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Mohamed Khider University of Biskra
Faculty of Science and Technology
Department of Process Engineering

COURSE HANDOUT

CHEMICAL KINETICS & HOMOGENEOUS CATALYSIS

Process Engineering Curriculum

PREPARED BY

Dr. Adaika Kaltoum
Associate Professor (MCA)

Target Audience:

3rd Year Bachelor (Licence) in Process Engineering

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General Introduction

Welcome to the module of **Chemical Kinetics and Homogeneous Catalysis**. This pedagogical handout is carefully designed and prepared specifically for the **3rd-year Bachelor (Licence) students in Process Engineering** at the Faculty of Science and Technology, Mohamed Khider University of Biskra.

CONTEXT AND IMPORTANCE OF THE COURSE

In the realm of process engineering and chemical industries, understanding thermodynamics is only half the battle; it tells us whether a chemical reaction is possible. However, **Chemical Kinetics** provides the crucial missing piece: it tells us *how fast* that reaction will occur and the specific pathway it follows. This knowledge is the fundamental cornerstone for the design, optimization, and safe operation of industrial chemical reactors.

Furthermore, the integration of **Homogeneous Catalysis** introduces students to one of the most powerful tools in modern chemistry and engineering. By utilizing catalysts that exist in the same phase as the reactants, engineers can significantly accelerate reaction rates, lower energy consumption, and control the selectivity of desired products, which is vital for sustainable and economically viable industrial processes.

OBJECTIVES OF THIS HANDOUT

The primary goal of this document is to bridge the gap between fundamental chemical theories and practical engineering applications. By studying this handout, students will be able to:

- Formulate rate laws and understand the factors affecting the speed of chemical reactions.
- Analyze elementary and complex reaction mechanisms.

- Comprehend the principles, kinetic models, and industrial applications of homogeneous catalysis.
- Develop the mathematical and analytical skills required to solve practical kinetic problems.

STRUCTURE AND PEDAGOGICAL APPROACH

This handout has been structured logically to facilitate a smooth learning curve. It progresses gradually from basic definitions and macroscopic kinetic concepts to microscopic mechanisms and advanced catalytic cycles. Each chapter is enriched with clear theoretical explanations, essential mathematical derivations, and illustrative examples to ensure a comprehensive understanding of the physical phenomena behind the equations.

A WORD TO THE STUDENTS

I highly encourage you to actively engage with this material—not just by reading, but by practicing the derivations and solving the related exercises. Process engineering is a field built on applied problem-solving.

I hope this document serves as a valuable and accessible resource throughout your studies and helps lay a solid foundation for your future careers as successful process engineers. I wish you a fruitful and highly successful academic year.

Dr. Adaika Kaltoum

Associate Professor (MCA)

Department of Process Engineering

TABLE OF CONTENTS

General Introduction

Chapter 1: Fundamentals of Chemical Kinetics

- 1.1 Reaction Rates and Stoichiometry
- 1.2 Rate Laws, Order, and Molecularity
- 1.3 Integral Form of Rate Equations (0, 1st, 2nd, and nth Order)

Chapter 2: Experimental Methods & Determination of Reaction Orders

- 2.1 Measurement Techniques for Reaction Rates
- 2.2 The Differential Method
- 2.3 The Integral Method
- 2.4 Fractional Life and Isolation Methods

Chapter 3: Complex and Multiple Reactions

- 3.1 Reversible (Opposing) Reactions
- 3.2 Parallel (Competing) Reactions
- 3.3 Series (Consecutive) Reactions

Chapter 4: Theories of Chemical Kinetics

- 4.1 Temperature Dependence: The Arrhenius Equation
- 4.2 Collision Theory
- 4.3 Transition State Theory (Activated Complex)

Chapter 5: Reaction Mechanisms

- 5.1 Elementary Steps and Reaction Intermediates

- 5.2 The Steady-State Approximation (Bodenstein Principle)
- 5.3 Rate-Determining Step Approximation
- 5.4 Chain Reactions (Free Radicals)

Chapter 6: Introduction to Catalysis

- 6.1 Definition and General Properties of Catalysts
- 6.2 Classification: Homogeneous, Heterogeneous, and Enzymatic
- 6.3 Energy Profile of a Catalyzed Reaction

Chapter 7: Homogeneous Catalysis

- 7.1 Acid-Base Catalysis
- 7.2 Enzyme Kinetics (Michaelis-Menten Equation)
- 7.3 Organometallic Catalysis in Industry

General Conclusion

Chapter 1: Fundamental Concepts of Chemical Kinetics

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1 Introduction

Chemical kinetics is the branch of physical chemistry that studies the rates at which chemical reactions occur, the factors affecting these rates, and the macroscopic mechanisms by which reactants are transformed into products. For process engineers, mastering chemical kinetics is critical for the rational design, scaling, and optimization of chemical reactors in industrial processes.

2 The Rate of Reaction

Consider a generalized chemical reaction occurring in a closed system under constant volume:

$$aA + bB \longrightarrow cC + dD \tag{1}$$

Where A and B are reactants, C and D are products, and a, b, c, d are the stoichiometric coefficients.

The reaction rate (v) is defined as the change in the extent of reaction (ξ) per unit volume (V) per unit time (t):

$$v = \frac{1}{V}\frac{d\xi}{dt} \tag{2}$$

In terms of the molar concentration of any species i (denoted as $[i]$ or C_i), the global reaction rate is expressed using its stoichiometric coefficient ν_i (negative for reactants, positive for products):

$$v = -\frac{1}{a}\frac{d[A]}{dt} = -\frac{1}{b}\frac{d[B]}{dt} = \frac{1}{c}\frac{d[C]}{dt} = \frac{1}{d}\frac{d[D]}{dt} \tag{3}$$

3 Rate Laws, Reaction Order, and Molecularity

3.1 The Empirical Rate Law

Experimental observations show that the reaction rate often depends on the concentrations of the reactants. The empirical rate law is typically written as:

$$v = k[A]^{\alpha}[B]^{\beta} \tag{4}$$

Where:

- k: The specific rate constant (highly dependent on temperature).

- α: The partial order of reaction with respect to reactant A.
- β: The partial order of reaction with respect to reactant B.
- $n = \alpha + \beta$: The overall order of the reaction.

Important Note: The reaction orders (α and β) are determined strictly by experiment and do not necessarily correspond to the stoichiometric coefficients (a and b), unless the reaction is an **elementary step**.

3.2 Molecularity vs. Order

- **Molecularity:** A theoretical concept representing the number of molecules or ions that collide simultaneously to trigger an elementary reaction step (e.g., unimolecular, bimolecular). It is always a positive integer.
- **Reaction Order:** An empirical macroscopic quantity that can be zero, fractional, or negative.

4 Integrated Rate Equations for Constant Volume Systems

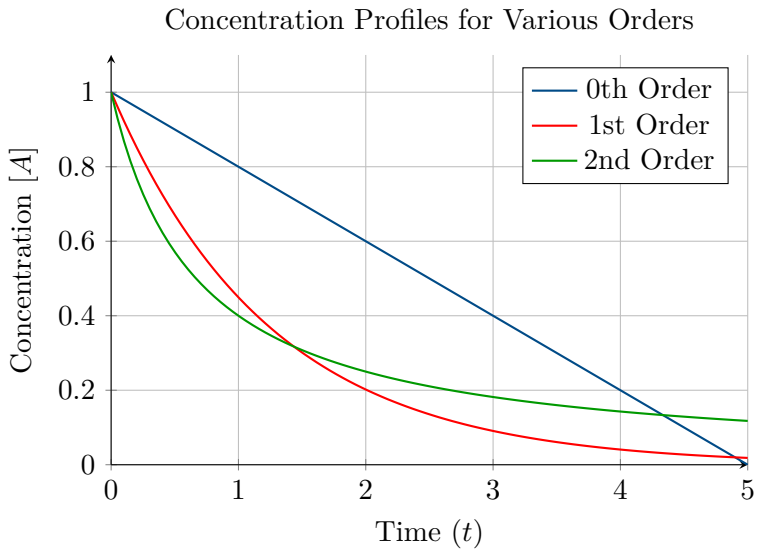
By integrating the differential rate laws, we obtain expressions that relate reactant concentration directly to time.

Table 1: Summary of Kinetic Parameters for Common Reaction Orders (Type $A \rightarrow$ Products)

Order (n)	**Differential Rate Law**	**Integrated Equation**	**Half-Life ($t_{1/2}$)**	**Units of k**
0	$-\frac{d[A]}{dt} = k$	$[A] = [A]_0 - kt$	$\frac{[A]_0}{2k}$	$\text{mol} \cdot \text{L}^{-1} \cdot \text{s}^{-1}$
1	$-\frac{d[A]}{dt} = k[A]$	$\ln\left(\frac{[A]}{[A]_0}\right) = -kt$	$\frac{\ln(2)}{k}$	s^{-1}
2	$-\frac{d[A]}{dt} = k[A]^2$	$\frac{1}{[A]} - \frac{1}{[A]_0} = kt$	$\frac{1}{k[A]_0}$	$\text{L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$

4.1 Kinetic Profiles

The following plots illustrate the behavior of reactant concentration over time for different reaction orders.



5 Effect of Temperature: The Arrhenius Equation

Chemical reaction rates typically increase exponentially with an increase in temperature. This dependence is mathematically modeled by the Arrhenius equation:

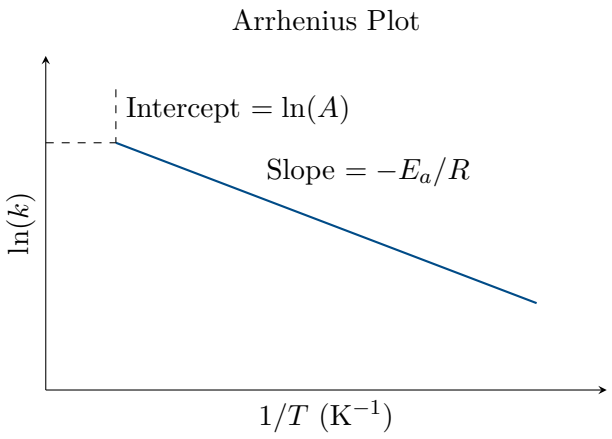
$$k(T) = A \exp\left(-\frac{E_a}{RT}\right) \tag{5}$$

Where:

- A: The pre-exponential factor or frequency factor (same units as k).
- E_a: The activation energy ($\mathrm{J \cdot mol^{-1}}$), representing the minimum energy barrier the reactants must overcome.
- R: The universal gas constant ($8.314\,\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$).
- T: Absolute temperature in Kelvin (K).

To determine E_a and A experimentally, we use the linearized form of the Arrhenius equation:

$$\ln(k) = \ln(A) - \frac{E_a}{R}\left(\frac{1}{T}\right) \tag{6}$$



6 Elementary and Complex Reactions

- **Elementary Reaction:** Occurs in a single kinetic step. The rate law can be written directly from the stoichiometry.
- **Complex Reaction:** Occurs in multiple sequence steps (the reaction mechanism). Examples include consecutive reactions ($A \rightarrow B \rightarrow C$), parallel reactions, and reversible reactions. The overall rate is often dictated by the **Rate-Determining Step (RDS)**, which is the slowest step in the mechanism.

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Chapter 2: Kinetics of Complex Reactions and Mechanistic Analysis

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1 Introduction to Complex Systems

In Chapter 1, we treated reactions as occurring in a single elementary step. However, in industrial chemical processes, most reactions are **complex**, meaning they proceed through a sequence of elementary steps known as the reaction mechanism. For process engineers, understanding these complex networks is essential for optimizing reactor residence times, maximizing the yield of desired products, and minimizing unwanted by-products.

Complex reactions can be broadly classified into three fundamental types: Reversible (opposing), Parallel (competing), and Consecutive (series) reactions.

2 Reversible (Opposing) Reactions

In many chemical processes, the products can react to reform the original reactants. The simplest case is a first-order reversible reaction:

$$A \rightleftharpoons B \tag{1}$$

Where k_1 is the forward rate constant and k_{-1} is the reverse rate constant.

2.1 Kinetic Equations

Let $[A]_0$ be the initial concentration of A, and assume $[B]_0 = 0$. At any time t, if x moles of A have reacted, then $[A] = [A]_0 - x$ and $[B] = x$. The net rate of disappearance of A is:

$$-\frac{d[A]}{dt} = \frac{dx}{dt} = k_1([A]_0 - x) - k_{-1}x \tag{2}$$

At equilibrium, the net rate is zero ($dx/dt = 0$), and the equilibrium conversion is x_e:

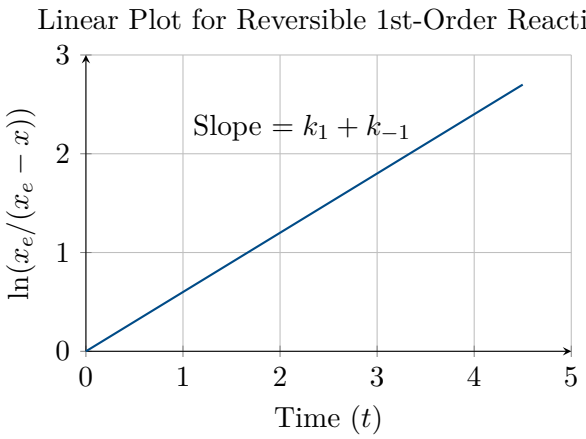
$$k_1([A]_0 - x_e) = k_{-1}x_e \implies K_c = \frac{k_1}{k_{-1}} = \frac{x_e}{[A]_0 - x_e} \tag{3}$$

Where K_c is the thermodynamic equilibrium constant.

2.2 Integrated Form

Integrating the rate equation yields:

$$\ln\left(\frac{x_e}{x_e - x}\right) = (k_1 + k_{-1})t \tag{4}$$



3 Parallel (Competing) Reactions

Parallel reactions occur when a reactant undergoes multiple separate reactions simultaneously to form different products. This is highly relevant in industrial synthesis where selectivity is a primary concern.

$$A \xrightarrow{k_1} B \quad \text{(Desired Product)}$$
$$A \xrightarrow{k_2} C \quad \text{(By-Product)}$$

3.1 Kinetic Equations

The rate of disappearance of A is the sum of the rates of the individual reactions (assuming both are first order):

$$-\frac{d[A]}{dt} = k_1[A] + k_2[A] = (k_1 + k_2)[A] \tag{5}$$

Integration gives:

$$[A] = [A]_0 \exp(-(k_1 + k_2)t) \tag{6}$$

The rates of formation of B and C are:

$$\frac{d[B]}{dt} = k_1[A] \quad \text{and} \quad \frac{d[C]}{dt} = k_2[A] \tag{7}$$

3.2 Product Distribution and Selectivity

The ratio of the products formed at any given time is constant and equal to the ratio of their rate constants:

$$\frac{[B]}{[C]} = \frac{k_1}{k_2} \tag{8}$$

To maximize the selectivity of B over C, process engineers must adjust operating conditions (like temperature) based on the activation energies (E_{a1} and E_{a2}) of the two pathways.

4 Consecutive (Series) Reactions

Consecutive reactions occur when the product of an initial reaction serves as the reactant for a subsequent reaction.

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \tag{9}$$

4.1 Differential Rate Equations

Assuming both steps are irreversible and first-order:

$$\frac{d[A]}{dt} = -k_1[A] \tag{10}$$

$$\frac{d[B]}{dt} = k_1[A] - k_2[B] \tag{11}$$

$$\frac{d[C]}{dt} = k_2[B] \tag{12}$$

4.2 Integrated Profiles

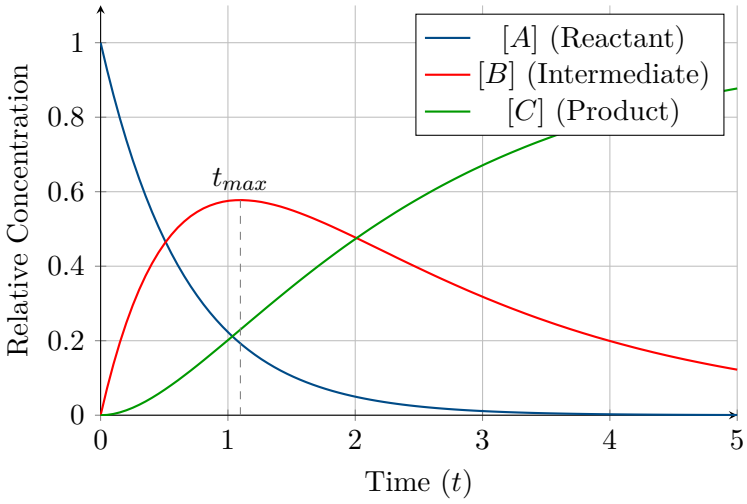
Solving this system of linear differential equations (with $[A] = [A]_0$ and $[B]_0 = [C]_0 = 0$) yields:

$$[A] = [A]_0 e^{-k_1 t} \tag{13}$$

$$[B] = [A]_0 \frac{k_1}{k_2 - k_1} \left(e^{-k_1 t} - e^{-k_2 t} \right) \tag{14}$$

$$[C] = [A]_0 \left(1 - \frac{k_2}{k_2 - k_1} e^{-k_1 t} + \frac{k_1}{k_2 - k_1} e^{-k_2 t} \right) \tag{15}$$

Concentration Profiles for Consecutive Reactions ($A \to B \to C$)



Optimum Time (t_{max}): To maximize the yield of intermediate B, the reaction must be quenched at a specific time:

$$t_{max} = \frac{\ln(k_2/k_1)}{k_2 - k_1} \tag{16}$$

5 Analytical Tools for Complex Mechanisms

To solve complex kinetic mechanisms without resolving exhaustive differential equations, kineticists employ approximations.

5.1 The Steady-State Approximation (Bodenstein's Principle)

For an intermediate I^*:

$$\frac{d[I^*]}{dt} = \sum(\text{Rates of Formation}) - \sum(\text{Rates of Consumption}) \approx 0 \tag{17}$$

Table 1: Key Mechanistic Approximations

Approximation	Principle	Application Conditions
Rate-Determining Step (RDS)	The overall reaction rate is governed by the slowest elementary step.	One step has a significantly smaller rate constant (k) than all others.
Steady-State Approximation (SSA)	The concentration of highly reactive intermediates remains constant.	$d[Intermediate]/dt \approx 0$. Used for radicals or unstable complexes.
Pre-Equilibrium	A fast reversible step reaches equilibrium before the subsequent slow step.	The reverse rate is much faster than the forward rate of the subsequent step.

This algebraic manipulation allows us to express the unmeasurable concentration of reactive intermediates in terms of the stable, measurable reactants. This principle will be extensively used in **Chapter 3** when we derive the Michaelis-Menten kinetics for homogeneous catalysis.

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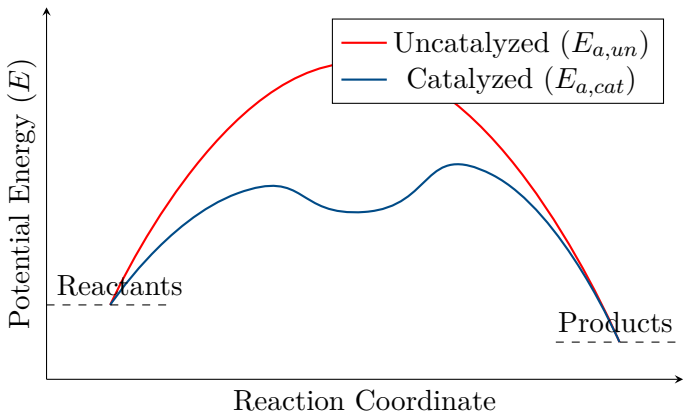
Chapter 3: Fundamentals of Homogeneous Catalysis

1 Introduction to Catalysis

A catalyst is a substance that increases the rate of a chemical reaction without being consumed in the overall stoichiometry. In **homogeneous catalysis**, the catalyst is in the same phase (usually liquid or gas) as the reactants. This allows for excellent molecular-level mixing and high selectivity compared to heterogeneous systems, though separation of the catalyst from the products can be challenging.

The fundamental action of a catalyst is to provide an alternative reaction pathway with a lower activation energy (E_a).

Energy Profile: Uncatalyzed vs. Catalyzed Pathways



2 Mechanisms of Homogeneous Catalysis

A generalized homogeneous catalytic cycle involves the catalyst (C) binding to the reactant (A) to form a reactive intermediate (AC^*), which subsequently decomposes into the product (P) and regenerates the catalyst:

$$A + C \rightleftharpoons AC^* \quad \text{(Fast equilibrium)} \tag{1}$$

$$AC^* \xrightarrow{k_2} P + C \quad \text{(Slow, Rate-Determining Step)} \tag{2}$$

Since the catalyst is regenerated, even a very small concentration of C can turn over a large number of reactant molecules.

3 Acid-Base Catalysis

Acid-base catalysis is the most common form of homogeneous catalysis in liquid solutions, particularly in organic synthesis and hydrolysis reactions.

3.1 Specific Acid and Base Catalysis

In specific catalysis, the reaction rate depends solely on the concentration of the solvated proton (e.g., H_3O^+) or the specific base (e.g., OH^-) from the solvent. The observed first-order rate constant (k_{obs}) can be written as:

$$k_{obs} = k_0 + k_{H^+}[H^+] + k_{OH^-}[OH^-] \tag{3}$$

Where:

- k_0: Rate constant of the uncatalyzed (neutral solvent) reaction.
- k_{H^+}: Catalytic constant for the specific acid.
- k_{OH^-}: Catalytic constant for the specific base.

At low pH (acidic), $k_{obs} \approx k_{H^+}[H^+]$. At high pH (basic), $k_{obs} \approx k_{OH^-}[OH^-]$.

3.2 General Acid-Base Catalysis

In general acid-base catalysis, undissociated weak acids (HA) or weak bases (B) in the buffer solution also participate directly in the proton transfer during the transition state.

$$k_{obs} = k_0 + k_{H^+}[H^+] + k_{OH^-}[OH^-] + k_{HA}[HA] + k_B[B] \tag{4}$$

4 Enzymatic Catalysis: Michaelis-Menten Kinetics

Enzymes are highly specific, highly efficient biological catalysts that operate in aqueous solutions (a prime example of homogeneous catalysis). The kinetics of many single-substrate enzymatic reactions are described by the Michaelis-Menten model.

4.1 The Kinetic Model

Let E be the free enzyme, S the substrate, ES the enzyme-substrate complex, and P the product.

$$E + S[k_{-1}]k_1 ES \xrightarrow{k_2} E + P \tag{5}$$

Applying the **Steady-State Approximation (SSA)** to the intermediate ES:

$$\frac{d[ES]}{dt} = k_1[E][S] - k_{-1}[ES] - k_2[ES] \approx 0 \tag{6}$$

By recognizing that the total enzyme concentration $[E]_0 = [E] + [ES]$, we can substitute $[E] = [E]_0 - [ES]$ and solve for $[ES]$. The initial reaction rate ($v_0 = k_2[ES]$) is then derived as the **Michaelis-Menten Equation**:

$$v_0 = \frac{V_{max}[S]}{K_m + [S]} \tag{7}$$

Key Kinetic Parameters:

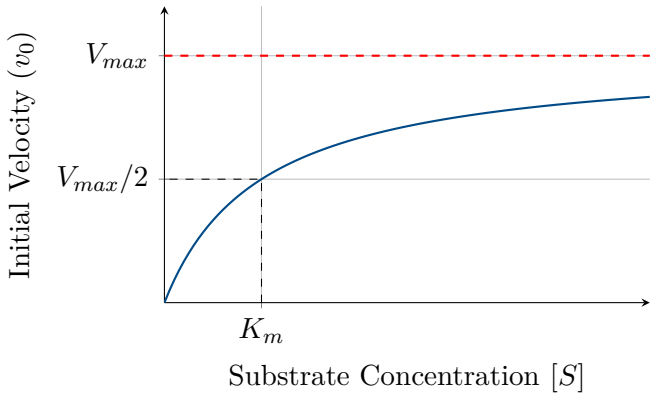
- $V_{max} = k_2[E]_0$: The maximum velocity of the reaction when the enzyme is fully saturated with substrate.
- $K_m = \frac{k_{-1}+k_2}{k_1}$: The Michaelis Constant. It represents the substrate concentration at which the reaction rate is exactly half of V_{max} ($v_0 = V_{max}/2$). It is an inverse measure of the enzyme's affinity for the substrate.

4.2 Graphical Determinations of Parameters

4.2.1 1. Michaelis-Menten Plot (v_0 vs. $[S]$)

A plot of initial velocity versus substrate concentration yields a rectangular hyperbola.

Michaelis-Menten Saturation Curve

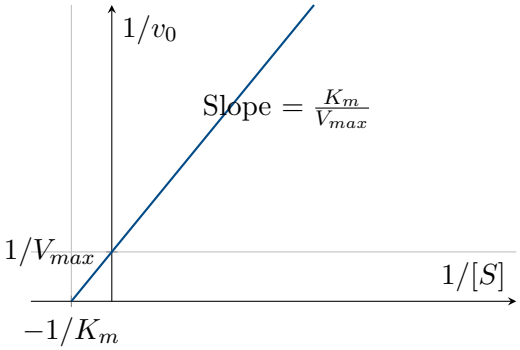


4.2.2 2. Lineweaver-Burk Plot (Double Reciprocal)

To extract accurate values of V_{max} and K_m from experimental data, the Michaelis-Menten equation is linearized by taking the reciprocal of both sides:

$$\frac{1}{v_0} = \left(\frac{K_m}{V_{max}}\right)\frac{1}{[S]} + \frac{1}{V_{max}} \tag{8}$$

Lineweaver-Burk Double Reciprocal Plot



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Chapter 4: Catalysis by Transition Metal Complexes

1 Introduction to Organometallic Catalysis

In modern industrial chemistry, homogeneous catalysis frequently employs transition metal complexes. These complexes consist of a central metal atom surrounded by molecules or ions called ligands. Unlike heterogeneous catalysts where active sites are on a solid surface, homogeneous metal complexes are dissolved in the reaction medium, allowing every single molecule to act as an active site.

This chapter covers the fundamental elementary steps that make up an organometallic catalytic cycle and analyzes the kinetics of such systems.

2 Fundamental Elementary Steps

A catalytic cycle in homogeneous organometallic chemistry is built from a sequence of specific elementary reactions. The most important steps are:

2.1 1. Ligand Substitution (Association and Dissociation)

To create an open coordination site for a reactant to bind, a ligand (L) must often dissociate from the metal (M):

$$ML_n \rightleftharpoons ML_{n-1} + L \quad (1)$$

Kinetically, this step can be purely dissociative (first-order) or associative (second-order).

2.2 2. Oxidative Addition and Reductive Elimination

Oxidative Addition involves the cleavage of a covalent bond in a reactant (e.g., H_2, RX) and the addition of the two fragments to the metal. The formal oxidation state of the metal increases by +2, and its coordination number increases by 2.

$$L_nM^{(x)} + A - B \xrightarrow{k_{oa}} L_nM^{(x+2)}(A)(B) \quad (2)$$

Reductive Elimination is the reverse process, where two ligands couple together to form a product molecule which then leaves the metal complex, decreasing the metal's oxidation state by 2.

$$L_nM^{(x+2)}(A)(B) \xrightarrow{k_{re}} L_nM^{(x)} + A - B \quad (3)$$

2.3 3. Migratory Insertion and β-Elimination

In Migratory Insertion, an unsaturated ligand (like an alkene or CO) inserts itself into an adjacent Metal-Ligand bond (usually Metal-Hydride or Metal-Alkyl).

$$L_nM(H)(CH_2 = CH_2) \rightleftharpoons L_nM - CH_2 - CH_3 \quad (4)$$

The reverse process is called β-Hydride Elimination.

3 Kinetics of a Catalytic Cycle

Let us consider a simplified catalytic cycle, such as homogeneous hydrogenation of an alkene by Wilkinson's Catalyst ($RhCl(PPh_3)_3$). The general cycle can be abstracted as follows:

- 1. Catalyst (C)
- - Product P (k_4)
- + Reactant 1 (k_1)
- 4. $C - P$
- 2. $C - R_1$
- Insertion (k_3)
- 3. $C - R_1 - R_2$
- + Reactant 2 (k_2)

3.1 Deriving the Rate Law using the Steady-State Approximation

If we assume that step 3 (migratory insertion, k_3) is the Rate-Determining Step (RDS), and steps 1 and 2 are in rapid pre-equilibrium, we can express the global rate v:

$$v = k_3[C - R_1 - R_2] \quad (5)$$

From the pre-equilibria (with equilibrium constants K_1 and K_2):

$$[C - R_1] = K_1[C][R_1] \quad (6)$$

$$[C - R_1 - R_2] = K_2[C - R_1][R_2] = K_1K_2[C][R_1][R_2] \quad (7)$$

Applying the total catalyst mass balance:

$$[C]_0 = [C] + [C - R_1] + [C - R_1 - R_2] \approx [C](1 + K_1[R_1] + K_1K_2[R_1][R_2]) \quad (8)$$

Substituting $[C]$ back into the rate expression gives a saturation kinetics profile (similar to Michaelis-Menten):

$$v = \frac{k_3 K_1 K_2 [C]_0 [R_1][R_2]}{1 + K_1[R_1] + K_1 K_2 [R_1][R_2]} \quad (9)$$

This rate law explains why increasing reactant concentrations indefinitely does not indefinitely increase the rate; eventually, all the catalyst is tied up in the $[C - R_1 - R_2]$ state, and the rate approaches a maximum $v_{max} = k_3[C]_0$.

4 Comparison: Homogeneous vs. Heterogeneous Catalysis

Process engineers must choose between homogeneous and heterogeneous catalysis based on industrial requirements.

Table 1: Key Differences between Homogeneous and Heterogeneous Catalysis

Property	Homogeneous Catalysis	Heterogeneous Catalysis
Phase	Same as reactants (liquid/gas)	Different (usually solid)
Active Sites	All metal atoms are active	Only surface atoms are active
Selectivity & Yield	Excellent (single-site behavior)	Often lower (multiple site types)
Catalyst Separation	Difficult (requires distillation/extraction)	Easy (filtration/fixed bed)
Heat Transfer	Excellent	Can be problematic (hotspots)
Operating Conditions	Mild (low T, P)	Severe (high T, P)

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Chapter 5: Industrial Applications and Detailed Kinetic Modeling of Homogeneous Processes

1 Introduction

Building upon the elementary steps of organometallic catalysis discussed in Chapter 4, this chapter provides a highly detailed kinetic analysis of major industrial processes that rely on homogeneous catalysis. For process engineers, deriving the accurate rate law from a proposed catalytic cycle is crucial for reactor sizing, process optimization, and economic evaluation. We will analyze three cornerstone processes: The Wacker Oxidation, Hydroformylation, and the Monsanto Acetic Acid Process.

2 The Wacker Process: Oxidation of Ethylene

The Wacker process is a major industrial method for the production of acetaldehyde from ethylene using a homogeneous Palladium/Copper catalyst system.

$$C_2H_4 + \frac{1}{2}O_2 \xrightarrow{PdCl_2/CuCl_2/HCl(aq)} CH_3CHO$$

2.1 Detailed Kinetic Mechanism

The reaction proceeds in aqueous solution. The widely accepted mechanism involves the following pre-equilibria before the rate-determining step (RDS):

1. **Alkene Coordination:** Substitution of a chloride ligand by ethylene.

$$[PdCl_4]^{2-} + C_2H_4 \rightleftharpoons [PdCl_3(C_2H_4)]^- + Cl^-$$

2. **Aquation:** Substitution of a trans chloride by water.

$$[PdCl_3(C_2H_4)]^- + H_2O \rightleftharpoons [PdCl_2(H_2O)(C_2H_4)] + Cl^-$$

3. **Deprotonation:** The coordinated water acts as an acid.

$$[PdCl_2(H_2O)(C_2H_4)] \rightleftharpoons [PdCl_2(OH)(C_2H_4)]^- + H^+$$

4. **Rate-Determining Step (RDS):** Migratory insertion of the alkene into the Pd-OH bond.

$$[PdCl_2(OH)(C_2H_4)]^- \xrightarrow{k_{RDS}} [PdCl_2(CH_2CH_2OH)]^- \quad \text{(Slow)}$$

2.2 Derivation of the Rate Law

The global rate of acetaldehyde formation (v) is dictated by the RDS:

$$v = k_{RDS}[[PdCl_2(OH)(C_2H_4)]^-]$$

Using the equilibrium expressions for steps 1, 2, and 3:

$$K_1 = \frac{[[PdCl_3(C_2H_4)]^-][Cl^-]}{[[PdCl_4]^{2-}][C_2H_4]}$$

$$K_2 = \frac{[[PdCl_2(H_2O)(C_2H_4)]][Cl^-]}{[[PdCl_3(C_2H_4)]^-]} \quad (\text{assuming } [H_2O] \approx const)$$

$$K_3 = \frac{[[PdCl_2(OH)(C_2H_4)]^-][H^+]}{[[PdCl_2(H_2O)(C_2H_4)]]}$$

By substituting these sequentially into the rate equation, we obtain the highly specific empirical rate law:

$$v = k_{RDS} K_1 K_2 K_3 \frac{[[PdCl_4]^{2-}][C_2H_4]}{[Cl^-]^2[H^+]} = k_{obs} \frac{[Pd_{\text{total}}][C_2H_4]}{[Cl^-]^2[H^+]}$$

Process Engineering Implication: The rate law explicitly shows an inverse square dependence on chloride concentration ($[Cl^-]^{-2}$) and an inverse first-order dependence on proton concentration ($[H^+]^{-1}$). Thus, operating at highly acidic or highly concentrated chloride conditions severely inhibits the reaction rate.

3 The Monsanto Acetic Acid Process

The synthesis of acetic acid from methanol and carbon monoxide is one of the most successful homogeneous catalytic processes, operating with $> 99\%$ selectivity.

$$CH_3OH + CO \xrightarrow{[Rh(CO)_2I_2]^-/HI} CH_3COOH$$

3.1 The Catalytic Cycle

The cycle utilizes a Rhodium(I) catalyst promoted by Methyl Iodide (CH_3I). The cycle involves Rh(I) (16-electron) and Rh(III) (18-electron) species.

- **Oxidative Addition:** $[Rh(CO)_2I_2]^- + CH_3I \rightarrow [Rh(CH_3)(CO)_2I_3]^-$ (Slow)
- **Migratory Insertion:** $[Rh(CH_3)(CO)_2I_3]^- \rightarrow [Rh(COCH_3)(CO)I_3]^-$
- **Coordination:** $[Rh(COCH_3)(CO)I_3]^- + CO \rightarrow [Rh(COCH_3)(CO)_2I_3]^-$
- **Reductive Elimination:** $[Rh(COCH_3)(CO)_2I_3]^- \rightarrow [Rh(CO)_2I_2]^-$

3.2 Kinetic Analysis

Experimental data reveals that the reaction rate is completely independent of the partial pressure of carbon monoxide (P_{CO}) and the concentration of methanol. The empirical rate law is:

$$v = k_{obs}[Rh_{\text{total}}][CH_3I]$$

This first-order dependence on both the rhodium complex and the methyl iodide promoter confirms that the Oxidative Addition of CH_3I to the square planar $[Rh(CO)_2I_2]^-$ complex is the strictly rate-determining step.

4 Hydroformylation (The Oxo Process)

Hydroformylation converts alkenes, CO, and H_2 (syngas) into aldehydes. It is the largest-volume homogeneously catalyzed industrial process.

$$\text{R-CH} = \text{CH}_2 + \text{CO} + \text{H}_2 \xrightarrow{\text{HCo(CO)}_4 \text{ or HRh(CO)}_2(\text{PPh}_3)_2} \text{R-CH}_2\text{-CH}_2\text{-CHO (Linear)}$$

4.1 Kinetic Features and Substrate Inhibition

When using the classic Cobalt catalyst [$HCo(CO)_4$], an interesting kinetic phenomenon occurs: the rate of reaction is inversely proportional to the partial pressure of carbon monoxide at high pressures.

$$v = k\frac{[\text{Alkene}][\text{H}_2][\text{Co}_{\text{total}}]}{P_{CO}}$$

This occurs because CO competes with the alkene for the active coordination site on the metal. High P_{CO} forces the equilibrium towards the saturated, inactive [$HCo(CO)_4$] species, preventing the necessary dissociation of a CO ligand to form the active 16-electron species [$HCo(CO)_3$].

Table 1: Comparison of Industrial Hydroformylation Catalysts

Parameter	**Unmodified Cobalt** ($HCo(CO)_4$)	**Rhodium-Phosphine** ($HRh(CO)_2L_2$)
Operating Temp.	$110 - 180°C$	$60 - 120°C$
Operating Pressure	200-300 bar	10-50 bar
Linear:Branched Ratio	$\sim 3:1$ to $4:1$	$\geq 10:1$ (Excellent)
Catalyst Cost	Low	Very High
Kinetics	Inhibited by high P_{CO}	Highly active, mild conditions

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Chapter 6: Ideal Chemical Reactors and Isothermal Design

1 Introduction to Reactor Design

In the previous chapters, we determined the rate of reaction ($-r_A$) based on the underlying chemical mechanisms and homogeneous catalysis. For a process engineer, the ultimate goal is to use this kinetic data to design chemical reactors specifically, to determine the reactor volume (V) or residence time (τ) required to achieve a desired conversion (X_A).

2 The General Mole Balance Equation

Reactor design is founded on the principle of conservation of mass. For any chemical species A entering a system volume V, the mole balance is defined as:

$$[Rate\ In] - [Rate\ Out] + [Rate\ of\ Generation] = [Rate\ of\ Accumulation]$$

Mathematically, this is expressed as:

$$F_{A0} - F_A + \int r_A \, dV = dN_A / dt \qquad (1)$$

Where:

- F_{A0}, F_A: Molar flow rates of A in and out (mol/s).
- r_A: Rate of generation of A per unit volume (mol/L·s). Since A is a reactant, r_A is negative.
- N_A: Number of moles of A inside the reactor at time t.

We define the conversion X_A as the fraction of reactant A converted into product: $X_A = (N_{A0} - N_A) / N_{A0}$ (for batch) or $X_A = (F_{A0} - F_A) / F_{A0}$ (for flow systems).

3 Ideal Batch Reactor

A batch reactor is a closed system with no inflow or outflow ($F_{A0} = F_A = 0$). It is heavily used in fine chemicals, pharmaceuticals, and homogeneous catalytic systems where long reaction times are required.

3.1 Design Equation

Assuming the reactor is perfectly mixed (spatially uniform temperature and concentration), the mole balance simplifies to:

$$dN_A / dt = r_A V$$

Expressed in terms of conversion (X_A):

$$N_{A0}\,(dX_A/dt) = -r_A V \;\Rightarrow\; t = N_{A0}\int_0^{X_A} dX_A/(-r_A V)$$

For a constant volume batch reactor ($V = V_0$), this becomes:

$$t = C_{A0}\int_0^{X_A} dX_A/(-r_A)$$

4 Continuous Stirred-Tank Reactor (CSTR)

A CSTR operates at steady state ($dN_A / dt = 0$) and is perfectly mixed. The conditions (concentration, temperature) inside the reactor are uniform and perfectly match the conditions of the exit stream.

4.1 Design Equation

Because the rate $-r_A$ is uniform throughout the reactor, the integral $\int r_A\, dV$ becomes $r_A V$. The balance is:

$$F_{A0} - F_A + r_A V = 0 \;\Rightarrow\; V = (F_{A0} - F_A)/(-r_A) = (F_{A0}X_A)/(-r_A)$$

The space-time (τ), which is the average time a fluid element spends in the reactor, is $\tau = V / v_0 = (C_{A0}X_A)/(-r_A)$ (where v_0 is volumetric flow rate).

5 Plug Flow Reactor (PFR)

A PFR (tubular reactor) operates at steady state. The fluid flows in a plug-like manner with no radial gradients and no axial mixing.

5.1 Design Equation

Applying the mole balance over a differential volume element dV gives:

$$dF_A = r_A\, dV \;\Rightarrow\; dV = dF_A / r_A$$

Integrating from $V = 0$ ($X_A = 0$) to $V(X_A)$:

$$V = F_{A0}\int_0^{X_A} dX_A/(-r_A) \quad \text{and} \quad \tau = C_{A0}\int_0^{X_A} dX_A/(-r_A)$$

6 Reactor Sizing and Levenspiel Plots

To visualize the volume required for a CSTR versus a PFR, we plot $F_{A0}/(-r_A)$ against conversion X_A. This is known as a Levenspiel Plot. For normal kinetics ($n > 0$), the reaction rate decreases as conversion increases, meaning $1/(-r_A)$ increases.

Reactor Comparison: As shown in the Levenspiel plot, for reaction orders $n > 0$, the area under the curve (PFR volume) is strictly less than the area of the rectangle (CSTR volume). Therefore, to achieve the same conversion, $V_{PFR} < V_{CSTR}$.

References for Chapter 6

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Chapter 7: Non-Isothermal Reactor Design and Energy Balances

1 Introduction and Rationale

In Chapter 6, we designed ideal chemical reactors under the assumption of isothermal operation (constant temperature). However, in industrial process engineering, true isothermal conditions are rarely achieved. The vast majority of chemical reactions are either significantly exothermic (releasing heat) or endothermic (absorbing heat).

When heat is released or absorbed, the temperature of the reacting fluid changes. Because the specific rate constant, $k(T)$, is exponentially dependent on temperature (via the Arrhenius equation), even a small change in temperature can drastically alter the reaction rate, the required reactor volume, and the product distribution (selectivity).

This chapter introduces the fundamental thermodynamic principles and the Energy Balance equations required to design non-isothermal continuous and batch reactors.

2 Reaction Thermodynamics Review

Before writing energy balances, we must rigorously define the thermodynamic properties of the reacting mixture.

2.1 Heat of Reaction (ΔH_{rxn})

The heat of reaction is the enthalpy change associated with the chemical transformation. For a general reaction:

$$aA + bB \rightarrow cC + dD \qquad (1)$$

Normalized per mole of the limiting reactant A:

$$A + (b/a)B \rightarrow (c/a)C + (d/a)D \qquad (2)$$

The standard heat of reaction at a reference temperature T_R (typically 298.15 K) is calculated from the standard heats of formation ($\Delta H°_{f,i}$):

$$\Delta H°_{rxn}(T_R) = \Sigma\, \nu_i \Delta H°_{f,i}(T_R) = (c/a)\Delta H°_{f,C} + (d/a)\Delta H°_{f,D} - \Delta H°_{f,A} - (b/a)\Delta H°_{f,B} \qquad (3)$$

2.2 Temperature Dependence of ΔH_{rxn}

The heat of reaction at any temperature T is obtained using Kirchhoff's Law, which integrates the difference in heat capacities (ΔC_p) between products and reactants:

$$\Delta H_{rxn}(T) = \Delta H°_{rxn}(T_R) + \int_{T_R}^{T} \Delta C_p \, dT \qquad (4)$$

Where $\Delta C_p = (c/a)C_{p,C} + (d/a)C_{p,D} - C_{p,A} - (b/a)C_{p,B}$. If ΔC_p is approximately constant over the temperature range, this simplifies to:

$$\Delta H_{rxn}(T) = \Delta H°_{rxn}(T_R) + \Delta C_p(T - T_R) \qquad (5)$$

2.3 Temperature Dependence of the Equilibrium Constant (K_{eq})

For reversible complex reactions (covered in Chapter 2), the maximum achievable conversion is dictated by thermodynamics. The variation of the equilibrium constant with temperature is given by the Van't Hoff Equation:

$$d \ln K_{eq} / dT = \Delta H_{rxn}(T) / (RT^2) \qquad (6)$$

Integrating this equation (assuming ΔH_{rxn} is constant) yields:

$$K_{eq}(T) = K_{eq}(T_1) \exp [(-\Delta H_{rxn} / R) (1/T - 1/T_1)] \qquad (7)$$

Crucial Insight: For exothermic reactions ($\Delta H_{rxn} < 0$), K_{eq} decreases as temperature increases, thereby lowering the maximum possible conversion. For endothermic reactions ($\Delta H_{rxn} > 0$), K_{eq} increases with temperature.

3 The General Energy Balance

The first law of thermodynamics for an open flow system operating at steady state is:

$$\dot{Q} - \dot{W_s} + \Sigma F_{i0}H_{i0} - \Sigma F_iH_i = 0 \qquad (8)$$

Where:

- $\dot{Q}$: Rate of heat added to the system from the surroundings (J/s or W).
- $\dot{W_s}$: Rate of shaft work done by the system (typically negligible in chemical reactors, ≈ 0).
- F_{i0}, F_i: Molar flow rates of species i entering and leaving (mol/s).
- H_{i0}, H_i: Molar enthalpies of species i entering and leaving (J/mol).

3.1 Expressing the Balance in Terms of Conversion (X)

Using the stoichiometry $F_i = F_{A0}(\Theta_i + \nu_i X)$ where $\Theta_i = F_{i0}/F_{A0}$, we can rewrite the enthalpy terms. Assuming no phase changes and constant heat capacities, the generic energy balance simplifies to the foundational equation for reactor design:

$$\dot{Q} - F_{A0}X [\Delta H°_{rxn}(T_R) + \Delta C_p(T - T_R)] = F_{A0} \Sigma \Theta_i C_{pi}(T - T_0) \qquad (9)$$

This equation essentially states:

(Heat Added) + (Heat Generated by Reaction) = (Sensible Heat needed to raise fluid from T_0 to T)

4 Adiabatic Reactor Operation

In adiabatic operation, the reactor is perfectly insulated, meaning no heat is added or removed ($\dot{Q} = 0$).

4.1 The Adiabatic Energy Balance

Setting $\dot{Q} = 0$ in our general energy balance allows us to solve directly for the reactor temperature T as a function of conversion X:

$$T = T_0 + \{ X[-\Delta H_{rxn}(T)] \} / \{ \Sigma \Theta_i C_{pi} + X\Delta C_p \} \qquad (10)$$

If the reaction is dilute, or if $\Delta C_p \approx 0$, the term $X\Delta C_p$ can be neglected, yielding a strictly linear relationship between temperature and conversion:

$$T = T_0 + \{ [-\Delta H°_{rxn}] / [\Sigma \Theta_i C_{pi}] \} X \qquad (11)$$

4.2 Adiabatic Conversion-Temperature Profiles

> **Adiabatic Operating Lines and Equilibrium Curves Analysis:**
> For an *exothermic reaction*, the temperature increases as conversion increases (positive slope). However, the equilibrium conversion X_{eq} drops at high temperatures. The reactor can only operate up to the intersection point.
>
> For an *endothermic reaction*, the fluid cools down as it reacts (negative slope). The equilibrium conversion also drops at lower temperatures, leading to an intersection that limits conversion.

5 Non-Isothermal Continuous Stirred-Tank Reactor (CSTR)

For a CSTR with a cooling jacket (or heating coil), $\dot{Q} \neq 0$. The heat transfer rate is typically governed by Newton's law of cooling:

$$\dot{Q} = U A_H (T_a - T) \qquad (12)$$

Where U is the overall heat transfer coefficient, A_H is the heat exchange area, and T_a is the ambient coolant temperature.

5.1 Coupling the Material and Energy Balances

From the mole balance for a CSTR: $V = F_{A0}X / [-r_A(X,T)] \Rightarrow X = -r_A V / F_{A0}$. Substituting this X into the energy balance yields an equation relating heat generation and heat removal.

Heat Generation Term, G(T):

$$G(T) = (-\Delta H_{rxn}) \times (-r_A V / F_{A0}) \qquad (13)$$

Because $-r_A$ increases exponentially with T initially, G(T) follows an S-shaped (sigmoidal) curve. At high temperatures, the rate levels off because the reactant is completely consumed.

Heat Removal Term, R(T):

$$R(T) = C_{p,s}(T - T_0) + (U A_H / F_{A0})(T - T_a) \qquad (14)$$

Where $C_{p,s} = \Sigma \Theta_i C_{pi}$. The R(T) term is a strictly linear function of the reactor temperature T.

5.2 Multiple Steady States and Ignition/Extinction

A steady-state operating point occurs where the heat generated exactly equals the heat removed:

$$G(T) = R(T) \qquad (15)$$

Because G(T) is sigmoidal and R(T) is linear, they can intersect in one, two, or three distinct locations.

5.2.1 Van Heerden's Stability Criteria

For a steady state to be strictly stable, the rate of heat removal must increase faster than the rate of heat generation if a small temperature perturbation occurs:

$$dR(T)/dT > dG(T)/dT \qquad (16)$$

In cases of multiple steady states, SS1 (low conversion, cold) and SS3 (high conversion, hot) satisfy this criteria. SS2 is unconditionally unstable; a slight increase in T causes G(T) > R(T), driving the reactor to runaway to SS3 (Ignition). A slight decrease in T causes R(T) > G(T), quenching the reactor to SS1 (Extinction).

6 Non-Isothermal Plug Flow Reactor (PFR)

In a tubular reactor with heat exchange across the walls, the temperature varies continuously along the length (or volume V) of the reactor. We must solve a system of coupled Ordinary Differential Equations (ODEs).

6.1 Coupled Differential Equations

1. The Mole Balance ODE:

$$dX / dV = -r_A(X, T) / F_{A0} \qquad (17)$$

2. The Energy Balance ODE: Applying the energy balance over a differential volume dV with a heat transfer area $dA_H = a \cdot dV$ (where a is the heat exchange area per unit volume of reactor, m^2/m^3):

$$dT / dV = [\ U\ a(T_a - T) + (-r_A)(-\Delta H_{rxn})\ ] / [\ F_{A0}\ \Sigma\ \Theta_i C_{pi}\ ] \qquad (18)$$

6.2 Coolant Temperature (T_a) Profile

If the coolant is not strictly at a constant ambient temperature (e.g., it is a flowing fluid absorbing heat), we must add a third ODE for the coolant temperature:

$$dT_a / dV = U\ a(T - T_a) / (\ \dot{m_c} C_{p,c}\ ) \quad \textit{(Co-current flow)} \qquad (19)$$

$$dT_a / dV = -\ U\ a(T - T_a) / (\ \dot{m_c} C_{p,c}\ ) \quad \textit{(Counter-current flow)} \qquad (20)$$

> **The Hot Spot:** The temperature profile in a cooled PFR often exhibits a maximum known as the "Hot Spot". Initially, reactant concentration is high, making $-r_A$ large, so heat generation outpaces heat removal (dT/dV > 0). As reactants are depleted, the rate drops, and cooling dominates (dT/dV < 0). Managing the hot spot is critical to avoid catalyst deactivation or explosive runaway.

7 Optimal Temperature Progression

For reversible exothermic reactions, process engineers face a dilemma:

- High temperature favors fast kinetics (smaller reactor volume).
- Low temperature favors high equilibrium conversion (better thermodynamics).

To minimize the required reactor volume, the system should operate at the Maximum Rate Locus. The optimum temperature T_{opt} at any given conversion X is found by setting the derivative of the reaction rate with respect to temperature to zero:

$$\partial(-r_A) / \partial T = 0 \qquad (21)$$

For a simple elementary reversible reaction $A \rightleftharpoons B$, T_{opt} can be explicitly derived as:

$$T_{opt} = \Delta H_{rxn} / \{\ R\ ln\ [\ (E_1 / E_{-1}) \cdot (k_{-1}(T_\infty) / k_1(T_\infty)) \cdot (X / (1-X))\ ]\ \} \qquad (22)$$

Where E_1 and E_{-1} are the activation energies of the forward and reverse reactions. In practice, to follow this optimal temperature trajectory, an industrial sequence often employs a series of adiabatic fixed-bed reactors with interstage cooling.

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GENERAL CONCLUSION

Throughout this pedagogical handout, we have systematically explored the core principles of **Chemical Kinetics and Homogeneous Catalysis**. These two interconnected fields form the very backbone of process engineering, providing the essential tools needed to understand, control, and optimize chemical transformations.

We began our journey by establishing the macroscopic foundations of chemical kinetics. By defining reaction rates, understanding experimental measurement techniques, and exploring complex reaction networks (reversible, parallel, and consecutive), we acquired the mathematical framework required to quantify how fast chemical processes occur over time.

Moving beyond mere macroscopic observations, we delved into the microscopic realm. Through the lens of Collision Theory and Transition State Theory, we gained profound insights into the temperature dependence of reactions and the energetic barriers molecules must overcome. Furthermore, analyzing reaction mechanisms using approximations such as the Steady-State Approximation (Bodenstein principle) allowed us to bridge the gap between elementary molecular steps and the overall observed macroscopic kinetics.

The final chapters of this document successfully transitioned from theoretical kinetics to powerful industrial applications through the study of **Catalysis**. We highlighted how homogeneous catalysts—whether they are simple acid-base ions, complex biological enzymes, or sophisticated organometallic transition metal complexes—can provide alternative reaction pathways with lower activation energies. This not only accelerates reactions but also grants engineers unprecedented control over product selectivity.

> *For a process engineer, mastering chemical kinetics and catalysis is not merely an academic exercise. It is the absolute prerequisite for designing efficient chemical*

> *reactors, scaling up industrial processes, maximizing economic yields, minimizing environmental waste, and ensuring the inherent safety of chemical plants.*

It is my sincere hope that this handout has demystified the complexities of kinetics and catalysis, equipping you with both the theoretical knowledge and the analytical problem-solving skills necessary for your future professional endeavors. As you advance in your careers as process engineers, the principles detailed in these pages will serve as a reliable reference and a solid foundation for continuous innovation in the chemical and energy industries.