

International Journal of Research Publication and Reviews

Journal homepage: www.ijrpr.com ISSN 2582-7421

Comprehensive Analysis of Reaction Kinetics: Mechanisms, Order, and Rate-Controlling Parameters

Anju Yadav¹, Mukta Rajotia^{2*}

Department of Education, Navyug Kanya Mahavidyalaya, Lucknow, U.P., 226004, India Department of Chemistry, Banasthali Vidyapith, Niwai, Rajasthan, 304022, India^{2*} Corresponding author Email: muktarajotia98@gmail.com

ABSTRACT:

The reaction kinetics is central to understanding chemical processes, as it governs how fast a reaction proceeds and the factors influencing it. This review provides an in-depth analysis of reaction kinetics, focusing on rate laws, reaction order, mechanisms, and factors that determine the rate-controlling step. Various reaction orders such as zero, first, second, third, and pseudo-first order are examined in the context of their kinetic behavior and relevance in real world systems. Detailed discussion is also presented on reaction mechanisms, including notable case studies such as soot formation, enzyme catalysis, and hydrocarbon combustion. Advanced analytical tools like steady-state approximation, Lindemann-Hinshelwood theory, and reaction progress kinetic analysis are also included. Furthermore, the effects of temperature, activation energy, pressure, and concentration on reaction rates are critically evaluated. This comprehensive analysis provides valuable insights for understanding and modelling complex chemical reactions in both academic and industrial contexts.

Keywords; Chemical kinetics, Reaction rate, Reaction order, Mechanism, Parameters

Introduction

The principle of chemical affinity, which emerged during the seventeenth century, evolved from the earlier alchemical concept of the "chemical wedding" a belief that similar substances have a natural tendency to combine, allowing for classification based on their interactions. By the late 17th and throughout the 18th century, this idea transitioned from a purely taxonomic perspective to a foundational concept for understanding chemical reactivity. Initially based on the assumption that substances interact due to inherent similarities, this early interpretation of chemical attraction was simplistic and reflected the nascent stage of chemical science. However, by the end of the 17th century, this intuitive idea was formalized into a qualitative framework that sought to explain and organize interactions between different substances. During this period, retrosynthetic analysis and pattern recognition became important tools for understanding the behavior of chemical reactions. The repetition of reactions and systematic experimentation played a significant role in the study of chemical constituents, marking the emergence of a more methodical and empirical approach to chemistry.

Wilhelm Homberg (1652–1715) is considered one of the earliest researchers to introduce a dynamic interpretation of chemical phenomena. He was among the first to propose a quantitative approach to chemical activity, suggesting that the strength of an acid could be assessed based on the sequence and timing of its neutralization reactions with various alkalis. This marked an important step toward measuring chemical reactivity in a systematic and time-dependent manner [1]. For a chemical reaction to occur under typical conditions, it must be both thermodynamically and kinetically favorable. These are relative criteria: the reaction should be thermodynamically favorable enough to produce a significant amount of the desired product, and kinetically favorable enough to proceed within a practical timeframe. The thermodynamic control of a reaction is governed by factors such as enthalpy, entropy, and temperature. In contrast, the kinetic control depends on the reaction pathway, its mechanism and the energy barrier that must be overcome (activation energy), the concentration of reactants, and again the temperature.

Speed of Reaction

The speed of a chemical reaction refers to the rate at which the concentration of reactants or products changes over a given period. While the rapidity of a reaction can often be observed qualitatively, its quantitative expression is determined by measuring the change in concentration over time. In precise terms, the rate of a chemical reaction is defined as the change in the concentration of a specific component divided by the time interval during which the change is observed [3].

Rate =
$$\frac{\Delta \text{ Concentration}}{\Delta \text{ time}}$$
 (1)

For a reaction of type as A+B→C, rate can be stated in form of modification in absorption of any of its mechanisms

$$Rate = -\frac{\Delta[A]}{\Delta t} \tag{2}$$

$$Rate = -\frac{\Delta[B]}{\Delta t} \tag{3}$$

$$Rate = -\frac{\Delta[C]}{\Delta t} \tag{4}$$

Where, $\Delta[A]$ =Difference amongst absorption of component A through time interval $t_2 - t_1$:

$$\Delta [A] = [A_2 - A_1]$$

Rate Law

A rate law is an expression that relates the rate of a reaction to the rate constant and the concentrations of the reactants. A rate constant i.e. k is a proportionality continual aimed at a prearranged reaction as shown;

$$v = k [A]a[B]b[C]c...$$
 (5)

The reaction rate is proportional to the concentrations of the reactants, each raised to a certain power. The proportionality constant is known as the rate constant (k). The exponent of a particular reactant represents the order of the reaction with respect to that reactant, which may be fractional rather than a whole number. The sum of these exponents is called the overall order of the reaction. Even though many reactions proceed through several elementary steps, their experimentally determined rate laws often follow this general form, and the reaction orders do not necessarily correspond to the stoichiometric coefficients in the balanced chemical equation [2].

Order of reaction

The reaction rate for a given process is an important tool that allows us to determine the specific order of a reaction. Knowing the reaction order is essential, as it helps classify chemical reactions quickly and efficiently. It also provides insights into various aspects of the reaction, such as the rate law, the units of the rate constant, the half-life, and more. The order of a reaction can be determined from the rate law by adding the exponents of the reactant concentrations. It is important to note that, although the reaction order is obtained from the rate law, it does not necessarily correspond to the stoichiometric coefficients in the balanced chemical equation [3].

$$Rate = k[A]^s[B]^t \tag{6}$$

Reaction Order =
$$s + t$$
 (7)

First Order Speed of Reaction

If a reaction speeding on a solitary reactant and value of exponent is 1, reaction is supposed to be first order. Rate ν of a first-order reaction $A \to P$ can be stated as:

$$v = \frac{dp}{dt} = -\frac{da'}{dt} = k \ a = k \ (a_0 - p)$$
 (8)

in which a and p both are absorptions of A and P correspondingly at any period t, k is a first-order rate constant and a_0 is a constant.

The first two equality signs in the rate expression represent alternative ways of defining the reaction rate: since each molecule of A consumed corresponds to the formation of one molecule of P, it makes no mathematical difference whether the rate is expressed in terms of the appearance of the product or the disappearance of the reactant. The third equality indicates that the reaction is first-order, as it shows that the rate is directly proportional to the concentration of reactant A [3].

Second Order Speed of Reaction

A reaction is supposed to be second order as soon as complete order is 2. Speed of a second-order reaction might be proportionate to one absorption squared i.e., $r = K [A]^2$ or to invention of two absorptions r = K [A] [B].

A common type of bimolecular reaction involves a system of the form $A+B\to P+Q$, where two different species, A and B, interact to form products. In such a case, the rate of the reaction generally depends on the concentrations of both reactants. Therefore, the rate law is expected to follow a *second-order expression*, with the rate being directly proportional to the concentration of A raised to the first power and the concentration of B raised to the first power. This means that doubling the concentration of either reactant, while keeping the other constant, will double the reaction rate, whereas doubling both simultaneously will increase the rate by a factor of four. Such reactions provide a clear illustration of how bimolecular processes typically exhibit second-order kinetics.

$$v = \frac{dp}{dt} = kab = k(a_0-p)(b_0-p)$$
in which k is a second-order rate constant [3].

Pseudo-first Order Speed of Reaction

When the concentration of one reactant remains effectively constant during a reaction, it can be incorporated into the rate constant, leading to a simplified expression known as a pseudo-first-order (or sometimes pseudo-second-order) rate equation. For example, in a typical second-order reaction with the rate law r = k[A][B], if the concentration of reactant B is held constant, the equation becomes r=k[A][B]=k'[A], where the pseudo-first-order

rate constant is defined as k'=k[B]. This transforms the second-order rate law into a pseudo-first-order form, making the derivation of the integrated rate equation significantly easier. A classic example is the acid-catalyzed hydrolysis of sucrose. Although the actual rate law is third-order, $r=k[sucrose][H^+][H_2O]$, the concentrations of both the catalyst H^+ and the solvent H_2O remain essentially constant throughout the process. As a result, the reaction is experimentally observed to follow pseudo-first-order kinetics, and its rate is expressed as r=k[sucrose] [4].

Third Order Speed of Reaction

A tri-molecular reaction such as $A + B + C \rightarrow P + ...$ rarely occurs in a single elementary step involving the simultaneous collision of three molecules, as the probability of such an event is extremely low. Instead, these reactions generally proceed through a sequence of two or more elementary steps. For example, the mechanism may involve $A + B \leftrightarrow X$, followed by $X + C \rightarrow P$. In such cases, the overall kinetics of the reaction is determined by the slowest step in the pathway, which is known as the *rate-limiting step*. A well-known example of a tri-molecular process is the atmospheric reaction leading to the formation of NO_3 :

 $NO+O_2+M \rightarrow NO_3+M$

Here, M represents a third body (often N_2 or O_2 in the atmosphere) that absorbs excess energy and stabilizes the NO_3 molecule. Although written as a three-body reaction, it does not occur through a single collision of NO, O_2 , and M. Instead, it proceeds via a stepwise mechanism where the third body plays a critical role in dissipating energy [3].

Zero Order Speed of Reaction

Some reactions exhibit zero-order kinetics, where the reaction rate remains constant and is independent of the concentration of the reactant. If a reaction is zero-order with respect to a single reactant, it often indicates that this reactant participates only after the rate-limiting step. In certain cases, reactions are overall zero-order, meaning the rate is unaffected by the concentrations of any reactants. Such behavior is commonly observed in catalyzed reactions, particularly when reactants are present in large excess so that the catalytic sites are fully saturated. Enzyme-catalyzed reactions frequently display zero-order kinetics at very high substrate concentrations [1]. In zero-order processes, altering the concentration of a reactant has no effect on the reaction rate. This occurs when there is a limiting factor such as the finite number of enzyme active sites or catalytic surface sites-that restricts the number of reactant molecules that can react at a given time.

Reaction Mechanism of Some Compounds

Soot Formation in Flames

The formation of polycyclic aromatic hydrocarbons (PAHs) and soot has become a major focus of research in the fields of hydrocarbon combustion and pyrolysis. Interest in this topic primarily arises from environmental concerns related to pollutant emissions generated during combustion processes. Research efforts experimental, theoretical, and computational have sought to understand the physics and chemistry of soot formation. This process generally involves four key stages: homogeneous nucleation of soot particles, particle growth, surface reactions, and particle agglomeration [5-11]. Several mechanisms have been proposed to explain the initiation of soot particles. These include pathways involving polyacetylenes [12], ionic species [7], and PAHs [6] as major gaseous precursors of soot. Among these, the prevailing view, supported by extensive experimental and modeling studies, is that soot particles primarily form through the aggregation of PAHs. The PAH-based hypothesis also incorporates the role of aromatic aliphatic linked hydrocarbons, which subsequently undergo structural transformations and graphitization during particle maturation [13, 14].

Alkaline Phosphate

Alkaline phosphatase (AP) is a widely distributed, non-specific phosphomonoesterase that functions through the formation of a covalent phosphoseryl intermediate. The enzyme also catalyses phosphoryl transfer reactions to various alcohols. *Escherichia coli* alkaline phosphatase is a homodimer, with each monomer consisting of 449 amino acid residues. It is a metalloenzyme, containing two Zn²⁺ ions and one Mg²⁺ ion at each active site. The crystal structure of the native *Escherichia coli* AP in complex with inorganic phosphate (Pi) which acts both as a strong competitive inhibitor and as a substrate for the reverse reaction has been resolved at 2.0 Å resolutions.

In *Escherichia coli*, alkaline phosphatase plays a key role in acquiring phosphate from esters when free inorganic phosphate is limited. The *Escherichia coli* enzyme has been extensively studied using a wide range of physicochemical techniques, including NMR and ESR analyses, on both the native and modified forms, making it a valuable model system. The enzyme is a dimer, with each of the two chemically identical subunits containing 449 amino acid residues. It is located in the periplasmic space and lacks both carbohydrate and fatty acid terminal groups [15].

Combustion of n-alkane to n-hexadecane from n-octane

The composition of hydrocarbon oils has a significant impact on their explosion characteristics and other combustion properties. Experimental studies have established correlations between molecular size, structural features, and detonation behavior of various hydrocarbons [16]. More recently, investigations have emphasized the importance of intrinsic kinetic properties of these hydrocarbons in determining detonation velocities [17–19]. Standard octane and cetane scales are defined using reference fuels, which provide practical benchmarks for measuring detonation tendencies. For both scales, one reference fuel is highly prone to ignition, while the other is resistant. On the octane scale, n-heptane represents a value of zero because it

ignites readily in spark-ignition engines. On the cetane scale, n-hexadecane (cetane) defines a value of 100, as it ignites easily in diesel engines. Thus, in both cases, the reference fuel that undergoes ignition most readily is an n-alkane.

An early detailed kinetic mechanism for n-hexadecane was developed by Chevalier et al. [20], incorporating both high- and low-temperature reaction pathways and applied to simulate engine combustion phenomena. This mechanism included approximately 1200 chemical species and 7000 elementary reactions, with rate parameters quantified for multiple reaction classes. Nehse et al. [21] later constructed detailed kinetic models for n-decane and nheptane to simulate intermediate-temperature shock tube experiments for both fuels. More recently, a study [22] demonstrated the capability to generate comprehensive kinetic mechanisms for alkanes of varying chain lengths, validated using experimental data for n-hexadecane. Cathonnet, Dagaut and co-workers have advanced a huge assortment of kinetic mechanisms as well as those aimed at n-decane and n hexadecane [23-25]. Dagaut et al. took ndecane by means of a proxy for kinetics of lamp oil for aircraft machine recreations. Newly, their exertion [24, 25] has intensive on via n-decane organized through additional proxy complexes, specifically cyclo-alkanes and aromatics to restored signify coal construction and emanations belongings of lamp oil. Dagaut et al. [26, 27] freshly prolonged this identical method to custom a kinetic mechanism aimed at n-hexadecane to pretend corrosion of rapeseed emollient methyl ester, a protruding biodiesel oil. Olchanski and Burcat [28] established a condensed high temperature kinetic mechanism aimed at n-decane to study replicated shudder movement explosion interruption researches. Bikas and Peters[29] industrialized a complete temperature assortment, slightly condensed kinetic mechanism to transport n-decane ignition reproductions in laminar combustions, aircraft stimulated containers and shudder cylinders. Zeppieri et al.[30] industrialized a emaciated kinetic mechanism aimed at higher and midway temperature n-decane corrosion that practices fractional steadiness amongst alkyl radicals [31] and has capability to transport very resourceful recreations underneath proper situations, but it does not consist of lower temperature reaction pathways. Current kinetic displaying of pyrolysis in n-dodecane through Herbinet et al. [32] and Dahm et al. [33] have used ex-gas method to afford kinetic mechanisms to research pyrolysis of n-dodecane. Lindstedt and Maurice [34, 35] industrialized n-heptane and n-decane rejoinder mechanisms and pragmatic them to ignition of aircraft oils.

Steady State Approximation

In chemistry, a *steady state* refers to a condition in which all state variables remain constant despite on-going processes that continuously act to change them. For a system to be in steady state there must be a continuous flow through the system. A simple example is a bathtub with the tap running and the drain left open: after some time, the rate of water entering and leaving becomes equal, the water level remains constant, and the system reaches a steady state

Lindermann / Lindmann-Hinshelhood Theory

Many gas-phase reactions display first-order kinetics and seem to involve only a single reactant molecule. Classic examples include the isomerization of cyclopropane to propene and the decomposition of azomethane ($CH_3N_2CH_3 \rightarrow C_2H_6 + N_2$), which experimentally follows the rate law $v = k[CH_3N_2CH_3]$. For a long time, it was unclear how such molecules obtained the necessary energy to undergo reaction, especially since the observed kinetics appeared inconsistent with a simple bimolecular mechanism. This puzzle was resolved by Lindemann in 1922, who proposed a mechanism for so-called thermal unimolecular reactions. According to this model, the process actually begins with a bimolecular collision in which a reactant molecule A is energized by a collision with a partner molecule M (which may be another reactant or an inert gas molecule):

$$A+M \rightarrow A^*+M$$

Here, A* represents the energized molecule. The activated species A* can then undergo unimolecular decomposition:

 $A^* \rightarrow Products$

Alternatively, the energized molecule may be deactivated through another collision:

$$A^{*+}M \rightarrow A^{+}M$$

Animated reactant A^* formerly suffers unimolecular reaction to produce product P. To regulate complete rate law rising as of this mechanism, we can put on SSA to excited state A^* .

$$\frac{d[A^*]}{dt} = 0 = k1[A][M] - k_{-1}[A^*][M] - k_2[A^*]$$
(10)

Reorganizing this appearance produces absorption $[A^*]$.

$$[A^*] = \frac{k_1[A][M]}{k_{-1}[M] + k_2}$$

Complete speed of reaction is;

$$v = \frac{d[P]}{dt} = k_2[A^*] = \frac{k_1 k_2[A][M]}{k_{-1}[M] + k_2}$$

Thus, while the reaction appears unimolecular at high pressures (where activation is frequent), its mechanism actually involves both bimolecular energy transfer and unimolecular decomposition steps. This model explained why unimolecular reactions show first-order behavior under certain conditions but can exhibit pressure dependence consistent with bimolecular processes [2].

Higher pressure

At higher pressures, frequent collisions occur, making collisional de-excitation of A* more likely than its unimolecular conversion to products. In this case, $k_1[A^*][M] >> k_2[A^*]$. Therefore, the k_2 term in the denominator can be neglected, and the rate law simplifies to:

$$v = \frac{k_1 k_2}{k_{-1}} [A] \tag{11}$$

This expression corresponds to first-order kinetics, with an effective rate constant as;

$$k_{uni} = \frac{k_1 k_2}{k_{-1}}$$

(12)

Hence, the mechanism accounts for the experimentally observed first-order kinetics at moderate to high pressures, where the unimolecular step becomes rate-determining.

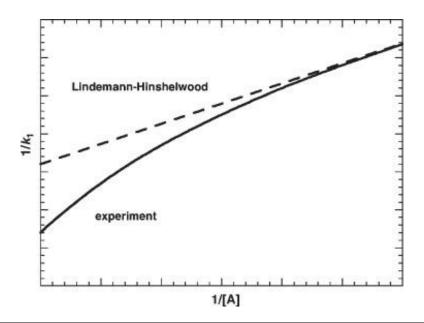
Lower pressure

At low pressures, collisions are infrequent, so the excited species A^* is more likely to undergo unimolecular reaction before collisional de-excitation. In this case, $k_2 >> k_{-1}[A^*][M]$. Thus the $k_{-1}[M]$ term in the denominator of Equation (12) can be neglected, and the rate law reduces to:

$$v = k_1[\mathbf{A}][\mathbf{M}] \tag{12}$$

At low pressures, the kinetics follows second-order behavior. This is because the formation of the excited intermediate A^* , a bimolecular process, becomes the rate-determining step. An example of such plots is shown below. Generally, good agreement is observed between theory and experiment at low pressures. However, at higher pressures, deviations appear, with experimental values of k being larger than those predicted by the Lindemann-Hinshelwood mechanism.

A plot of 1/k in contrast to $\frac{1}{[M]}$ would yield a straight line with an intercept of $\frac{k_{-1}}{k_1k_2}$ and a gradient of $1/k_1$. An example of such plots is shown below. Generally, good agreement is observed between theory and experiment at low pressures. However, at higher pressures, deviations appear, with experimental values of k being larger than those predicted by the Lindemann-Hinshelwood mechanism [2].



Reaction Progress Kinetics Analysis

In chemistry, reaction progress kinetic analysis (RPKA) is a specialized branch of kinetic methods used to determine the rate laws of chemical reactions and to aid in understanding their mechanisms. Although the basic concept behind RPKA is not new, the approach was formalized by Professor Donna Blackmond in the late 1990s and has since gained widespread application because reaction mechanisms can vary depending on the relative and absolute concentrations of the reacting species, this method provides results that more accurately reflect reaction behavior under commonly applied experimental conditions compared to traditional kinetic approaches.

1,3-Disiloxanediols as Hydrogen-Bonding Catalysts

Recent advancements in the understanding of hydrogen-bonding and anion-binding organocatalysts, particularly those based on thiourea derivatives (Figure 1), have revealed that the formation of higher-order supramolecular species can exert a pronounced influence on the kinetic profile, efficiency, and stereochemical outcome of catalytic reactions [36–38]. The dynamic interplay between individual catalyst molecules may result in either synergistic cooperative effects, wherein multiple catalytic units function in concert to enhance substrate activation and reaction turnover [39], or in contrast, non-productive aggregation phenomena, where catalyst self-association diminishes the availability of active sites, thereby reducing overall

catalytic efficiency and selectivity [40, 41].

Fig.1. Constructions of hydrogen-bonding catalytic agent estimated in this research [36].

1,3-Disiloxanediols, which feature a siloxane-linked 1,3-arrangement of two silanol groups, offer potential advantages in catalysis compared with conventional silanediols and other organocatalysts, owing to their enhanced solubility, acidity, and structural stability [42]. Previous investigations on 1,3-disiloxanediols have explored their anion-binding properties [43], supramolecular assembly behavior [44], and applications as organometallic ligands [45]. In the context of catalysis, these compounds are capable of engaging in multiple modes of intermolecular hydrogen bonding, which can lead either to cooperative catalytic activation or to unproductive catalyst aggregation [46]. In the solid state, 1,3-disiloxanediols are known to self-assemble into higher-order architectures through intermolecular hydrogen bonding [47], while in solution, 'H NMR diffusion-ordered spectroscopy (DOSY) studies have demonstrated their propensity for self-association at elevated concentrations. Building on recent findings, we have reported the use of 1,3-disiloxanediols as anion-binding catalysts [48] and have undertaken a detailed mechanistic investigation to elucidate their behavior as hydrogen-bonding organocatalysts.

Reaction calorimetry

Reaction calorimetry can be employed to monitor the progress of a chemical reaction, since the instantaneous heat flow generated is directly correlated with the *enthalpy change* of the process. This technique may be regarded as a *differential method*, as the primary data collected represent reaction rate as a function of time. From these data, the temporal evolution of substrate or product concentrations can be obtained by applying a simple integration of a polynomial function fitted to the experimental curve [49]. Although reaction calorimetry is not as widely utilized as several other kinetic methodologies, it has proven to be a powerful tool for catalyst evaluation. Moreover, it has been successfully applied in the mechanistic study of individual transformations, including the prolinate-catalysed α-amination of aldehydes [50] and, perhaps most notably, the palladium-catalysed Buchwald-Hartwig amination reaction [51].

In situ UV-Vis

In situ UV-visible absorbance spectroscopy can serve as a valuable technique for monitoring the real-time progress of chemical reactions, provided that either the reactant or the product exhibits a distinct absorbance feature within the UV-visible spectral region. By tracking changes in absorbance as a function of time, it is possible to determine the rate of substrate consumption and/or product formation, ultimately converting these spectral variations into quantitative kinetic information. This makes UV-Vis monitoring a type of indirect concentration-based method for evaluating reaction progress. Owing to the specific spectral window employed, UV-Vis methodologies are most frequently applied in the study of inorganic and organometallic systems, where metal-centered electronic transitions or charge-transfer bands are prominent. In contrast, their application in purely organic transformations is relatively limited, since many organic molecules either lack strong chromophores in the accessible range or display overlapping absorption features, complicating data interpretation. Nevertheless, when applicable, UV-Vis spectroscopy provides a non-invasive, rapid, and continuous monitoring tool that can yield valuable insights into both reaction kinetics and mechanistic pathways.

Rate Controlling Step

Activation Energy and Temperature

It is a well-established principle in chemical kinetics that reaction rates increase with rising temperature. When the concentrations of the reacting species are held constant, virtually all reactions proceed more rapidly as the temperature is elevated. This effect arises because an increase in temperature leads to a higher average kinetic energy of the reactant molecules. As a result, a larger fraction of molecules in the system acquire energies that are equal to or greater than the activation energy threshold necessary for a successful collision to occur. Consequently, the frequency of effective collisions those that can overcome the energy barrier and lead to product formation significantly increases. This phenomenon is commonly described using the Maxwell-Boltzmann distribution, which illustrates the spread of molecular kinetic energies within a population. As the temperature rises, this distribution shifts, broadens, and allows a greater proportion of molecules to possess sufficient energy to participate in the reaction, thereby accelerating the overall rate [52].

Concentration

Reaction speed rises through concentration as designated through rate law and explicated via collision concept. As reactant concentration rises, incidence of collision rises. Increasing concentration of one or more reactants will frequently increase rate of reaction. This arises due to a higher concentration of a reactant will chief to extra collisions of that reactant in a definite time period [53]. According to collision theory, rate of a reaction is directly proportional to number of effective collisions per second amongst reactant molecules. If concentration of reactants increases greater number of total collisions. Greater regularity of total collisions, greater regularity of effective collisions. If regularity of effective collisions increases, so does reaction rate [54].

Pressure

The rate of gaseous reactions increases with rising pressure, as higher pressure corresponds to an increase in the concentration of gas molecules. In accordance with Le Chatelier's principle, the reaction rate is enhanced in the direction that results in a decrease in the total number of gas moles, while it tends to slow down in the reverse direction. For reactions occurring in the condensed phase (liquids or solids), the influence of pressure is comparatively weak. In the case of gases, however, elevating the pressure increases the frequency of intermolecular collisions, thereby enhancing the likelihood of productive encounters between reactants and thus accelerating the overall reaction rate. As expected, this pressure effect plays a critical role in gas-phase reactions, but exerts only a minor influence on reactions involving liquids and solids, where molecular densities are already relatively high [55].

Conclusion

In summary, the course of a chemical reaction is dictated by the interplay of thermodynamics and kinetics. For a transformation to be practically useful, it must not only be thermodynamically favorable, ensuring sufficient product formation, but also kinetically accessible, proceeding within a reasonable timeframe. Reaction rates are strongly influenced by factors such as temperature, activation energy, and catalysis. An increase in temperature enhances the average kinetic energy of molecules, thereby raising the probability of successful collisions, a relationship quantitatively described by the Arrhenius equation. Catalysts, on the other hand, accelerate reactions by providing alternative pathways with lower activation barriers. Furthermore, the reaction order and rate laws highlight the dependence of reaction speed on reactant concentration or, in the case of gaseous systems, on pressure, both of which directly affect collision frequency. Collectively, these principles emphasize that a comprehensive understanding of both thermodynamic driving forces and kinetic parameters is essential for controlling and optimizing chemical reactivity.

Acknowledgement

Authors thank Banasthali Vidyapith for providing the necessary facilities.

Conflict of interest

"No conflict of interest".

Declarations

Ethical approval: Not applicable

Competing Interests: No known competing financial interest or personal relationships that could have appeared to influence the work reported in this paper.

Author's contributions: Mukta Rajotia: Formal analysis, Writing-Original drafting, Anju Yadav: Review & Editing.

The author declares no conflict of interest.

Funding: Not applicable.

Availability of data and materials: Not applicable.

REFERENCES:

- [1] V. patel, chemical kinetics, intech, Janeza Trdine 9, 51000 Rijeka, Croatia, (2012).
- [2] C. Vallance, Reaction Kinetics, 2017.
- [3] A. Cornish-Bowden, A. Cornish-Bowden, Fundamentals of enzyme kinetics, Wiley-Blackwell Weinheim, Germany2012.

- [4] J.H. Espenson, Chemical kinetics and reaction mechanisms, Citeseer1995.
- [5] R.L. Vander Wal, A.J. Tomasek, Soot oxidation: dependence upon initial nanostructure, Combustion and Flame, 134 (2003) 1-9.
- [6] B.S. Haynes, H.G. Wagner, Soot formation, Progress in Energy and Combustion Science, 7 (1981) 229-273.
- [7] H.F. Calcote, Mechanisms of soot nucleation in flames—A critical review, Combustion and Flame, 42 (1981) 215-242.
- [8] K.H. Homann, Formation of large molecules, particulates and ions in premixed hydrocarbon flames; Progress and unresolved questions, Symposium (International) on Combustion, 20 (1985) 857-870.
- [9] I. Glassman, Soot formation in combustion processes, Symposium (International) on Combustion, 22 (1989) 295-311.
- [10] M. Frenklach, H. Wang, Detailed Mechanism and Modeling of Soot Particle Formation, in: H. Bockhorn (Ed.) Soot Formation in Combustion: Mechanisms and Models, Springer Berlin Heidelberg, Berlin, Heidelberg, 1994, pp. 165-192.
- [11] H. Richter, J.B. Howard, Formation of polycyclic aromatic hydrocarbons and their growth to soot—a review of chemical reaction pathways, Progress in Energy and Combustion Science, 26 (2000) 565-608.
- [12] K.H. Homann, H.G. Wagner, Some new aspects of the mechanism of carbon formation in premixed flames, Symposium (International) on Combustion, 11 (1967) 371-379.
- [13] H. Bockhorn, Soot formation in combustion: mechanisms and models, Springer Science & Business Media2013.
- [14] R.A. Dobbins, H. Subramaniasivam, Soot Precursor Particles in Flames, in: H. Bockhorn (Ed.) Soot Formation in Combustion: Mechanisms and Models, Springer Berlin Heidelberg, Berlin, Heidelberg, 1994, pp. 290-301.
- [15] E.E. Kim, H.W. Wyckoff, Reaction mechanism of alkaline phosphatase based on crystal structures: Two-metal ion catalysis, Journal of Molecular Biology, 218 (1991) 449-464.
- [16] W.G. Lovell, Knocking Characteristics of Hydrocarbons, Industrial & Engineering Chemistry, 40 (1948) 2388-2438.
- [17] H.J. Curran, P. Gaffuri, W.J. Pitz, C.K. Westbrook, W.R. Leppard, Autoignition chemistry in a motored engine: An experimental and kinetic modeling study, Symposium (International) on Combustion, 26 (1996) 2669-2677.
- [18] C.K. Westbrook, W.J. Pitz, J.E. Boercker, H.J. Curran, J.F. Griffiths, C. Mohamed, M. Ribaucour, Detailed chemical kinetic reaction mechanisms for autoignition of isomers of heptane under rapid compression, Proceedings of the Combustion Institute, 29 (2002) 1311-1318.
- [19] M. Ribaucour, R. Minetti, L.R. Sochet, H.J. Curran, W.J. Pitz, C.K. Westbrook, Ignition of isomers of pentane: An experimental and kinetic modeling study, Proceedings of the Combustion Institute, 28 (2000) 1671-1678.
- [20] C. Chevalier, W.J. Pitz, J. Warnatz, C.K. Westbrook, H. Melenk, Hydrocarbon ignition: Automatic generation of reaction mechanisms and applications to modeling of engine knock, Symposium (International) on Combustion, 24 (1992) 93-101.
- [21] M. Nehse, J. Warnat, C. Chevalier, Kinetic modeling of the oxidation of large aliphatic hydrocarbons, Symposium (International) on Combustion, 26 (1996) 773-780.
- [22] Y. Muharam, J. Warnatz, Kinetic modelling of the oxidation of large aliphatic hydrocarbons using an automatic mechanism generation, Physical Chemistry Chemical Physics, 9 (2007) 4218-4229.
- [23] A. Ristori, P. Dagaut, M. Cathonnet, The oxidation of n-Hexadecane: experimental and detailed kinetic modeling, Combustion and Flame, 125 (2001) 1128-1137.
- [24] P. Dagaut, On the kinetics of hydrocarbons oxidation from natural gas to kerosene and diesel fuel, Physical Chemistry Chemical Physics, 4 (2002) 2079-2094.
- [25] P. Dagaut, A. El Bakali, A. Ristori, The combustion of kerosene: Experimental results and kinetic modelling using 1- to 3-component surrogate model fuels, Fuel, 85 (2006) 944-956.
- [26] P. Dagaut, S. Gaïl, Chemical Kinetic Study of the Effect of a Biofuel Additive on Jet-A1 Combustion, The Journal of Physical Chemistry A, 111 (2007) 3992-4000.
- [27] P. Dagaut, S. Gar"l, M. Sahasrabudhe, Rapeseed oil methyl ester oxidation over extended ranges of pressure, temperature, and equivalence ratio: Experimental and modeling kinetic study, Proceedings of the Combustion Institute, 31 (2007) 2955-2961.
- [28] O. Erna, B. Alexander, Decane oxidation in a shock tube, International Journal of Chemical Kinetics, 38 (2006) 703-713.
- [29] G. Bikas, N. Peters, Kinetic modelling of n-decane combustion and autoignition: Modeling combustion of n-decanem, Combustion and Flame, 126 (2001) 1456-1475.
- [30] S.P. Zeppieri, S.D. Klotz, F.L. Dryer, Modeling concepts for larger carbon number alkanes: A partially reduced skeletal mechanism for n-decane oxidation and pyrolysis, Proceedings of the Combustion Institute, 28 (2000) 1587-1595.
- [31] T. Held, A. Marchese, F. Dryer, A semi-empirical reaction mechanism for n-heptane oxidation and pyrolysis, Combustion Science and Technology, 123 (1997) 107-146.
- [32] O. Herbinet, P.-M. Marquaire, F. Battin-Leclerc, R. Fournet, Thermal decomposition of n-dodecane: Experiments and kinetic modeling, Journal of Analytical and Applied Pyrolysis, 78 (2007) 419-429.
- [33] K.D. Dahm, P.S. Virk, R. Bounaceur, F. Battin-Leclerc, P.M. Marquaire, R. Fournet, E. Daniau, M. Bouchez, Experimental and modelling investigation of the thermal decomposition of n-dodecane, Journal of Analytical and Applied Pyrolysis, 71 (2004) 865-881.
- [34] R. Lindstedt, L. Maurice, Detailed kinetic modelling of n-heptane combustion, Combustion Science and Technology, 107 (1995) 317-353.
- [35] R. Lindstedt, L. Maurice, Detailed chemical-kinetic model for aviation fuels, Journal of Propulsion and Power, 16 (2000) 187-195.
- [36] M.C. Gimeno, R.P. Herrera, Hydrogen Bonding Networks in Chiral Thiourea Organocatalysts: Evidence on the Importance of the Aminoindanol Moiety, Crystal Growth & Design, 16 (2016) 5091-5099.
- [37] G. Tárkányi, P. Király, S. Varga, B. Vakulya, T. Soós, Edge-to-Face CH/π Aromatic Interaction and Molecular Self-Recognition in epi-Cinchona-Based Bifunctional Thiourea Organocatalysis, Chemistry-a European Journal, 14 (2008) 6078-6086.
- [38] M.C. Etter, Z. Urbanczyk-Lipkowska, M. Zia-Ebrahimi, T.W. Panunto, Hydrogen bond-directed cocrystallization and molecular recognition properties of diarylureas, Journal of the American Chemical Society, 112 (1990) 8415-8426.

- [39] D.D. Ford, D. Lehnherr, C.R. Kennedy, E.N. Jacobsen, On-and off-cycle catalyst cooperativity in anion-binding catalysis, Journal of the American Chemical Society, 138 (2016) 7860-7863.
- [40] H.B. Jang, H.S. Rho, J.S. Oh, E.H. Nam, S.E. Park, H.Y. Bae, C.E. Song, DOSY NMR for monitoring self aggregation of bifunctional organocatalysts: increasing enantioselectivity with decreasing catalyst concentration, Organic & Biomolecular Chemistry, 8 (2010) 3918-3922.
- [41] W. Yang, D.-M. Du, Chiral squaramide-catalyzed highly diastereo- and enantioselective direct Michael addition of nitroalkanes to nitroalkenes, Chemical Communications, 47 (2011) 12706-12708.
- [42] M. Liu, N.T. Tran, A.K. Franz, J.K. Lee, Gas-Phase Acidity Studies of Dual Hydrogen-Bonding Organic Silanols and Organocatalysts, The Journal of Organic Chemistry, 76 (2011) 7186-7194.
- [43] S.-i. Kondo, A. Fukuda, T. Yamamura, R. Tanaka, M. Unno, Anion recognition by a disiloxane-1,3-diol in organic solvents, Tetrahedron Letters, 48 (2007) 7946-7949.
- [44] M. Unno, T. Matsumoto, H. Matsumoto, Synthesis of laddersiloxanes by novel stereocontrolled approach, Journal of Organometallic Chemistry, 692 (2007) 307-312.
- [45] M. Ojeda, R. Fandos, J.L.G. Fierro, A. Otero, C. Pastor, A. Rodríguez, M.J. Ruiz, P. Terreros, Synthesis and reactivity of heterometallic RhO–M (M=Si, Ti) complexes: Memory effect in their catalytic performance in CO hydrogenation, Journal of Molecular Catalysis A: Chemical, 247 (2006) 44-51
- [46] V. Chandrasekhar, R. Boomishankar, S. Nagendran, Recent Developments in the Synthesis and Structure of Organosilanols, Chemical Reviews, 104 (2004) 5847-5910.
- [47] B. O'Leary, T.R. Spalding, G. Ferguson, C. Glidewell, Oligosiloxanediols as building blocks for supramolecular chemistry: hydrogen-bonded adducts with amines form supramolecular structures in zero, one and two dimensions, Acta Crystallographica Section B: Structural Science, 56 (2000) 273-286.
- [48] D.K. M., W.S. O., F.A. K., Synthesis of Structurally Varied 1,3-Disiloxanediols and Their Activity as Anion-Binding Catalysts, Chemistry A European Journal, 22 (2016) 18349-18353.
- [49] W.K. Purves, W.K. Purves, G.H. Orians, D. Sadava, H.C. Heller, Life: The Science of Biology: Volume III: Plants and Animals, Macmillan 2003.
- [50] L. Berg, Introductory botany: plants, people, and the environment, Nelson Education 2007.
- [51] G. Sarton, E. Gilpatrick, Twelfth Critical Bibliography of the History and Philosophy of Science and of the History of Civilization (to March 1922), William Dawson and Sons Limited, 1922.
- [52] H. Eyring, The activated complex in chemical reactions, The Journal of Chemical Physics, 3 (1935) 107-115.
- [53] T. Dwars, E. Paetzold, G. Oehme, Reactions in micellar systems, Angewandte Chemie International Edition, 44 (2005) 7174-7199.
- [54] J.E. Leffler, E. Grunwald, Rates and equilibria of organic reactions: as treated by statistical, thermodynamic and extrathermodynamic methods, Courier Corporation 2013.
- [55] S. Schnell, T. Turner, Reaction kinetics in intracellular environments with macromolecular crowding: simulations and rate laws, Progress in biophysics and molecular biology, 85 (2004) 235-260.