac{F_{A0}[\Theta_D + (d/a)X]}{v} &&= \frac{F_{A0}[\Theta_D + (d/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} &&= C_{A0}\left(\frac{\Theta_D + (d/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)\\
C_I &= \frac{F_I}{v} = \frac{F_{A0}\Theta_I}{v} &&= \frac{F_{A0}\Theta_I}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} &&= \frac{C_{A0}\Theta_I}{1+\varepsilon X}\left(\frac{T_0}{T}\right)\frac{P}{P_0}
\end{aligned}
$$

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

Isothermal gas phase concentration

For isothermal reaction, there is no change in the temperature, thus $T=T_0$.

$$\begin{tikzcd}
 & \boxed{C_j = \frac{F_j}{\upsilon}} \arrow[d] & \\
\boxed{F_j = F_{j0} + \nu_j (F_{A0} X) = F_{A0}(\Theta_j + \nu_j X)} & {} \arrow[d] & \boxed{\upsilon = \upsilon_0 (1 + \varepsilon X) \frac{P_0}{P}} \\
 & \boxed{C_j = \frac{F_{A0}(\Theta_j + \nu_j X)}{\upsilon_0 \left((1 + \varepsilon X) \frac{P_0}{P} \cancel{\frac{T}{T_0}} \right)}} \arrow[d] & \\
 & \boxed{C_j = \frac{C_{A0}(\Theta_j + \nu_j X)}{1 + \varepsilon X} \left(\frac{P}{P_0} \right)} &
\end{tikzcd}$$

4.2 EXPLAIN THE STOICHIOMETRIC RELATIONSHIPS BETWEEN REACTING MOLECULES FOR SINGLE REACTION

Isothermal gas phase concentration and no pressure drop

For isothermal reaction, there is no change in the temperature, thus $T=T_0$.

No pressure drop, thus $P=P_0$.

$$\begin{tikzcd}
 & \boxed{C_j = \frac{F_j}{\upsilon}} \arrow[dd] & \\
\boxed{F_j = F_{j0} + v_j(F_{A0}X) = F_{A0}(\Theta_j + v_j X)} & & \boxed{\upsilon = \upsilon_0(1+\varepsilon X)} \\
 & \boxed{C_j = \frac{F_{A0}(\Theta_j + v_j X)}{\upsilon_0\left((1+\varepsilon X)\cancel{\frac{P_0}{P}\frac{T}{T_0}}\right)}} \arrow[d] & \\
 & \boxed{C_j = \frac{C_{A0}(\Theta_j + v_j X)}{1+\varepsilon X}} &
\end{tikzcd}$$

TUTORIAL CHAPTER FOUR

Chapter 4:

1. Write the rate law for the following reation:
   i. $C_2H_6 \rightarrow C_2H_4 + H_2$

   ii. $C_2H_4 + \frac{1}{2}O_2 \rightarrow C_2H_4O$

   iii. $n - C_4H_{10} \leftrightarrow i - C_4H_{10}$

2. Given the following reaction:
   $C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$
   If the r_{CO_2} is 8 mol/m^{3}s, find $r_{C_2H_4}, r_{O_2}, r_{H_2O}$.

3. Given the reaction of
   $2A + B \rightarrow C$
   The rate constant of A, $k_A = 15(dm^3/mol)^2$/s. Express the rate of disappearance of A in terms of C_A and C_B. Then, find k_B and k_C.
   [clue: make the stoichiometry of A equal to 1]

4. Determine the rate law, $-r_A$ for reaction:

$$\frac{1}{2}A + \frac{3}{2}B \leftrightarrow C$$

5. Table below contain reaction rate constant at several temperature.

K (min^{-1})	0.005	0.05
T (°C)	5.0	100.0

   i. Find the activation energy, in kJ/mol

   ii. Calculate the frequency factor, A in min^{-1}

6. In a constant volume vessel, the saponification process between fat and sodium hydroxide will form glycerol and crude soap. The chemical equation for this reaction is as follows:

$$3NaOH + (C_{15}H_{31}COO)_3C_3H_5 \rightarrow 3CH_3(CH_2)_{14}CO_3Na + C_3H_5(OH)_3$$

By using NaOH as basis and X represent the conversion of NaOH, set up a stoichiometric table expressing the concentration of each species in terms of its initial concentration and the conversion, X.

7. Given the initial concentration of sodium hydroxide and fats are 20mol/L and 5 mol/L respectively. Using the same stoichiometric table in question (6), find the concentration of glycerol and remaining fats when the conversion of sodium hydroxide is at 35%.

8. A reversible gas-phase decomposition of nitrogen tetroxide, N_2O_4 to nitrogen dioxide, NO_2:

$$N_2O_4 \leftrightarrow 2NO_2$$

Is to be carried out at a constant temperature. The feed consists of pure N_2O_4 at 10°C and 2 atm. The concentration equilibrium constant, K_C at the mentioned condition is 0.1 mol/dm^3. By considering this reaction takes place in a batch system;

i. Construct the stoichiometric table

ii. Calculate the initial concentration of N_2O_4. Use $R = 0.082\, atm \cdot dm^3/mol \cdot K$.

iii. Determine the possible value of equilibrium conversion, X_e.

9. The production of ethylene oxide from oxidation of ethylene and air at 6 atm and 260°C which takes place in PBR is as follow:

$$C_2H_4 + \frac{1}{2}O_2 \rightarrow C_2H_4O$$

i. Construct the stoichiometric table for all components

ii. Write up the concentration equation, C_i for each component that present at the exit of PBR.

05

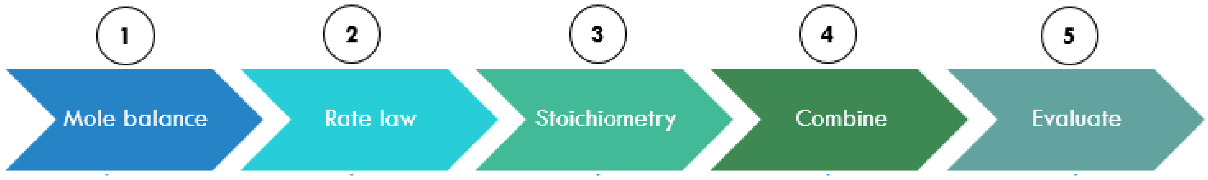
Isothermal Reactor Design

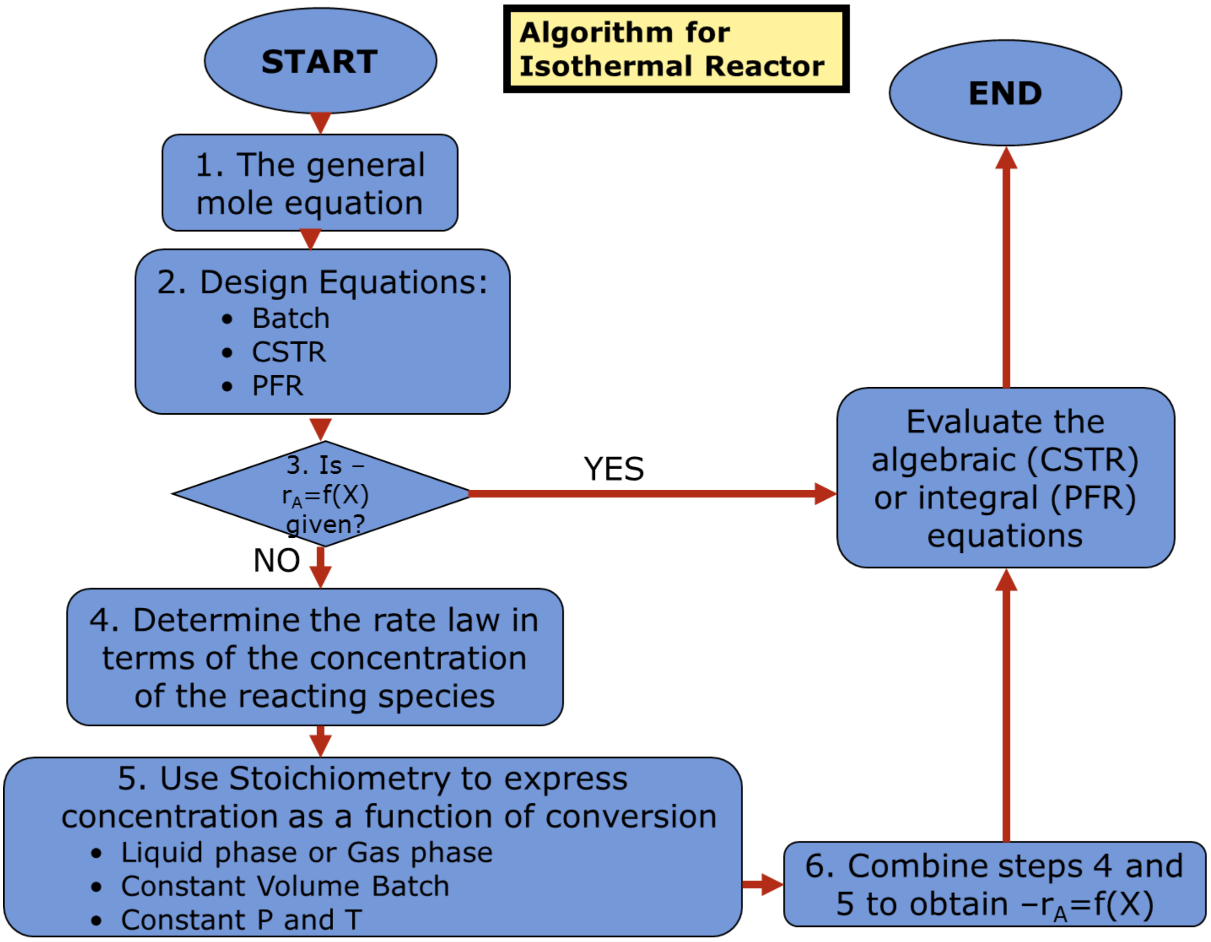
This topic will expose students to:

- Discover structure for isothermal reactors design
- Figure out the scale up of liquid-phase batch reactor data to the design of a CSTR/ Batch
- Discover Tubular Reactors
- Determine Pressure Drop in Reactors

5.1 Discover structure for isothermal reactors design

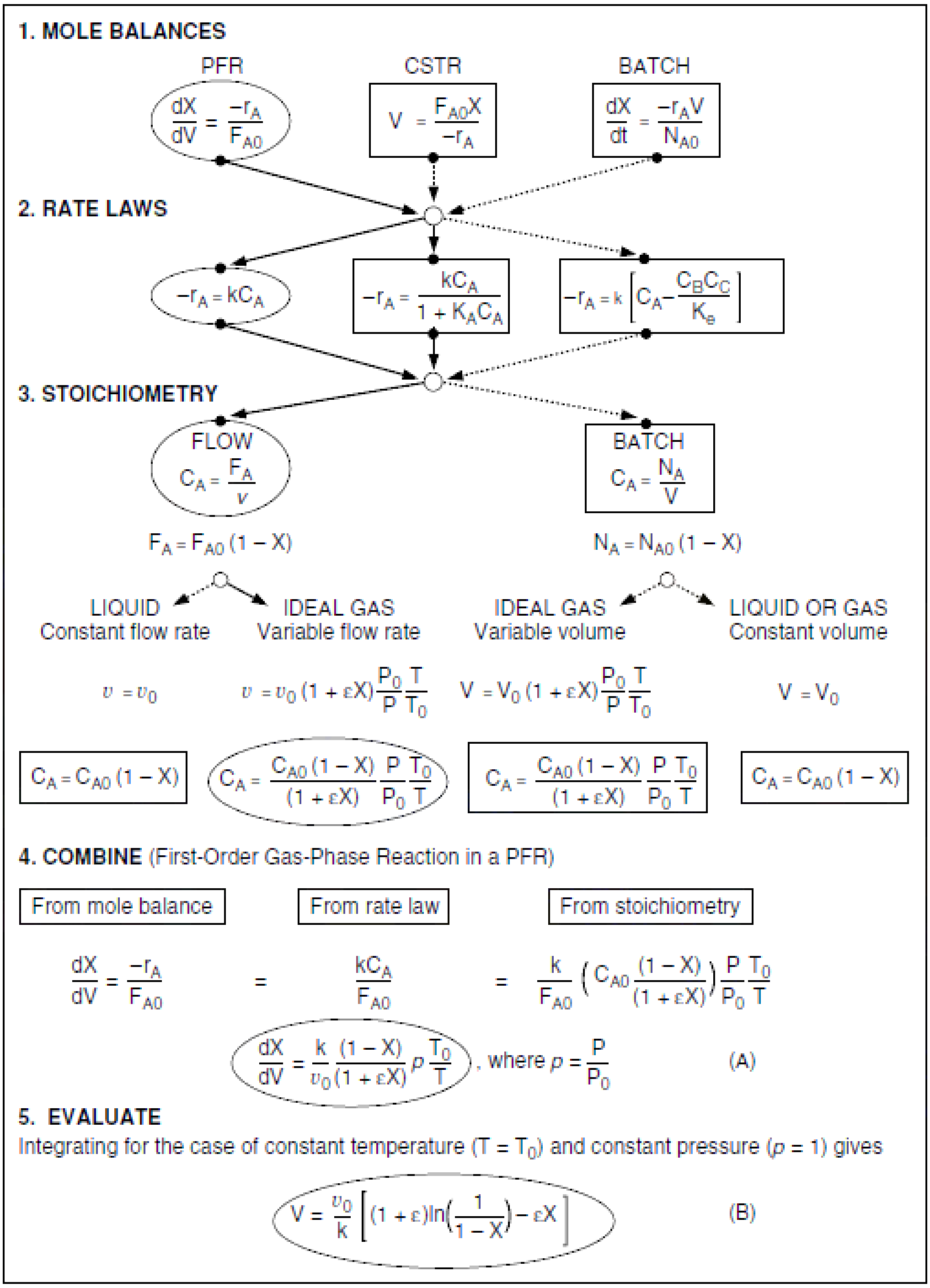
To design an isothermal reactors, use the following sequence;





5.1 Discover structure for isothermal reactors design

For example; let's formulate the equation to calculate the PFR reactor volume for a first-order & gas phase reaction.



1. MOLE BALANCES

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

CSTR: $V = \frac{F_{A0}X}{-r_A}$

BATCH: $\frac{dX}{dt} = \frac{-r_A V}{N_{A0}}$

2. RATE LAWS

$-r_A = kC_A$

$-r_A = \frac{kC_A}{1 + K_A C_A}$

$-r_A = k\left[C_A - \frac{C_B C_C}{K_e}\right]$

3. STOICHIOMETRY

FLOW $C_A = \frac{F_A}{v}$

BATCH $C_A = \frac{N_A}{V}$

$F_A = F_{A0}(1 - X)$

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

LIQUID
Constant flow rate

$\upsilon = \upsilon_0$

$C_A = C_{A0}(1 - X)$

IDEAL GAS
Variable flow rate

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

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

IDEAL GAS
Variable volume

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

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

LIQUID OR GAS
Constant volume

$V = V_0$

$C_A = C_{A0}(1 - X)$

4. COMBINE (First-Order Gas-Phase Reaction in a PFR)

From mole balance / From rate law / From stoichiometry

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}} = \frac{kC_A}{F_{A0}} = \frac{k}{F_{A0}}\left(C_{A0}\frac{(1 - X)}{(1 + \varepsilon X)}\right)\frac{P}{P_0}\frac{T_0}{T}$$

$$\frac{dX}{dV} = \frac{k}{\upsilon_0}\frac{(1 - X)}{(1 + \varepsilon X)} p \frac{T_0}{T}, \text{ where } p = \frac{P}{P_0} \quad \text{(A)}$$

5. EVALUATE

Integrating for the case of constant temperature ($T = T_0$) and constant pressure ($p = 1$) gives

$$V = \frac{\upsilon_0}{k}\left[(1 + \varepsilon)\ln\left(\frac{1}{1 - X}\right) - \varepsilon X\right] \quad \text{(B)}$$

5.2 Figure out the scale up of liquid-phase batch reactor data to the design of a CSTR

5.2.1 Batch operation

In a batch operation, assume that;

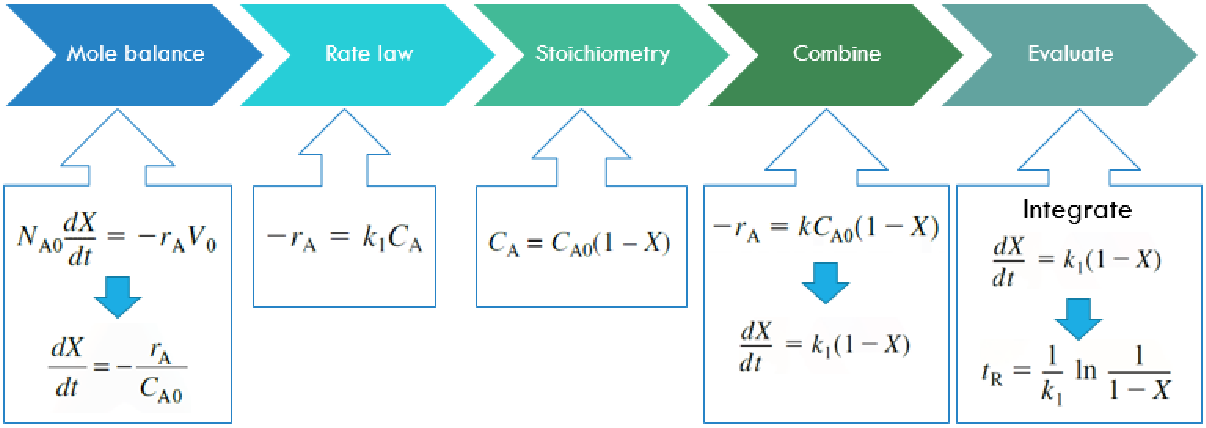
- No inflow or outdlow of material
- Well mixed
- Constant volume (V=V_0)

Batch reaction time is the time necessary to achieve a specific conversion depends upon how fast the reaction takes place.

It depends on the rate constant and the reactant concentration.

First-order batch reaction time

$$\boxed{A \rightarrow B}$$



5.2 Figure out the scale up of liquid-phase batch reactor data to the design of a CSTR

Example 1;

Calculate the batch reaction time for the first-order reaction in order to reach 90% conversion. Given the value of k is 10^{-4} s^{-1}.

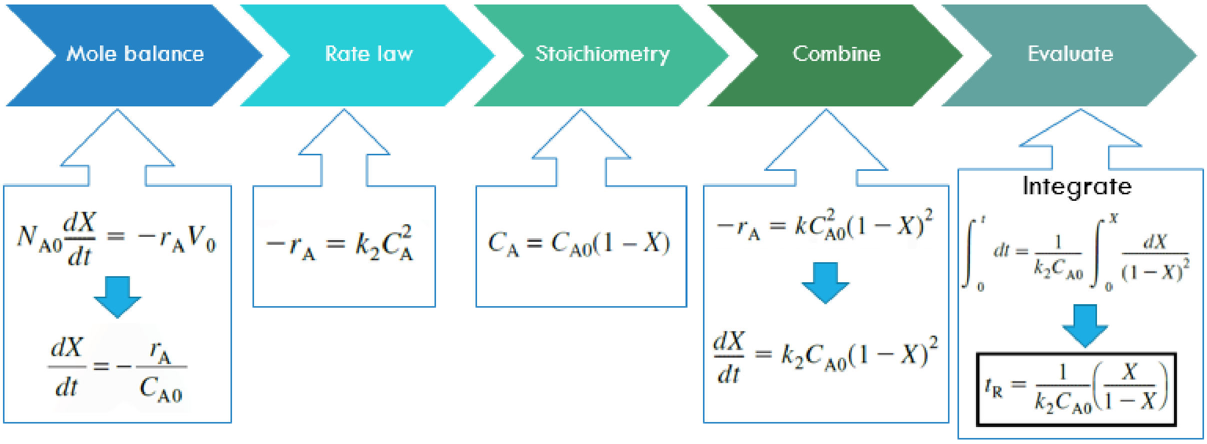
$$t_R = \frac{1}{k_1} \ln \frac{1}{1-X} = \frac{1}{k_1} \ln \frac{1}{1-0.9} = \frac{2.3}{k_1}$$

If $k_1 = 10^{-4}\ \mathrm{s}^{-1}$,

$$t_R = \frac{2.3}{10^{-4}\ \mathrm{s}^{-1}} = 23{,}000\ \mathrm{s} = 6.4\ \mathrm{h}$$

Second-order batch reaction time

$$\boxed{2A \rightarrow B + C}$$



5.2 Figure out the scale up of liquid-phase batch reactor data to the design of a CSTR

Example 2;

Calculate the batch reaction time for the second-order reaction in order to reach 90% conversion. Given the value of kC_{A0} is 10^{-3} s^{-1}.

$$t_R = \frac{1}{k_2 C_{A0}} \frac{X}{1-X} = \frac{0.9}{k_2 C_{A0}(1-0.9)} = \frac{9}{k_2 C_{A0}}$$

If $k_2 C_{A0} = 10^{-3}\ \mathrm{s}^{-1}$,

$$t_R = \frac{9}{10^{-3}\ \mathrm{s}^{-1}} = 9000\ \mathrm{s} = 2.5\ \mathrm{h}$$

5.2.2 Design of CSTRs

Space time for CSTR

$$V = \frac{F_{A0} X}{(-r_A)_{\text{exit}}}$$

$$\Big\downarrow \quad \boxed{F_{A0} = v_0 C_{A0}}$$

$$V = \frac{v_0 C_{A0} X}{(-r_A)_{\text{exit}}}$$

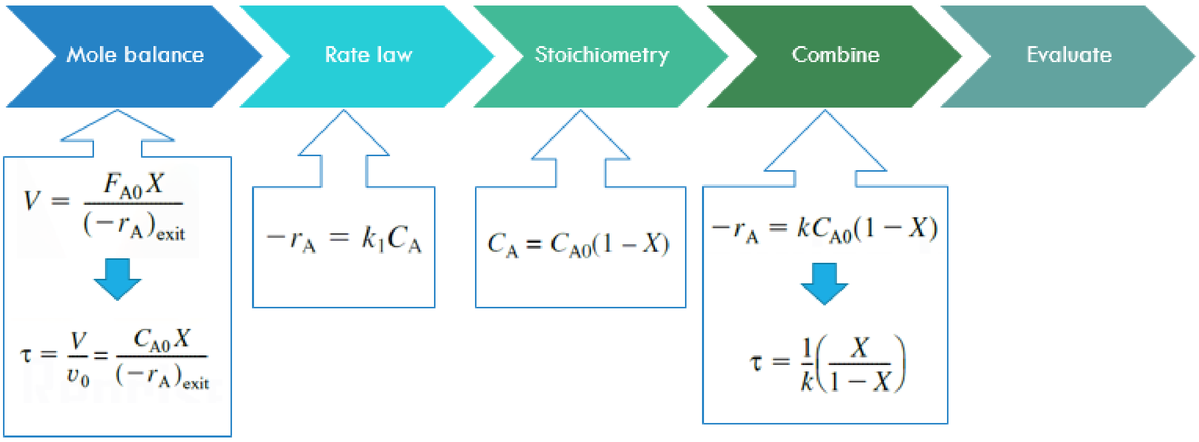
$$\Big\downarrow$$

$$\boxed{\tau = \frac{V}{v_0} = \frac{C_{A0} X}{(-r_A)_{\text{exit}}}}$$

5.2 Figure out the scale up of liquid-phase batch reactor data to the design of a CSTR

First-order for a single CSTR

$$\boxed{A \rightarrow B}$$



$$V = \frac{F_{A0}X}{(-r_A)_{exit}}$$

$$\tau = \frac{V}{v_0} = \frac{C_{A0}X}{(-r_A)_{exit}}$$

$$-r_A = k_1 C_A$$

$$C_A = C_{A0}(1-X)$$

$$-r_A = kC_{A0}(1-X)$$

$$\tau = \frac{1}{k}\left(\frac{X}{1-X}\right)$$

$$\tau = \frac{1}{k}\left(\frac{X}{1-X}\right)$$

Rearrange

$$\boxed{X = \frac{\tau k}{1+\tau k}}$$

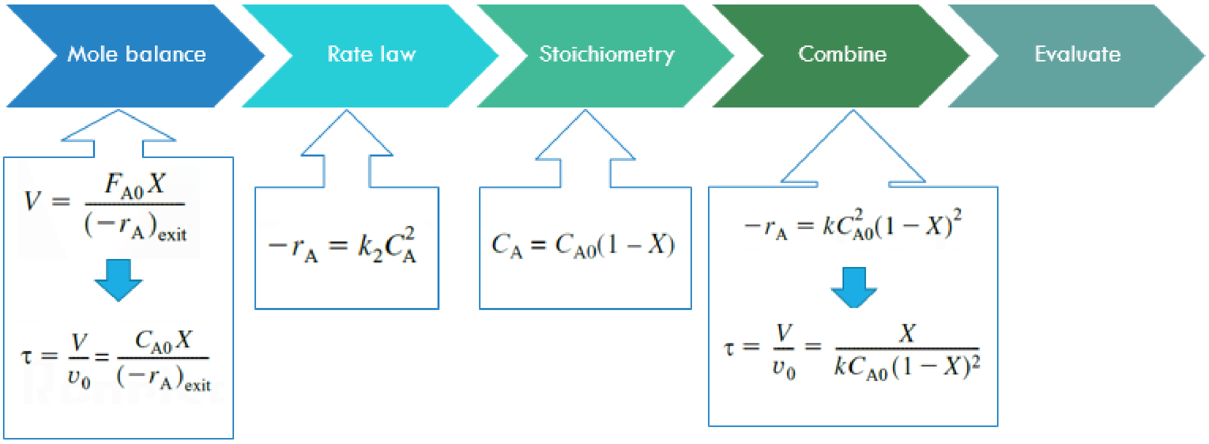
τk → Damköhler Number, Da

$$\boxed{X = \frac{\text{Da}_1}{1+\text{Da}_1}}$$

5.2 Figure out the scale up of liquid-phase batch reactor data to the design of a CSTR

Second-order for a single CSTR

$$\boxed{2A \rightarrow B + C}$$



$$V = \frac{F_{A0}X}{(-r_A)_{exit}}$$

$$\tau = \frac{V}{v_0} = \frac{C_{A0}X}{(-r_A)_{exit}}$$

$$-r_A = k_2 C_A^2$$

$$C_A = C_{A0}(1 - X)$$

$$-r_A = kC_{A0}^2(1 - X)^2$$

$$\tau = \frac{V}{v_0} = \frac{X}{kC_{A0}(1 - X)^2}$$

$$\tau = \frac{V}{v_0} = \frac{X}{kC_{A0}(1 - X)^2}$$

Rearrange

$$\boxed{X = \frac{(1 + 2\tau kC_{A0}) - \sqrt{1 + 4\tau kC_{A0}}}{2\tau kC_{A0}}}$$

Damköhler Number, Da

$$\boxed{X = \frac{(1 + 2\text{Da}_2) - \sqrt{1 + 4\text{Da}_2}}{2\text{Da}_2}}$$

5.2 Figure out the scale up of liquid-phase batch reactor data to the design of a CSTR

Damköhler number, Da

- Damköhler Number, Da is a dimensionless number to estimate the degree of conversion in CSTR.
- Damköhler Number, Da is the ratio of the rate of reaction of A to the rate of convective transport of A at the entrance to the reactor.

$$\mathrm{Da} = \frac{-r_{A0}V}{F_{A0}} = \frac{\text{Rate of reaction at entrance}}{\text{Entering flow rate of A}} = \frac{\text{“A reaction rate”}}{\text{“A convection rate”}}$$

The Damköhler number for a first-order irreversible reaction is

$$\mathrm{Da}_1 = \frac{-r_{A0}V}{F_{A0}} = \frac{k_1 C_{A0} V}{v_0 C_{A0}} = \tau k_1$$

For a second-order irreversible reaction, the Damköhler number is

$$\mathrm{Da}_2 = \frac{-r_{A0}V}{F_{A0}} = \frac{k_2 C_{A0}^2 V}{v_0 C_{A0}} = \tau k_2 C_{A0}$$

The rule of thumb;

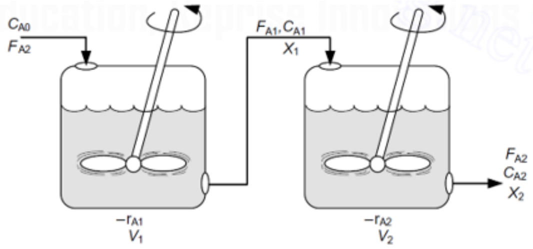
- If the value of Da is 0.1 or less, the conversion would be less than 10%.
- If the value of Da is 10 or greater, the conversion would be more than 90%.

$$\text{if } \mathrm{Da} < 0.1, \text{ then } X < 0.1$$

$$\text{if } \mathrm{Da} > 10, \text{ then } X > 0.9$$

5.2 Figure out the scale up of liquid-phase batch reactor data to the design of a CSTR

CSTRs in series



$$\tau = \frac{1}{k}\left(\frac{X}{1-X}\right)$$

Rearrange

$$1 - X = \frac{X}{\tau k}$$

$$\boxed{X = \frac{\tau k}{1+\tau k}}$$

$$\boxed{1 - X = \frac{1}{1+\tau k}}$$

$$C_A = C_{A0}(1-X)$$

$$\boxed{1 - X = \frac{1}{1+\tau k}}$$

$$\boxed{C_A = \frac{C_{A0}}{1+\tau k}}$$

$$C_{An} = \frac{C_{A0}}{(1+\tau k)^n} = \frac{C_{A0}}{(1+\mathrm{Da}_1)^n}$$

$$\boxed{C_{A0}(1-X) = \frac{C_{A0}}{(1+\mathrm{Da}_1)^n}}$$

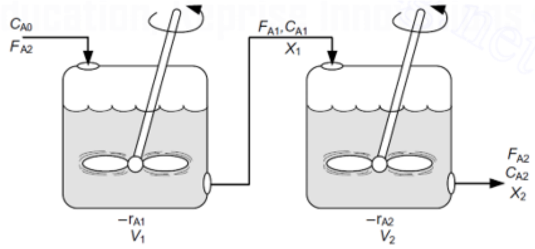
Rearrange

$$\boxed{X = 1 - \frac{1}{(1+\mathrm{Da}_1)^n} \equiv 1 - \frac{1}{(1+\tau k)^n}}$$

Conversion for identical *n* reactors in series

5.2 Figure out the scale up of liquid-phase batch reactor data to the design of a CSTR

CSTRs in series



The effluent concentration of reactant A from the first CSTR;

$$C_{A1} = \frac{C_{A0}}{1 + \tau_1 k_1}$$

The effluent concentration of reactant A from the second CSTR;

$$C_{A2} = \frac{C_{A1}}{1 + \tau_2 k_2} = \frac{C_{A0}}{(1 + \tau_2 k_2)(1 + \tau_1 k_1)}$$

If both reactors are equal in size thus, $\tau_1 = \tau_2 = \tau$

If both reactors are operated at the same temperature thus, $k_1 = k_2 = k$

$$C_{A2} = \frac{C_{A0}}{(1 + \tau k)^2}$$

5.3 Discover tubular reactors

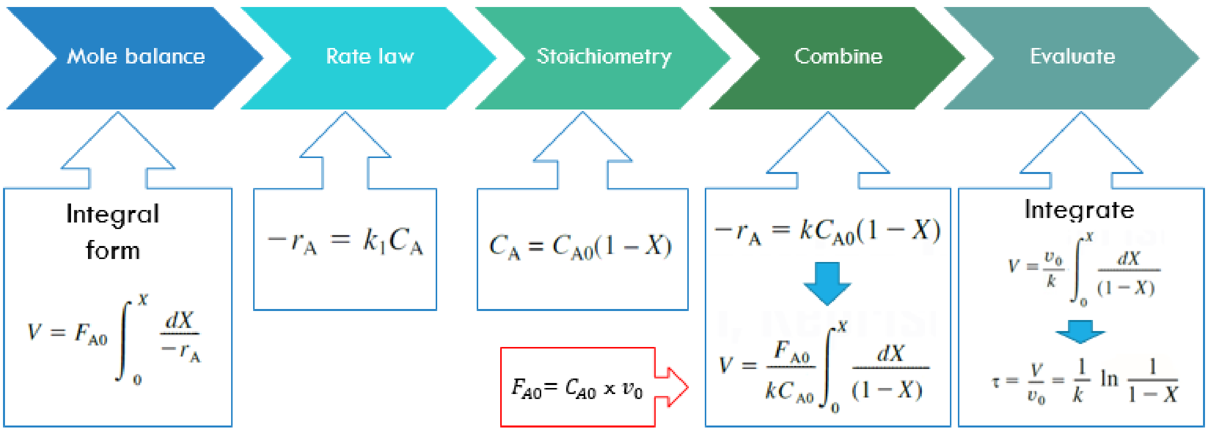
Tubular reactors

Assumptions:

- No dispersion
- No radial gradients in either temperature, velocity, concentration, or reaction rate

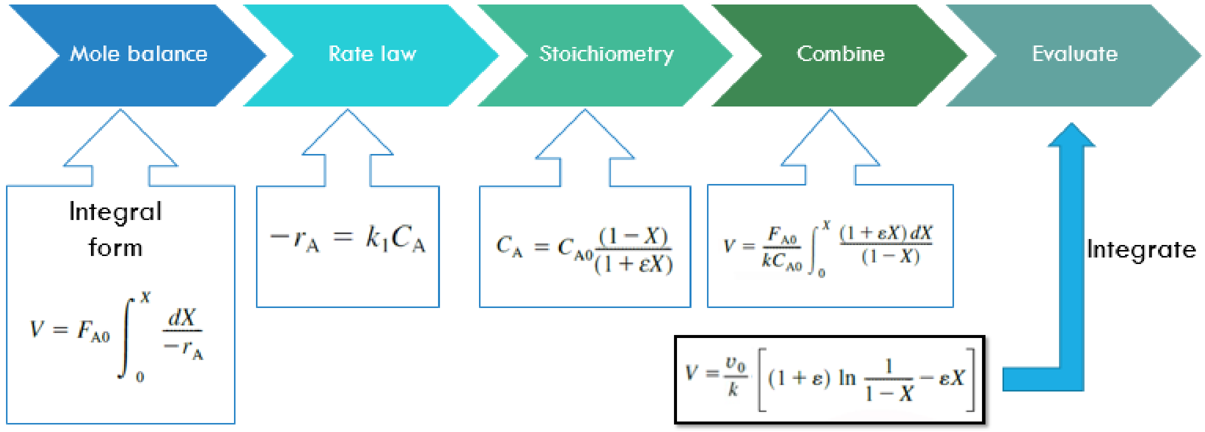
PFR: first-order and liquid phase (No pressure drop)

A → B



PFR: first-order and gas phase (No pressure drop $P=P_0$ & $T=T_0$)

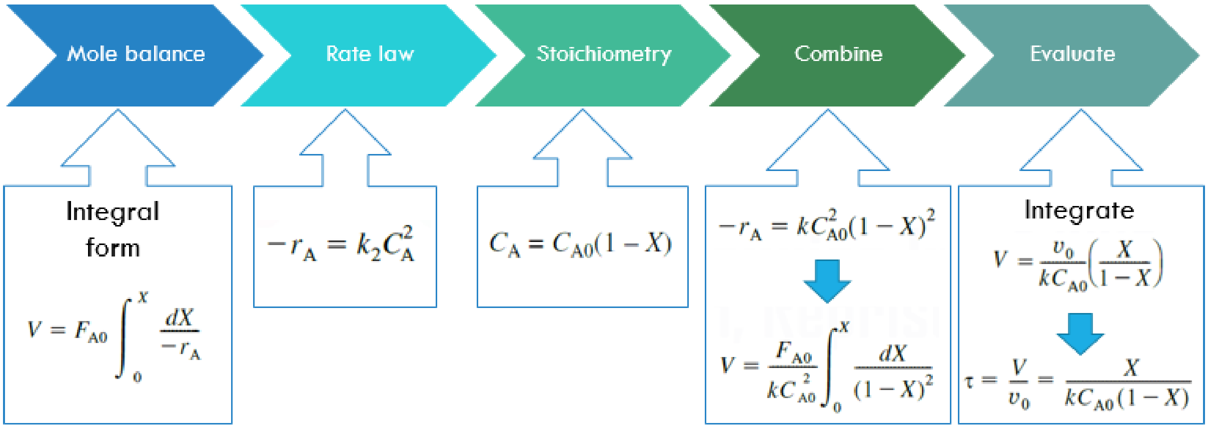
A → B



5.3 Discover tubular reactors

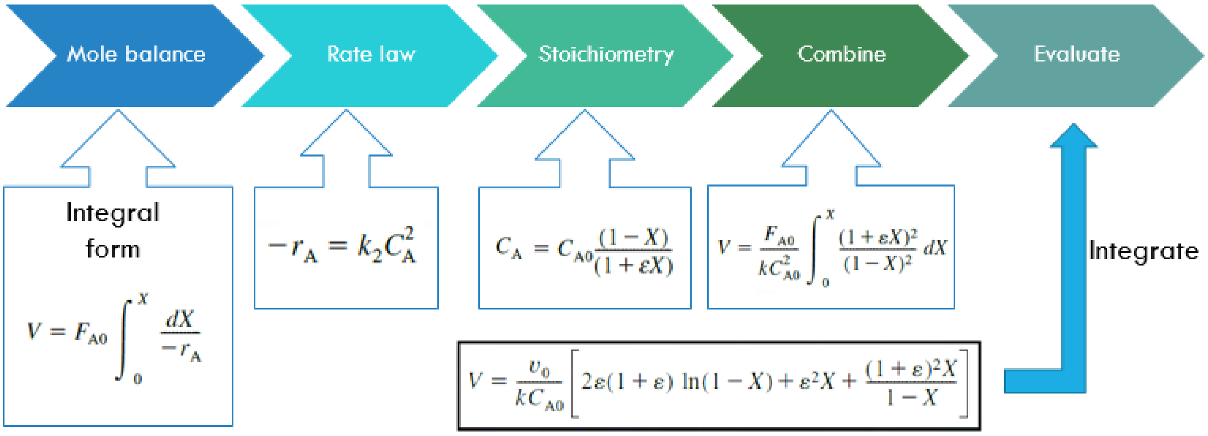
PFR: second-order and liquid phase (No pressure drop)

2A → B



PFR: second-order and gas phase (No pressure drop $P=P_0$ & $T=T_0$)

2A → B



TUTORIAL CHAPTER FIVE

1. Production of ethylene glycol (EG) was carried out in an isothermal CSTR. It is desired to produce 200 million pounds EG per year. A 1 lbmol/ft^3 solution of ethylene oxide (EO) in water is fed to reactor with an equal volumetric solution of water containing 0.9 wt% of catalyst H_2SO_4. The specific reaction rate, k = 0.311 min^{-1}. Assume that only EG is the only reaction product formed, calculate the CSTR volume if 80 % conversion is to be achieved.

   $C_2H_4O + H_2O \xrightarrow{H_2SO_4} C_2H_4(OH)_2$

2. Referring to question (1), how would the reactor volume change if the conversion is set to only 50%.

3. A reaction of:

$$A + B \rightarrow C$$

Follows an elementary rate law and is carried out isothermally in a flow system. The concentrations of A abd B feed stream are 2M before mixing. The volumetric flow rate of each stream is 5 dm^3/min, and the entering temperature is 300K. The streams are mixed before entering CSTR. The activation energy is measured to be 20kcal/mol. Given the volume of CSTR and specific rate of reaction at 300K are 200 dm^3 and 0.07 dm^3/mol-min, determine the conversion at 350K.

4. The elementary gas-phase reaction

$(CH_3)_3COOC(CH_3)_3 \rightarrow C_2H_4 + 2CH_3COCH_3$

Is carried out in a flow reactor with no pressure drop. The specific reaction rate at 323K is 10^{-4} min^{-1} and activation energy is 85 kJ/mol. Pure di-tert-butyl peroxide enters the reactor at 10 atm and 127°C and a molar flow rate of 2.5 mol/min.

i. Calculate the PFR volume to achieve 90 % conversion

ii. Calculate the CSTR volume to achieve 90 % conversion.

5. A gaseous reaction of $A \rightarrow B$ has reaction rate constant of 0.0015 m^{-1} at 26.7°C. the reaction takes place under a pressure of 1011 kPa and 126.7°C. A production rate of 453.6 kg/h of B is required. Assuming an activation energy of 104.6 kJ/mol. Find the total volume of tubes needed if the conversion of A is 90 %.
   i. Assume it is in perfect gas law condition
   ii. A and B each have molecular weight of 58 kg/kmol

06

Catalysis and Catalytic Reactors

This chapter explain the catalyst in terms of the definition and the properties of the catalyst. This topic also introduces the steps in a Catalytic Reaction for Adsorption Isotherms, Surface Reaction, Desorption and The Rate-Limiting Step.

6.1 CATALYST

6.1.1 Definition.

- A catalyst is a substance that affects the rate of a reaction but emerges from the process unchanged.
- A catalyst usually changes a reaction rate by promoting a different molecular path ("mechanism") for the reaction.

Catalyst affect yield and selectivity

Changes only the rate of reaction; it does not affect the equilibrium.

Example of catalyst process:

- H_2 and O_2 to form water; with Platinum as catalyst

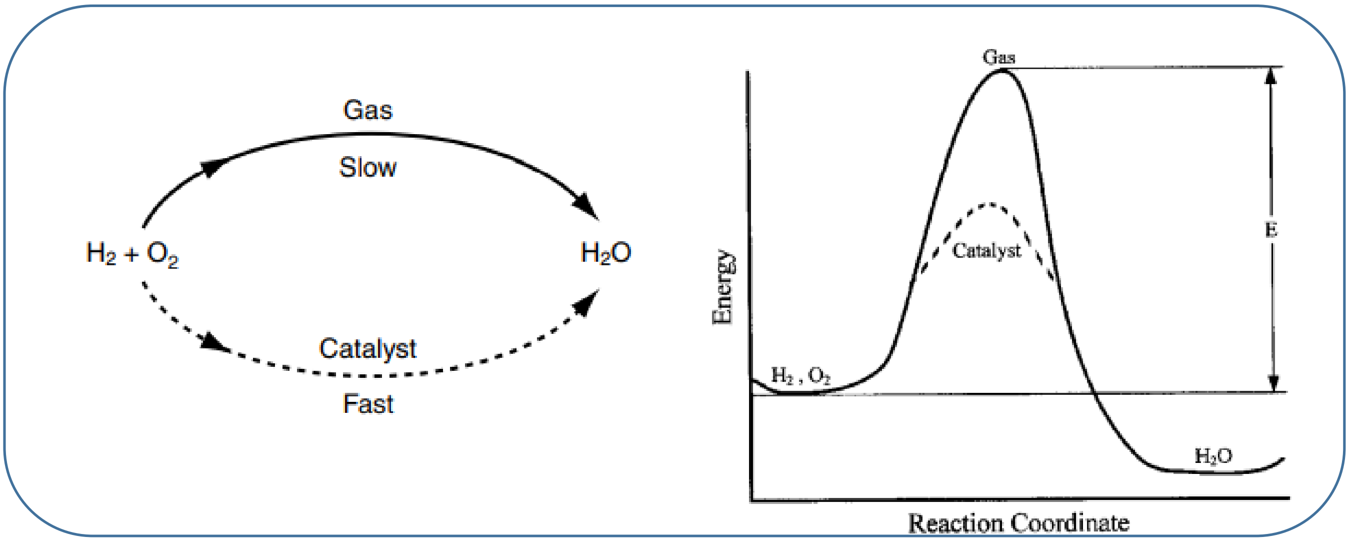


Figure 6.1 Different reaction path

(Source: Fogler 2016)

- Usually for “Faster” reaction design
- Less Activation Energy/Less free energy is required to reach the transition state

6.1.2 Uses

- 1/3 of chemical processes will need the use of a catalyst

- Catalyst was being used first in wine, cheese and bread production.
- Now, major uses were in petroleum refining, chemical processes and automotive


Cylindrical Extrusions
Spheres
Tri lobe Extrusions
Tablets /Pellets

Figure 3.2: Different shapes of catalyst

(Source: Kishore Ravindran, G. Madhu (2020))

6.1.3 Type of catalyst

HOMOGENEOUS	HETEROGENEOUS
• In solution with at least one of the reactants • catalysis reactants and catalyst are in the same face • mostly observed in liquid and gases catalysis • products cannot be separated • has low selectivity • Example; ○ 0xo process for manufacturing normal isobutylaldehyde	• more than one phase – typical solid catalyst in liquid/gaseous reactants • catalysis the reactant and catalysis are in a different phase. • observed when the catalyst is in solid form • high selectivity. • Example; ○ The dehydrogenation of cyclohexane

6.1.4 Properties of catalyst

1) Porous-Catalyst with large area resulting from pores
2) Molecular sieve - Small pores
3) Monolithic- can be either porous or nonporous
4) Supported-consists of minute particles of an active material dispersed over a less active substance.
5) Unsupported- mainly promoters that increase activity

6.1.5 Classification Of Catalyst

REACTION	**CATALYST**	**APPLICATION**
1. Halogenation-dehalogenation	$CuCl_2$, AgCl, Pd	-Halogenation of hydrocarbon -hydrochlorination reactions with mercury copper or zinc halides.
2. Hydration-dehydration	Al_2O_3, MgO	-Dehydration of alcohol to form olefins, -synthesis of ethanol from ethylene.
3. Alkylation-dealkylation	$AlCl_3$, Pd, Zeolites	-formation of ethyl benzene from benzene and ethylene -cracking of petrochemical product by dealkylation reaction.
4. Hydrogenation-dehydrogenation	Co, Pt, Cr_2O_3, Ni	-dehydrogenation of ethyl benzene to form styrene -formation of cyclohexane from n-hexane
5. Oxidation	Cu, Ag, Ni, V_2O_5	-oxygenolysis of carbon-hydrogen bond -oxygenation of nitrogen-hydorogen bonds -complete combustion of hydrocarbon
6. Isomerization	$AlCl_3$, Pt/Al_2O_3, Zeolites	-n-pentane isomerized to i-pentane -conversion of paraffins to isoparaffins

6.2 STEPS IN CATALYTIC REACTION

6.2 Steps in Catalytic Reaction

* Steps 3, 4 and 5 are MOST important

1. Mass transfer (diffusion) of the reactant from the bulk to the external transport.
2. Internal diffusion
3. Adsorption
4. Reaction on the surface
5. Desorption
6. Diffusion of the reactant
7. Mass transfer of the product

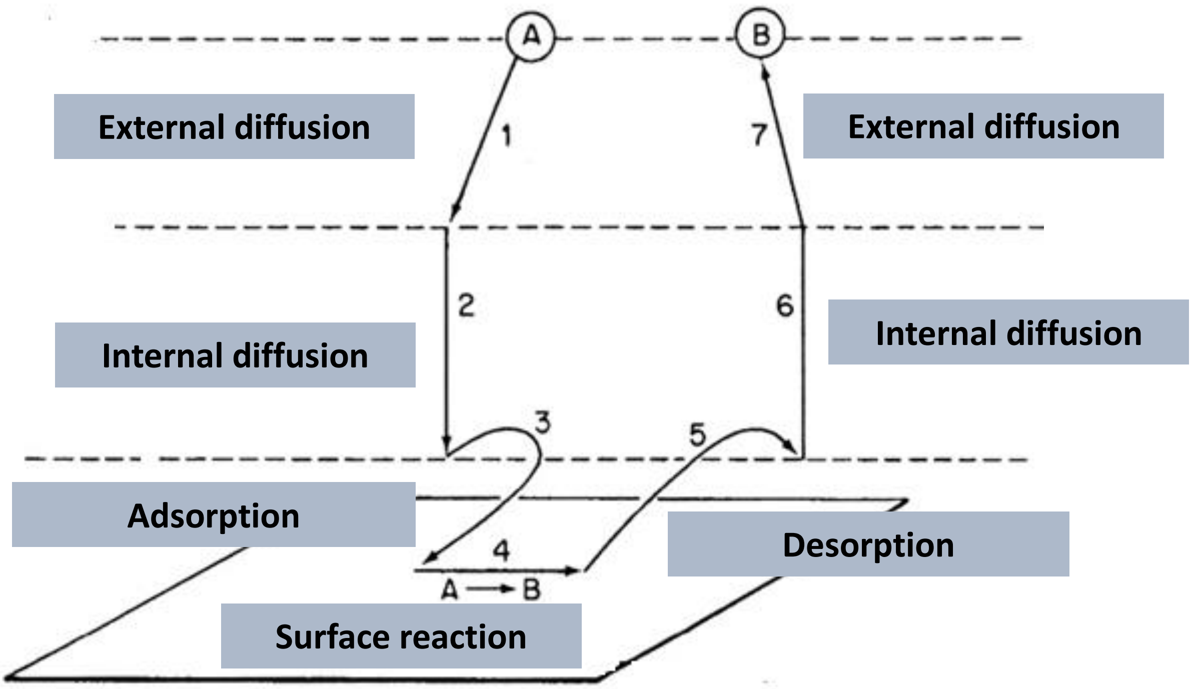
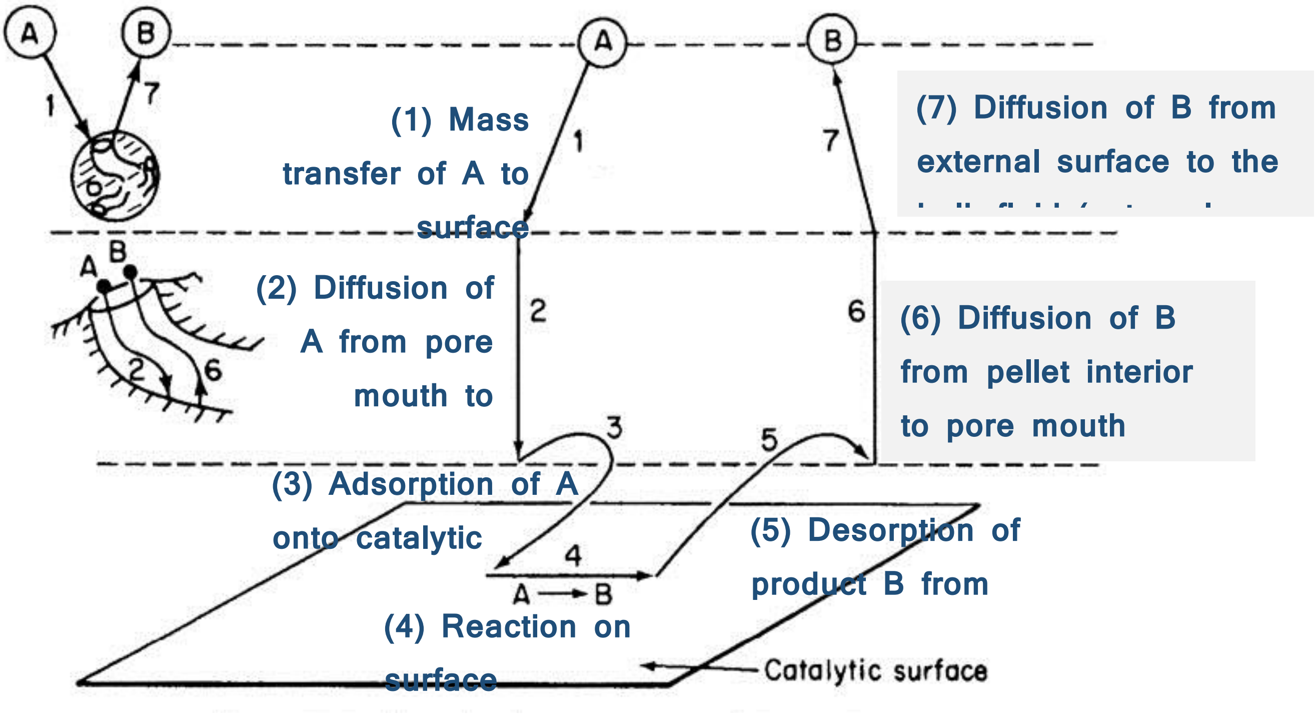


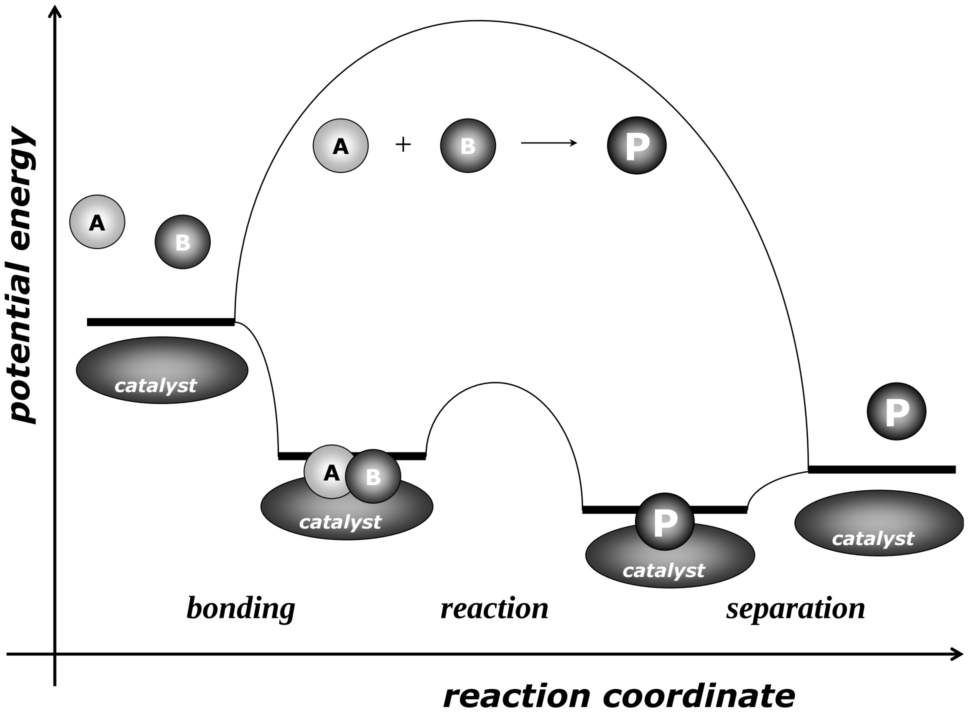
Figure 6.3: Steps in Catalytic Reaction



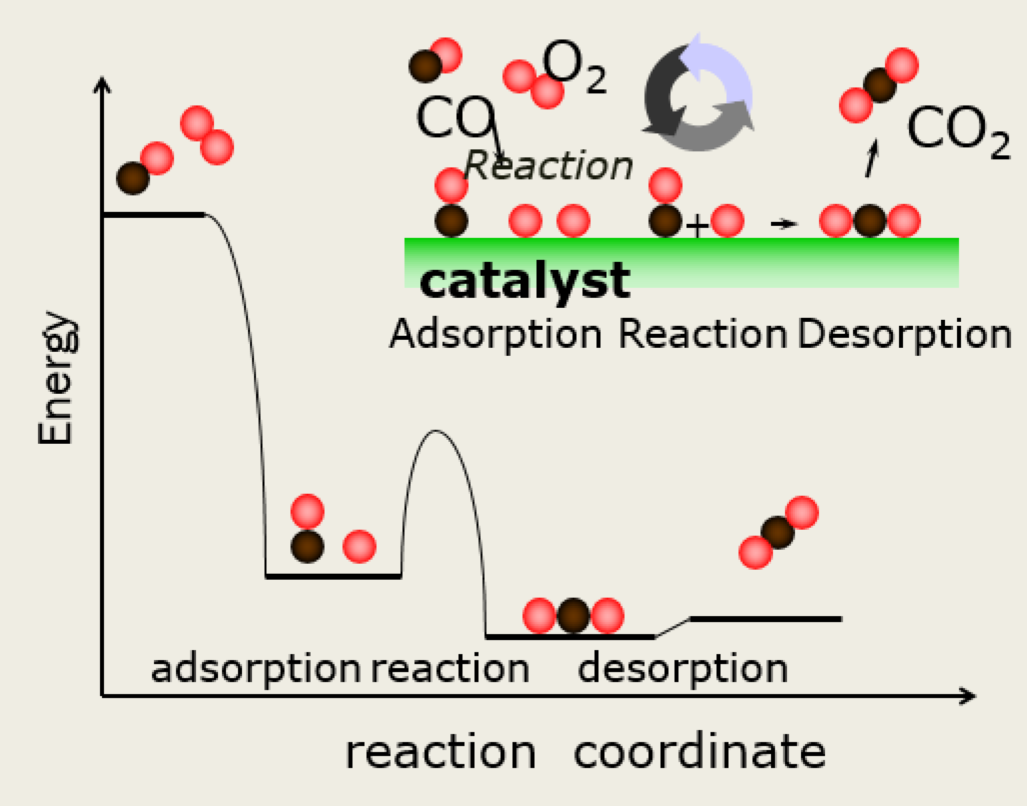
**Steps 1,2,6 & 7 are fast, so only steps 3, 4, and 5 need to be considered

Figure 6.4: Mechanism in Catalytic Reaction Steps

6.2.1 Basic surface interactions

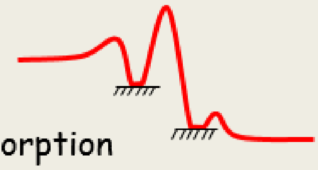


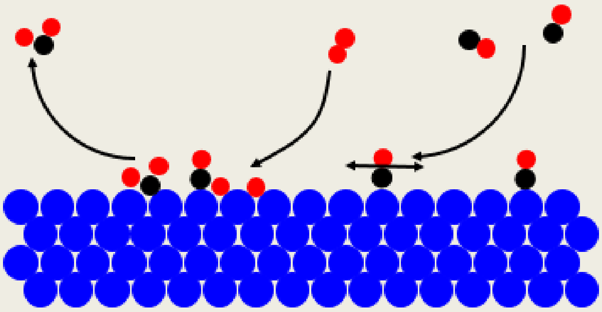
Reaction Scheme



Heterogeneous Catalysis

- Reactions take place on the metal surface





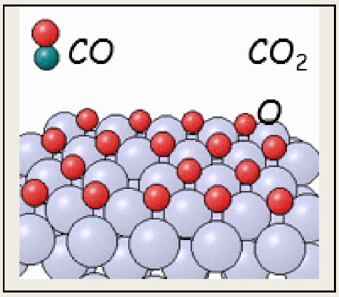
Molecular adsorption

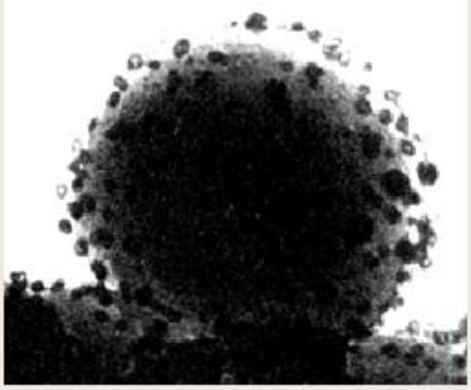
Dissociativ adsorption

Diffusion

Reaction

Desorption





Adsorption

$$O_2 + 2* \Leftrightarrow 2O*$$

$$CO + * \Leftrightarrow CO*$$

Reaction

$$CO* + O* \Leftrightarrow CO_2* + 2*$$

Desorption

$$CO_2* \Leftrightarrow CO_2 + *$$

Guidelines for Deducing Mechanisms

- **More than 70% of heterogeneous reaction mechanisms are surface reaction limited**
    - When you need to propose a rate limiting step, start with a surface reaction limited mechanism unless you are told otherwise
- If a species appears in the numerator of the rate law, it is probably a reactant
- If a species appears in the denominator of the rate law, it is probably adsorbed in the surface

$$i + j \rightarrow k$$

$$\text{Generic equation: } -r'_A = \frac{kP_iP_j}{1 + K_iP_i + K_jP_j + K_kP_k}$$

STEP 1: Diffusion of the reactant from the bulk to the external transport.

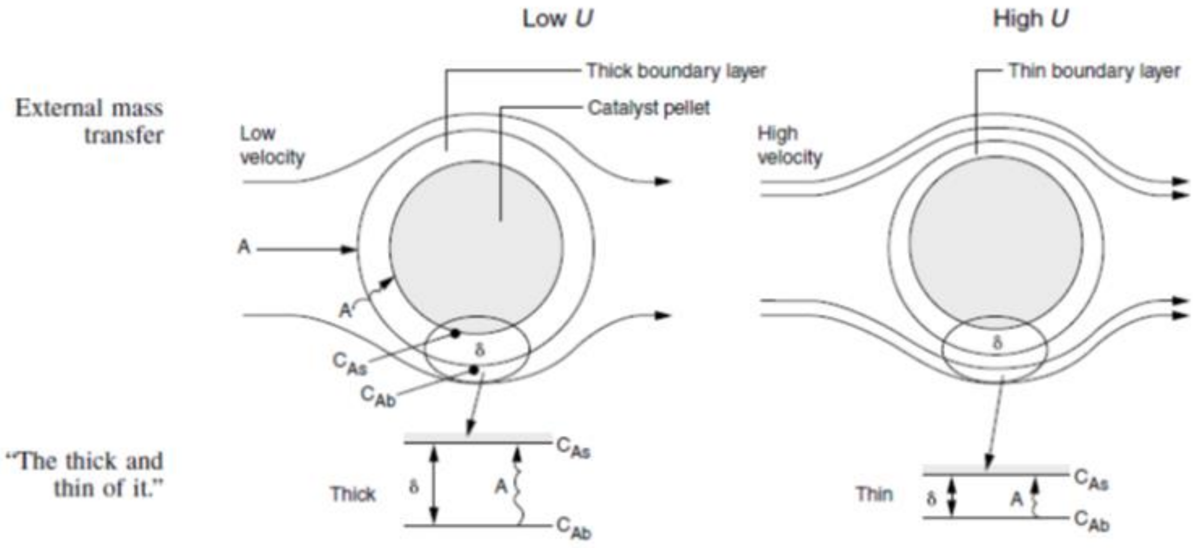


Figure 6.5: Diffusion through the external boundary layer

$$Rate = k_C(C_{Ab} - C_{As})$$

- mass-transfer coefficient, k_C, is a function of the hydrodynamic conditions,namely the fluid velocity, U, and the particle diameter, Dp

$$k_C = \frac{D_{AB}}{\delta}$$

- At low U, the boundary layer across which A and B must diffuse is thick, and it takes a long time for A to travel to the surface- small mass-transfer coefficient k_C.
- As the velocity over the pellet is increased, the boundary layer becomes thinner and the mass-transfer rate is increased

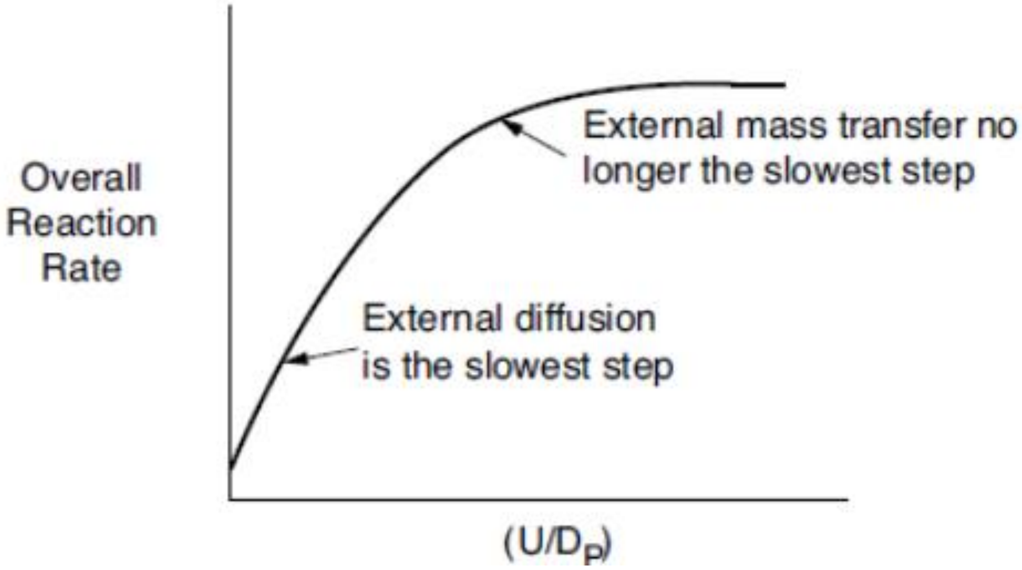


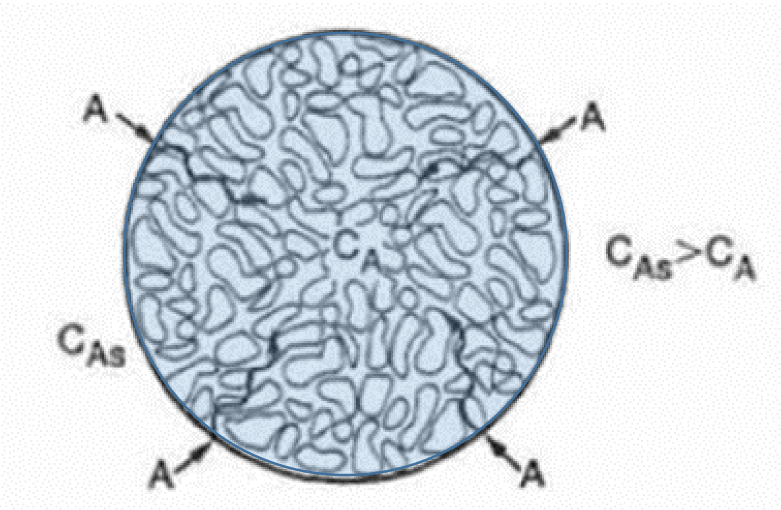
Figure 6.6: Effect of particle size and fluid velocity on the overall reaction rate.

STEP 2: Internal Diffusion

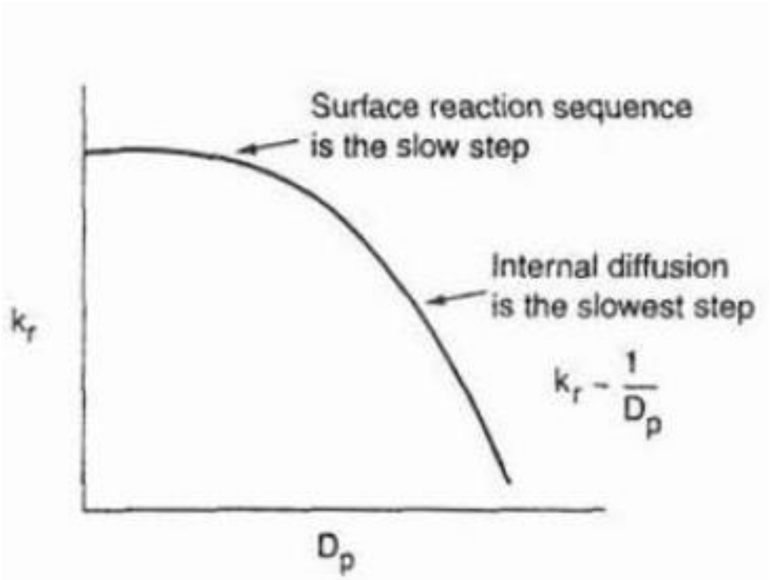
$$k_r = C_{As}$$

- C_{As} is the concentration at the external pellet surface and k_r is an overall rate constant, which is a function of particle size.

- The overall rate constant, *k_r*, increases as the pellet diameter decreases.



(a)

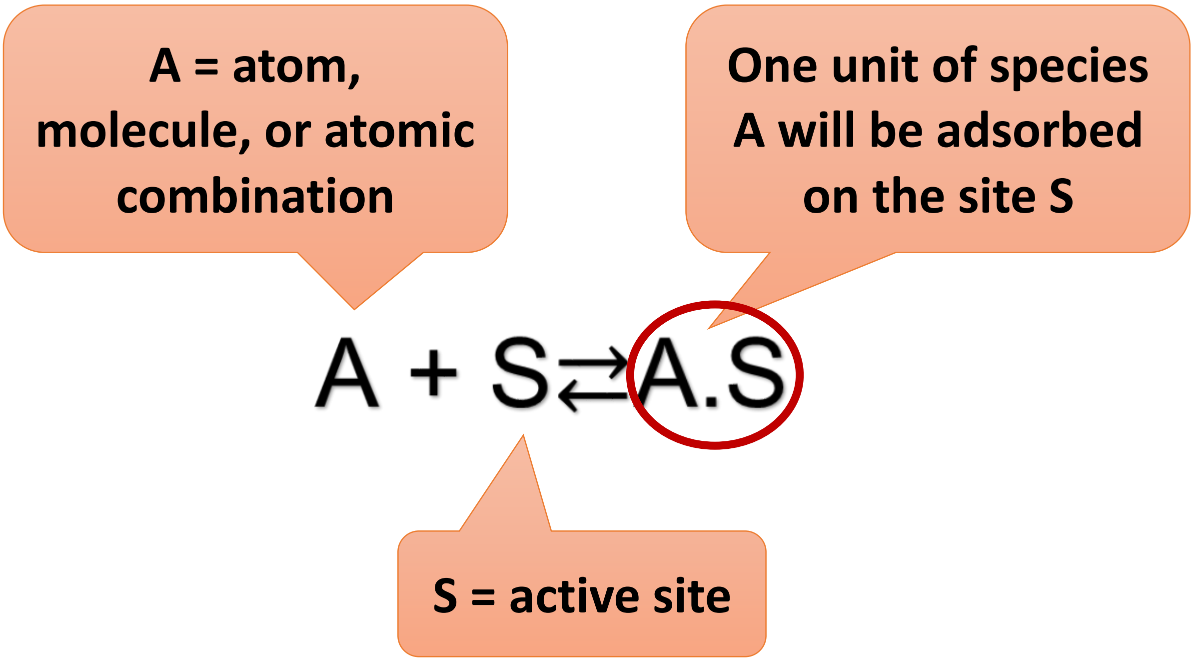


(b)

Figure 6.7: Effect of particle size on the overall reaction-rate constant.

(a) Branching of a single pore with deposited metal; (b) decrease in rate constant with increasing particle diameter.

STEP 3: Adsorption Isotherms



A = atom, molecule, or atomic combination

One unit of species A will be adsorbed on the site S

$$A + S \rightleftarrows A.S$$

S = active site

Active Sites

- Reactions are not catalyzed over the entire surface but only at certain active sites or centers that result from unsaturated atoms in the surface.
- An ***active site*** is a point on the surface that can form strong chemical bonds with an adsorbed atom or molecule.

STEP 4: SURFACE REACTION

THREE WAYS OF SURFACE REACTION MODEL:

1. SINGLE SITE

$$\mathrm{A \cdot S} \rightleftarrows \mathrm{B \cdot S} \qquad r_S = k_S\left(C_{A\cdot S} - \frac{C_{B\cdot S}}{K_S}\right)$$

2. DUAL SITE

$$\mathrm{A \cdot S + S} \rightleftarrows \mathrm{B \cdot S + S} \qquad r_S = k_S\left(C_{A\cdot S}C_v - \frac{C_{B\cdot S}C_v}{K_S}\right)$$

$$\mathrm{A \cdot S + B \cdot S} \rightleftarrows \mathrm{C \cdot S + D \cdot S} \qquad r_S = k_S\left(C_{A\cdot S}C_{B\cdot S} - \frac{C_{C\cdot S}C_{D\cdot S}}{K_S}\right)$$

3. ELEY-RIDEAL

$$A \cdot S + B(g) \rightleftarrows C \cdot S \qquad r_S = k_S\left(C_{A\cdot S}P_B - \frac{C_{C\cdot S}}{K_S}\right)$$

STEP 5: DESORPTION

$$\mathrm{C \cdot S} \rightleftarrows \mathrm{C + S}$$

The rate of desorption of C

$$r_{DC} = k_D\left(C_{C\cdot S} - \frac{P_C C_v}{K_{DC}}\right)$$

$$r_{DC} = -r_{ADC}$$

$$K_{DC} = \frac{1}{K_C}$$

$$r_{DC} = k_D(C_{C\cdot S} - K_C P_C C_v)$$

The Rate-Limiting Step

- When **heterogeneous reactions** are carried out at **steady state**. The rates of each of the three reaction steps in series (**adsorption, surface reaction and desorption)** are equal to one another:

$$\boxed{-r'_A = r_{AD} = r_S = r_D}$$

- **<u>One</u>** particular step in the series is usually found to be rate-limiting or rate-controlling.

TUTORIAL CHAPTER SIX

Chapter 6:

1. List out all five (5) types of catalyst that can be used in a chemical reaction.

2. Name two (2) types of attachment involved whereby the reactants attached to surface during catalytic reaction occur.

3. Name two (2) type of catalytic reactions concerns.

4. List out all six (6) types of chemical reaction which uses catalyst as part of the process.

5. In the hydration process of ethylene, cobalt is used as catalyst to speed up the reaction.

$$H_2 + C_2H_4 \rightarrow C_2H_6$$

At temperature 475K, the minimum and maximum turnover frequency, f are 0.01 and 100 molecules/site/sec respectively. Assume the dispersion is 65% and the amount of catalyst used is 0.8 %. Calculate the minimum and maximum rate of reaction in mol/s·g catalyst.

04

Appendix

Appendix I

Table of Unit Conversions Factor

Quantity	Equivalent Values
Mass	1 kg = 1000 g = 0.001 metric ton = 2.20462 Ib_m = 35.27392 oz 1 Ib_m = 16 oz = 5 X 10^{-4} ton = 453.593 g = 0.453593 kg
Length	1 m = 100 cm = 1000 mm = 10^6 microns (μm) = 10^{10} angstroms (A) = 39.37 in. = 3.2808 ft = 1.0936 yd = 0.0006214 mile
Volume	1 m^3 = 1000 liters = 10^6 cm^3 = 10^6 ml = 35.3145 ft^3 = 220.83 imperial gallons = 264.17 gal = 1056.68 qt 1 ft^3 = 1728 in^3 = 7.4805 gal = 0.028317 m^3 = 28.317 liters = 28 317 cm^3
Force	1 N = 1 kg.m/s^2 = 10^5 dynes = 10^5 g.cm/s^2 = 0.22481 Ib_f 1 Ib_f = 32.174 Ib_m.ft/s^2 = 4.4482 N = 4.4482 X 10^4 dynes
Pressure	1 atm = 1.01325 x 10^5 N/m^2 (Pa) = 101.325 kPa = 1.01325 bars = 1.01325 x 10^6 dynes/cm^2 = 760 mm Hg at 0 °C (torr) = 10.333 m H_2O at 4 °C = 14.696 Ib_f/in^2 (psi) = 33.9 ft H_2O at 4 °C = 29.921 in Hg at 0 °C
Energy	1 J = 1 N.m = 10^7 ergs = 10^7 dyne.cm = 2.778 x 10^{-7} kW.h = 0.23901 cal = 0.7376 ft-lbf = 9.486 x 10^{-4} Btu
Power	1 W = 1J/s = 0.23901 cal/s = 0.7376 ft.Ib_f/s = 9.468 x 10^{-4} Btu/s = 1.341 x 10^{-3} hp

Appendix II

CHAPTER 1

a) Rate of Reaction

1) $r_i = \frac{1}{V}\frac{dN_i}{dt} = \frac{moles\ i\ formed}{(volume\ of\ fluid)(time)}$
2) $r_i' = \frac{1}{W}\frac{dN_i}{dt} = \frac{moles\ i\ formed}{(mass\ of\ solid)(time)}$
3) $r_i'' = \frac{1}{S}\frac{dN_i}{dt} = \frac{moles\ i\ formed}{(surface)(time)}$
4) $r_i''' = \frac{1}{V_S}\frac{dN_i}{dt} = \frac{moles\ i\ formed}{(volume\ of\ solid)(time)}$
5) $r_i'''' = \frac{1}{V_r}\frac{dN_i}{dt} = \frac{moles\ i\ formed}{(volume\ of\ reactor)(time)}$
6) $-r_A = kC_A$ (first order reaction)
7) $-r_A = kC_A{}^2$ (Second order reaction)
8) $-r_A = \frac{k_1 C_A}{(1+k_2 C_A)}$

b) General mole balance:

1) F_{j0} - F_j + G_j = dN_j/dt
2) In - Out + Generation = Accumulation

c) Reactor Mole Balances Summary

Reactor	Differential	Algebraic	Integral
Batch Reactors	$\frac{dN_A}{dt} = r_A V$		$t_1 = \int_{N_{A0}}^{N_{A1}} \frac{dN_A}{r_A V} = \int_{N_{A1}}^{N_{A0}} \frac{dN_A}{-r_A V}$
CSTR		$V = \frac{F_{A0} - F_A}{-r_A}$	
PFR	$\frac{dF_A}{dV} = r_A$		$V_1 = \int_{F_{A0}}^{F_{A1}} \frac{dF_A}{r_A} = \int_{F_{A1}}^{F_{A0}} \frac{dF_A}{-r_A}$
PBR	$\frac{dF_A}{dW} = r_A'$		$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A'}$

d) The molar flow rate**, F_j** is a product of the concentration of species j **(C_j)** and the volumetric flow rate, **v**

$F_j = C_j$.v

CHAPTER 2

a) Conversion

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

b) Batch Reactor

$$X = \frac{(N_{A0} - N_A)}{N_{A0}}$$

c) Continuous Flow Reactor

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

d) Ideal gas law

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

Where,

P_0 *= entering total pressure of A ;*

y_{A0} *=entering mole fraction of A;*

C_{A0} *=entering concentration;*

T_0 *= initial temperature;*

R = 8.314 dm^3.kPa/mol.K

e) Design Equation for Isothermal Reactors in terms of conversion, X

Reactor	Differential	Algebraic	Integral
Batch Reactors	$N_{A0}\frac{dX}{dt} = -r_A V$		$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$

CSTR		$V = \frac{F_{A0}X}{-r_A}$	
PFR	$F_{A0}\frac{dX}{dV} = -r_A$		$V = \int_0^X \frac{F_{A0}dX}{-r_A}$
PBR	$F_{A0}\frac{dX}{dW} = -r'_A$		$W = \int_0^X \frac{F_{A0}dX}{-r'_A}$

f) Reactor Sizing: Sizing A PFR

1) Trapezoidal Rule (2-point):

$$\int_{X_0}^{X_1} f(X)dX = \frac{h}{2}\left[f(X_0) + f(X_1)\right]$$

$$where \quad h = X_1 - X$$

2) Simpson's One-Third Rule (3-point):

$$\int_{X_0}^{X_2} f(X)dX = \frac{h}{3}\left[f(X_0) + 4f(X_1) + f(X_2)\right]$$

$$where \quad h = \frac{X_2 - X_0}{2} \quad X_1 = X_0 + h$$

3) Simpson's Three-Eighths Rule (4-point):

$$\int_{X_0}^{X_3} f(X)dX = \frac{3}{8}h\left[f(X_0) + 3f(X_1) + 3f(X_2) + f(X_3)\right]$$

$$where \quad h = \frac{X_3 - X_0}{3} \quad X_1 = X_0 + h \quad X_2 = X_0 + 2h$$

4) Five-Point Quadrature Formula:

$$\int_{X_0}^{X_4} f(X)dX = \frac{h}{3}\left[f(X_0) + 4f(X_1) + 2f(X_2) + 4f(X_3) + f(X_4)\right]$$

$$where \quad h = \frac{X_4 - X_0}{4}$$

CHAPTER 3

a) Reactor Sizing For Reactors In Series

$$X_i = \frac{F_{A0} - F_{Ai}}{F_{A0}}$$

b) Reactor sizing for CSTR in series

$$V_1 = F_{A0}\left(\frac{1}{-r_{A1}}\right)X_1$$

$$V_2 = \frac{F_{A2} - F_{A1}}{r_{A2}} = \frac{F_{A1} - F_{A2}}{-r_{A2}}$$

$$V_2 = \frac{-F_{A0}X_1 + F_{A0}X_2}{-r_{A2}} = \frac{F_{A0}}{-r_{A2}}\left(X_2 - X_1\right)$$

$$V = \frac{F_{A0}\left(X_{out} - X_{in}\right)}{\left(-r_A\right)_{out}}$$

c) Reactor sizing for PFR in Series

$$\int_0^{X_2} F_{A0}\frac{dX}{-r_A} = \int_0^{X_1} F_{A0}\frac{dX}{-r_A} + \int_0^{X_2} F_{A0}\frac{dX}{-r_A}$$

$$V = \int_{X_{in}}^{X_{out}} \frac{F_{A0}}{-r_A}dX$$

$$V = V_1 + V_2$$

d) Space Time

$$\tau = \frac{V}{\nu_0}$$

e) Space Velocity

$$SV = \frac{\nu_0}{V} = \frac{1}{\tau}$$

CHAPTER 4

a) Irreversible Reactions

$$aA + bB \rightarrow cC + dD$$

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

$$k=\frac{(Concentration)^{1-n}}{Time}$$

Zero order (n=0); $-r_A = k_A$

First order (n=1);

$$-r_A = k_A C_A$$

b) Reversible Reactions

$$aA + bB \Leftrightarrow cC + dD$$

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

c) Arrhenius equation

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

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

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

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

d) Stoichiometric Table for Batch Systems

Species	Initially	Change	Remaining	*Concentration*
A	N_{A0}	$-(N_{A0}X)$	$N_A = N_{A0} - N_{A0}X$	$C_A = \frac{N_{A0}(1-X)}{V}$
B	N_{B0}	$-\frac{b}{a}(N_{A0}X)$	$N_B = N_{A0}\left(\Theta_B - \frac{b}{a}X\right)$	$C_B = \frac{N_{A0}[\Theta_B - (b/a)X]}{V}$
C	N_{C0}	$\frac{c}{a}(N_{A0}X)$	$N_C = N_{A0}\left(\Theta_C + \frac{c}{a}X\right)$	$C_C = \frac{N_{A0}[\Theta_C + (c/a)X]}{V}$

D	N_{D0}	$\frac{d}{a}(N_{A0}X)$	$N_D = N_{A0}\left(\Theta_D + \frac{d}{a}X\right)$	$C_D = \frac{N_{A0}[\Theta_D + (d/a)X]}{V}$
I	N_{I0}	-	$N_I = N_{I0}$	C_{IO}

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

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

δ = change in total number of mol per mol A reacted

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

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

e) In the case of ideal gases, relates volumetric flow rate to conversion.

Batch constant volume: $V = V_0$

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

Liquid: $v = v_0$

f) Flow Systems Stoichiometric Table

Species	Feed rate to reactor (mol/time)	Change within the reactor (mol/time)	Effluent rate from reactor (mol/time)	Concentration (mol/L)
A	F_{A0}	$-(F_{A0}X)$	$F_A = F_{A0} - F_{A0}X$	$C_A = \frac{F_{A0}(1-X)}{\upsilon}$
B	$F_{B0} = \Theta_B F_{A0}$	$-\frac{b}{a}(F_{A0}X)$	$F_B = F_{A0}\left(\Theta_B - \frac{b}{a}X\right)$	$C_B = \frac{F_{A0}[\Theta_B - (b/a)X]}{\upsilon}$

C	$F_{C0} = \Theta_C F_{A0}$	$\frac{c}{a}(F_{A0}X)$	$F_C = F_{A0}\left(\Theta_C + \frac{c}{a}X\right)$	$C_C = \frac{F_{A0}\left[\Theta_C + (c/a)X\right]}{\upsilon}$
D	$F_{D0} = \Theta_D F_{A0}$	$\frac{d}{a}(F_{A0}X)$	$F_D = F_{A0}\left(\Theta_D + \frac{d}{a}X\right)$	$C_D = \frac{F_{A0}\left[\Theta_D + (d/a)X\right]}{\upsilon}$
I	$F_{I0} = \Theta_i F_{A0}$	-	$F_I = F_{A0}\Theta_I$	$C_I = \frac{F_{A0}\Theta_I}{\upsilon}$
Totals	F_{T0}		$F_T = F_{T0} + \delta F_{A0}X$	

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

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

g) In terms of gas-phase molar flow rates, the concentration of species i is

$$C_i = C_{T0}\frac{F_i}{F_T}\frac{P}{P_0}\frac{T_0}{T}$$

<u>Ideal Gas Constant and Conversion Factor</u>

Ideal Gas Constant

R = 10.731573 ft^3·psia/°R·.lb.mol

R = 0.73 ft^3·atm/°R·.lb.mol

R = 82.0573383 (cm^3·.atm)/(K·.mol)

R = 0.083144 (L·bar)/(K·.mol)

R = 8.3144 J/(K . mol)

R = 8.3144 (m^3·Pa)/(K·.mol)

R = 0.083144 (m^3·bar)/(K·kg.mol)

R = 1.987 Btu/(°R·.lb.mol)

R = 1.987 cal/(K·.mol)

R =0.082 (m^3·.atm)/(K·.mol)

Boltzman's constant, $k_B = 1.381 \times 10^{-23}$ J/molecule .K

$$= 1.381 \times 10^{-23} \text{ kg m}^2/\text{s}^2/\text{molecule/K}$$

Volume of Ideal Gas

1 mol of ideal gas at 0^oC and 1 atm occupies22.4dm^3 (0.0446 mol/dm^3)

$$C_A = \frac{P_A}{RT} = \frac{y_A P}{RT}$$

Where; C_A = concentration of A, mol/dm^3

T = temperature, K

P = pressure, kPa

y_A = mole fraction of A

R = ideal gas constant, 8.314 kPa . dm^3/mol . K

1 M = 1 molar = 1 mol/liter = 1 mol/dm^3 = 1 kmol/m^3 = 0.062 Ibmol/ft^3

Appendix III

GRAPH PAPER

GRAPH PAPER

GRAPH PAPER

GRAPH PAPER

GRAPH PAPER

Appendix IV

05

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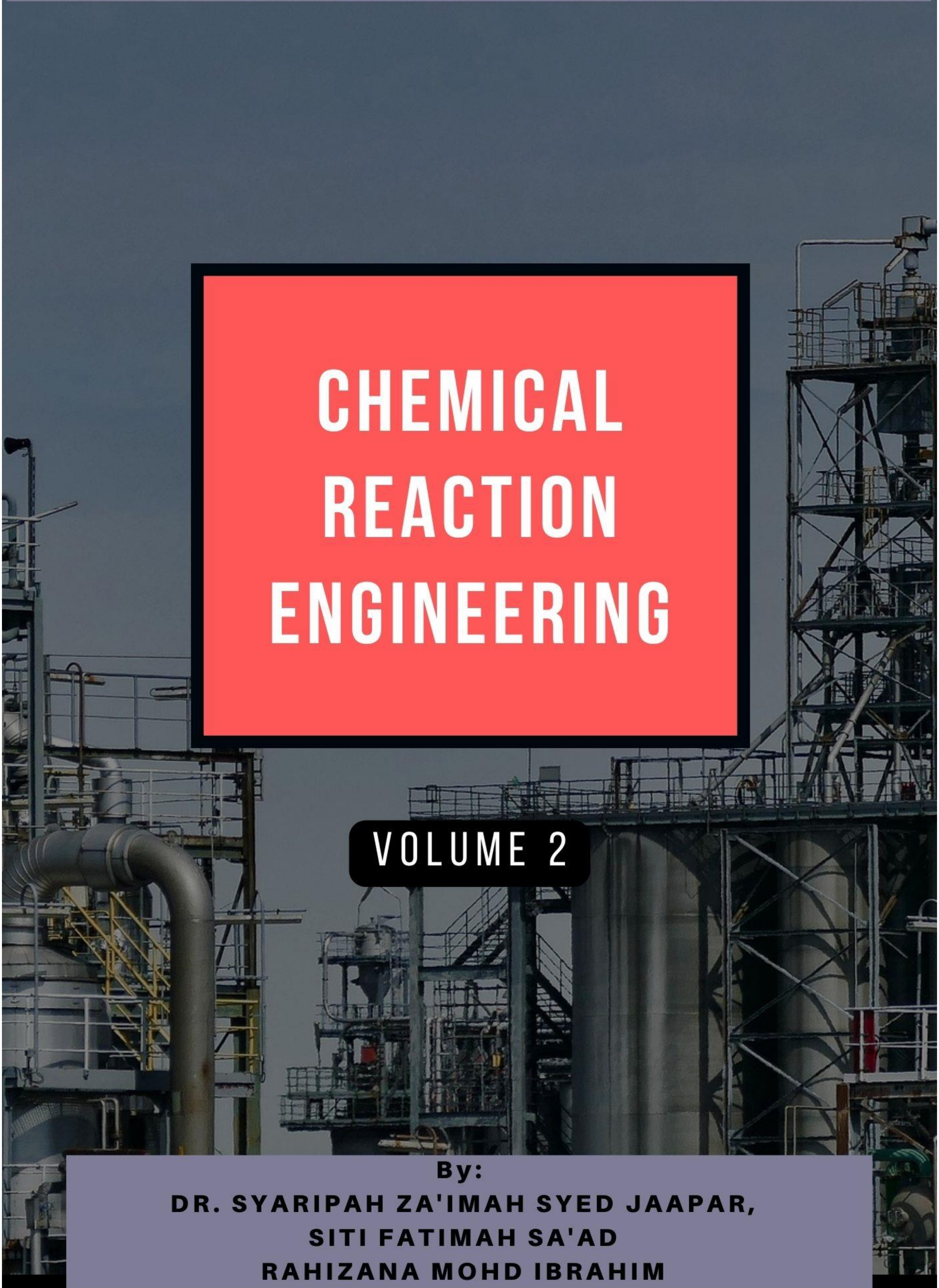

CHEMICAL REACTION ENGINEERING

VOLUME 2

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