



# How to Calculate and Determine Chemical Kinetics: Step-by-Step Interpretation of Experimental Data to Get Reaction Rate and Order

Asep Bayu Dani Nandiyanto\*, Risti Ragadhita, Meli Fiandini

Universitas Pendidikan Indonesia, Jl. Dr. Setiabudi No. 229, Bandung, Indonesia

\*Correspondence: E-mail: [nandiyanto@upi.edu](mailto:nandiyanto@upi.edu)

## ABSTRACT

Chemical kinetics is a fundamental field of study that focuses on the rates of chemical reactions and the factors influencing them. Determining the rate and order of the chemical reaction is an important aspect of understanding the reaction mechanism. This article presents a step-by-step guide to calculate and determine the rate and order of the reaction through a comprehensive analysis of experimental data. We discussed the concept of chemical kinetics, the integration of the kinetic order method, and the curve-fitting analysis technique. Several case studies are also included to provide practical applications of the theory outlined. This proposed guide aims to provide students, educators, researchers, and practitioners with a systematic approach to specify and verify prospective kinetic models, enabling them in decision-making, improving, and optimizing chemical reaction processes.

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## 1. INTRODUCTION

Chemical kinetics is a branch of science, that studies the rate of chemical reactions and the factors influencing the speed of the reactions (Jere & Mpeti, 2024; Arndt & Schomacker, 2022; Musah *et al.*, 2022; Campbell, 2017). Understanding reaction kinetics is essential in a variety of scientific disciplines, including industrial, pharmaceutical, and environmental chemistry, where reaction rate control plays a crucial role in process optimization (Zhang *et al.*, 2023; Aquilanti *et al.*, 2017; Mills *et al.*, 2007; Walker *et al.*, 2020). Reaction rate determination and kinetic model prediction do not only provide information about reaction rates but also provide insight into the underlying reaction mechanism (Motagamwala & Dumesic, 2020; Marin *et al.*, 2021). Indeed, the individual steps can make up the overall reaction (Bhandari *et al.*, 2020; Alnasif *et al.*, 2023). Therefore, kinetic studies serve as a basis for the development and improvement of chemical processes in industry and other scientific applications.

One of the main goals in kinetic studies is to determine reaction orders and rate constants, which describe the relationship between reactant concentration and reaction rate. The reaction order explains how changes in reactant concentration affect the rate, while the rate constant provides information about environmental factors influencing the rate, such as temperature, process condition, and existence of catalyst (Razdan *et al.*, 2023; Arcus & Mulholland, 2020; Faraji *et al.*, 2022; Lazaridou *et al.*, 2023; Cama *et al.*, 2002). Determination of these parameters is usually carried out through experimental observations and mathematical data analysis involving kinetic modeling. Commonly used experimental techniques include spectroscopy, titration, and chromatography to monitor changes in the concentration of reactants or products during the reaction (Marín-García *et al.*, 2022; Kukoc-Modun *et al.*, 2021; Srivastava, 2021; Tafazoli *et al.*, 2020; Blazheyevskiy *et al.*, 2022).

Various methods are used to determine reaction orders and rate constants. The initial rate method is an approach that is often used to determine the reaction order by measuring the reaction rate at different initial concentrations. Additionally, integral and differential methods are applied to analyze the concentration-versus-time dataset to verify the most appropriate kinetic models, such as zero-, first-, and second-order reactions (Taylor *et al.*, 2023, Liao *et al.*, 2024). These approaches provide flexibility in evaluating diverse kinetic mechanisms and allow in-depth interpretation of how external factors influence the reactions.

Chemical kinetics is not only theoretically useful but also has significant practical applications. In the chemical industry, a deep understanding of kinetics is essential for designing reactors and optimizing operating conditions for efficiency and safety (Westbrook *et al.*, 2021). Likewise, in the environmental field, knowledge of kinetics can be applied to understand pollutant degradation or effective waste processing (Ganiyu *et al.*, 2022; Ateia *et al.*, 2020). This article aims to explain the steps in determining the reaction order using integral and differential methods by analyzing concentration data over time to verify the most appropriate kinetic model.

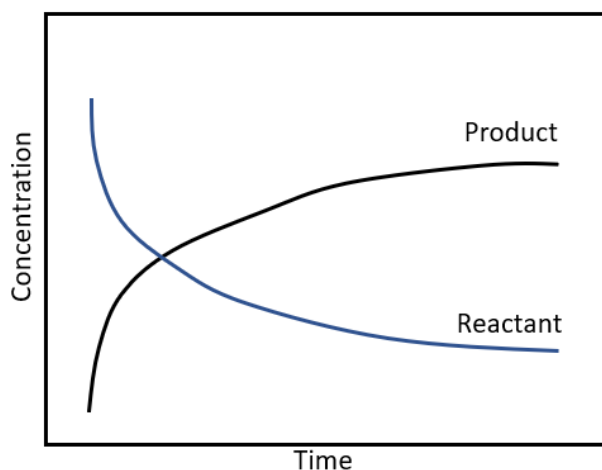
## 2. BASIC THEORY OF CHEMICAL KINETICS

### 2.1. Reaction Rate

Chemical kinetics or reaction kinetics studies the reaction rate in the chemical reaction. Analysis of the influence of various reaction conditions on the reaction rate provides information about the reaction mechanism and transition states in the chemical reaction. Chemical component changes are simply written in the reaction equation with balanced coefficients. However, the reaction equation cannot answer the main important issue

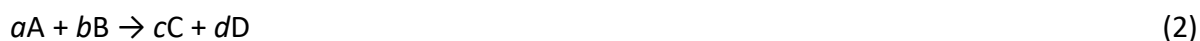
regarding how fast the reaction takes place. Chemical kinetics is the study of reaction rates and changes in the concentration (either reactants or products) as a function of time as illustrated in **Figure 1**. Reactions can take place at varying rates. Some occur immediately, require quite a long time (combustion), or take a very long time. We can find the reaction in the aging, coal formation, and some radioactive decay reactions. In general, the reaction rate is the rate of reduction of reactants per unit of processing time. Or, it can be the rate of product formation per unit of processing time. A simple explanation is shown in Eq. (1) (Dybeck *et al.*, 2017; Mavroudis *et al.*, 2019).

$$r = - \frac{\Delta [\text{reactant}]}{\Delta t} = \frac{\Delta [\text{product}]}{\Delta t} \quad (1)$$



**Figure 1.** Changes in the concentration of reactant and product concentrations per unit of processing time.

Based on Eq. (1), the  $\Delta$  sign is defined as the difference/change between the final condition and the initial condition. The negative sign in front of  $\Delta$  [reactant] indicates a decrease in the concentration of the reactant over time. In contrast, the positive sign in front of  $\Delta$  [product] indicates an increase in the concentration of the product over time. Here, square brackets, [ ], are used to express concentration. The expression of the reaction rate is based on the rate equation, depending on the concentration of reactants and products in the chemical reaction, as well as the stoichiometric coefficients of the reaction (see Eq. (2)):



where  $a$ ,  $b$ ,  $c$ , and  $d$ , are the stoichiometric coefficients of the reactants and products. A, B, C, and D are the chemical species involved in the reaction. The expression for the reaction rate ( $r$ ) from Eq. (2) can be written as in Eq. (3):

$$r = - \frac{1}{a} \frac{\Delta [A]}{\Delta t} = - \frac{1}{b} \frac{\Delta [B]}{\Delta t} = + \frac{1}{c} \frac{\Delta [C]}{\Delta t} = + \frac{1}{d} \frac{\Delta [D]}{\Delta t} \quad (3)$$

## 2.2. Factors Influencing the Reaction Rate

Chemical reactions may or may not take place and cannot be explained using collision theory only. Collisions between reactant/product components produce a reaction if they have sufficient energy and are in the right direction of collision (effective collision). Several factors are involved in getting excellent collisions to make a reaction:

- (i) Surface area. The surface area gives more possible contact between reactants to make reactions. Indeed, surface area can be obtained by the change in component size and

porosity. In short, reactants in liquid or powder form produce a faster reaction rate than those in flake form in the same concentration (Hu & Xia, 2016; Leng *et al.*, 2021; Qu *et al.*, 2021).

- (ii) Concentration. In most cases, if the reactant concentration increases, it creates more numbers of collisions, allowing a faster reaction rate (Li *et al.*, 2012).
- (iii) Temperature. In most cases, temperature accelerates the reaction rate. Increases in temperature cause the reactant components to move faster in the reactor, resulting in more opportunities for effective collisions. Many reactions proceed twice faster for every 10°C increase in temperature (Wei *et al.*, 2020).
- (iv) Catalyst and Inhibitor. Catalyst and inhibitor are involved in the collision process between reactants, but at the end of the reaction, they will be found again (exist in the final condition after the reaction is finished). In short, during the reaction, the catalyst can speed up the reaction rate, while the inhibitor can slow down the reaction rate. They play in creating an alternative (different) reaction mechanism, changing activation energy ( $E_a$ ) (Lin *et al.*, 2018).

### 2.3. Rate Law and Reaction Order

In chemical kinetics, the reaction order of a substance (such as reactants, catalysts, or products) is the number of concentration factors that influence the speed of the reaction. The reaction rate is shown in Eq. (4).

$$r = k [A]^m [B]^n \quad (4)$$

where  $m$  and  $n$  are the reaction orders of the reactants  $A$  and  $B$ .

In reaction kinetics, the reaction order is often not the same as the stoichiometric coefficient since it is determined from experiments. The reaction order for each reactant often has a positive number, but some are fractional or zero. Several examples in the reaction order are the following:

- (i) Zero-Order. The reaction rate is independent of the concentration of the reactants. The change in concentration does not change the reaction rate. The reaction can be done as long as the number of reactants is enough to be converted into a product. Examples are various reactions catalyzed by enzymes (Ray & Mandal, 2008).
- (ii) First-Order. The reaction rate is directly proportional to the concentration of one of the reactants. Any change in the concentration of a reactant will affect the reaction rate proportionally (Allen, 2018).
- (iii) Second-Order. The rate of reaction is affected by the concentration of one or more reactants by a total power of two (Haraldsrud & Odden, 2023).
- (iv) Kinetic Fractional Order. The rate of reaction is not in the cardinal number. Most reaction orders are in decimal and fractional numbers.

Kinetics with fractional order reactions include (Al-Basir *et al.*, 2015; Sokolov *et al.*, 2002; Elio *et al.*, 2018):

- (i) One-fourth order ( $m = \frac{1}{4}$ ). A reaction of one-fourth order is an example of fractional kinetics, which is often observed in complex reactions or reactions involving non-simple mechanisms. Unlike whole-order reactions (such as 0, 1, or 2), fractional kinetics show that the reaction rate is not directly proportional to the concentration of the reactants. A one-fourth reaction order shows that the reaction rate is not directly proportional to the concentration of the reactants, but rather depends on  $[A]$  as a power of 0.25. Changes in the concentration of the reactants will have a smaller effect on the reaction rate than a first- or second-order reaction.

- (ii) Half order ( $m = \frac{1}{2}$ ). Half-order kinetics is a form of fractional kinetics in which the reaction rate is proportional to the square root of the reactant concentration. Half-order reactions are often found in more complex processes, such as enzymatic reactions or reactions involving free radicals. Increasing reactant concentration will increase the reaction rate at a slower rate than in a first-order reaction.
- (iii) Three-quarter order ( $m = \frac{3}{4}$ ). In a three-quarter order reaction, the reaction rate increases more rapidly than in a lower order reaction (such as one-fourth or half orders), but it is slower than in the first-order reaction.

#### 2.4. Understanding Reaction Order in the Integration Theory

The reaction order can be determined by the existence of a rate law. The rate law for any chemical reaction must be determined from experiments and cannot be predicted from the chemical reaction equation directly. The initial rate method is often used to determine the rate law, namely by observing the effect of changes in the initial reactant concentration on the initial rate of the reaction. The integrated rate law equation is obtained by integrating the rate law. The following are the integration steps for zero, first, second, and fractional orders. In short, the integration process is done and derived from the concept in Eq. (4) to equations (5), (6), and (7):

$$r = k[A]^m \quad (5)$$

$$-\frac{d[A]}{dt} = k[A]^m \quad (6)$$

$$\frac{d[A]}{[A]^m} = -k dt \quad (7)$$

$$\int_{A_0}^A \frac{d[A]}{[A]^m} = -k \int_0^t dt \quad (8)$$

Then, the following steps are done:

- (i) For zero-order integration ( $m = 0$ ), we can get equations (9) and (10):

$$-\int_{A_0}^A d[A] = k \int_0^t dt \quad (9)$$

$$[A] = [A]_0 - kt \quad (10)$$

- (ii) For first-order integration ( $m = 1$ ), we can get equations (11), (12), and (13):

$$-\int_{A_0}^A \frac{d[A]}{[A]} = k \int_0^t dt \quad (11)$$

$$\ln \frac{[A]}{[A]_0} = -kt \quad (12)$$

$$\ln[A] = \ln[A]_0 - kt \quad (13)$$

- (iii) For second-order integration ( $m = 2$ ), we can get equations (14) and (15):

$$-\int_{A_0}^A \frac{d[A]}{[A]^2} = k \int_0^t dt \quad (14)$$

$$\frac{1}{[A]} = \frac{1}{[A]_0} + kt \quad (15)$$

- (iv) For kinetic fractional integration, such as  $m = \frac{1}{4}$ ,  $\frac{1}{2}$ , and  $\frac{3}{4}$ , using a similar method, we can get equations (15), (16), and (17), respectively:

$$[A]^{\frac{3}{4}} = [A_0]^{\frac{3}{4}} - \frac{3}{4}kt \tag{16}$$

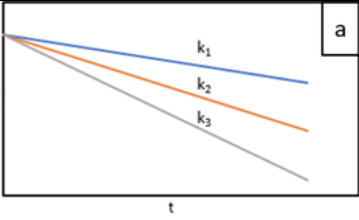
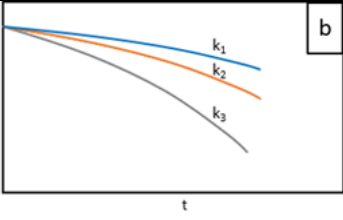
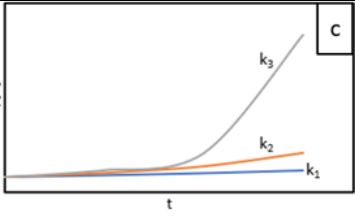
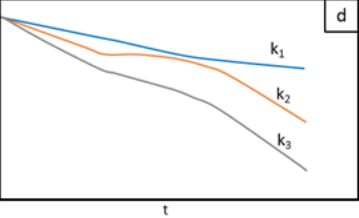
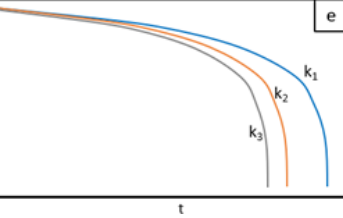
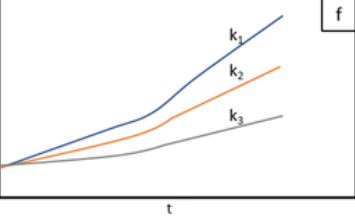
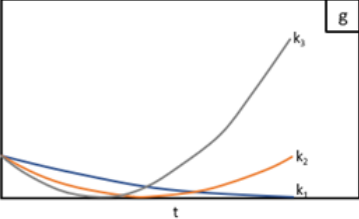
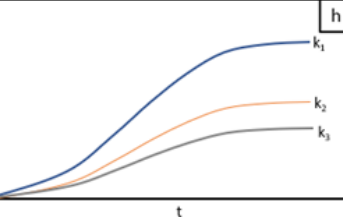
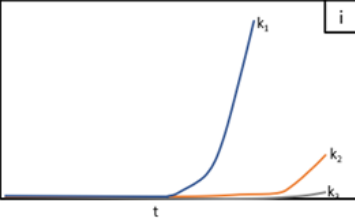
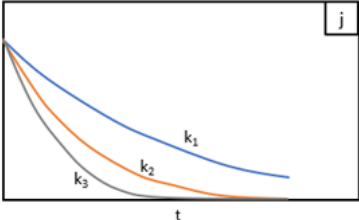
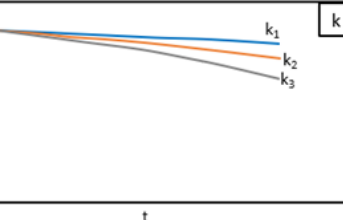
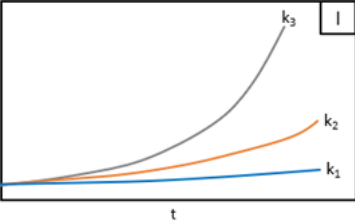
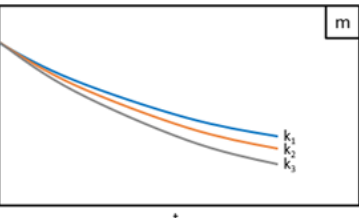
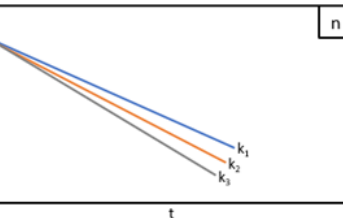
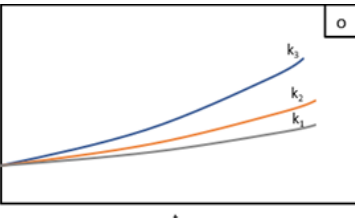
$$[A]^{\frac{1}{2}} = [A_0]^{\frac{1}{2}} - \frac{1}{2}kt \tag{17}$$

$$[A]^{\frac{1}{4}} = [A_0]^{\frac{1}{4}} - kt \tag{18}$$

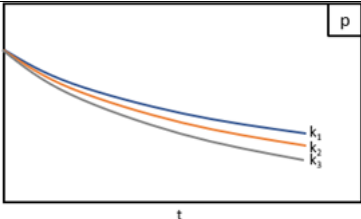
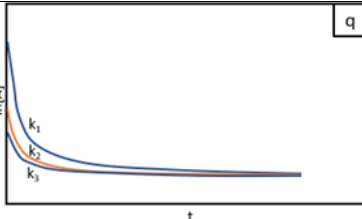
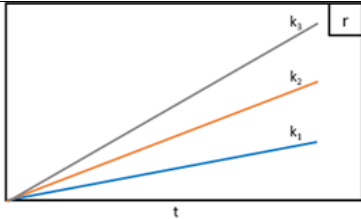
### 2.5. Reaction Order Determination

The unified rate allows the prediction of reaction order by plotting and regressing data of reactant concentration data against  $t$ . Each reaction order has different characteristics of the curve (**Table 1**). By analyzing the curve shape, the reaction order can be accurately determined. Then, the information regarding curve data fitting, calculations, and parameters of the kinetic order model is presented in **Table 2**.

**Table 1.** Reaction order characteristics in plotting concentration vs  $t$ .

Order	$[A]$ vs $t$	$\ln[A]$ vs $t$	$1/[A]$ vs $t$
0			
$\frac{1}{4}$			
$\frac{1}{2}$			
$\frac{3}{4}$			
1			

**Table 1 (Continue).** Reaction order characteristics in plotting concentration vs  $t$ .

Order	$[A]$ vs $t$	$\ln[A]$ vs $t$	$1/[A]$ vs $t$
2	 p	 q	 r

**Table 2.** Curve data fitting for zero-, first-, second-, and fraction-order reactions.

Kinetic Order	Linear Equation or Integrated Rate Law	Plotting	$k$ -value obtainment	Rate Law	Unit for $k$
Zero	$[A] = [A]_0 - kt$	$[A]_t$ vs $t$	- slope	$r = k$	mol/L.s
First	$\ln[A] = \ln[A]_0 - kt$	$\ln[A]_t$ vs $t$	- slope	$r = k[A]$	1/s
Second	$\frac{1}{[A]} = \frac{1}{[A]_0} + kt$	$1/[A]_t$ vs $t$	+ slope	$r = k[A]^2$	L/mol.s
$\frac{1}{4}$	$[A]^{\frac{3}{4}} = [A]_0^{\frac{3}{4}} - \frac{3}{4}kt$	$[A]^{\frac{3}{4}}$ vs $t$	- 4/3 slope	$r = k[A]^{\frac{3}{4}}$	mol <sup>0.75</sup> /L <sup>0.75</sup> s
$\frac{1}{2}$	$[A]^{\frac{1}{2}} = [A]_0^{\frac{1}{2}} - \frac{1}{2}kt$	$[A]^{\frac{1}{2}}$ vs $t$	- 2 slope	$r = k[A]^{\frac{1}{2}}$	mol <sup>0.5</sup> /L <sup>0.5</sup> s
$\frac{3}{4}$	$[A]^{\frac{1}{4}} = [A]_0^{\frac{1}{4}} - kt$	$[A]^{\frac{1}{4}}$ vs $t$	- 4 Slope	$r = k[A]^{\frac{1}{4}}$	mol <sup>0.25</sup> /L <sup>0.25</sup> s

### 3. METHOD

This study showed how to analyze experimental data to predict reaction order and kinetics. Data was obtained from literature in Internet sources, especially from articles published in international journals.

### 4. RESULTS AND DISCUSSION

For determining data, several steps are done:

- (i) Step 1: Take data from the experiment to obtain concentration  $[A]$  versus  $t$ .
- (ii) Step 2: Tabulate concentration  $[A]$  into other forms, including  $\ln[A]$  and  $1/[A]$ .
- (iii) Step 3: Plot data into:  $[A]$ ,  $\ln[A]$ ,  $1/[A]$  versus  $t$ .
- (iv) Step 4: Compare the curves created in step (iii) and the curves in **Table 1**. The nearest curve shape represents the type of reaction order.
- (v) Step 5: After analyzing and comparing data with curves in **Table 1** (as in step (iv)), predict the reaction order. Then, calculate the value for reaction order and constant as well as select possible reaction rate equation, as explained in **Table 2**.
- (vi) Step 6: Based on step (vi), take data from **Table 2** and select from the "plotting" column to understand what curve should be made (for the x- and y-axis) for getting the  $k$  value. Following the best curve fitting from **Table 2** in the "k-value" obtainment column, re-put the regression equation for understanding reaction kinetics.

#### 4.1. Example Case 1

For the chemical reaction of hydrazine to form water and oxygen (reaction (CR1)):



The determination of the reaction order is explained as follows:

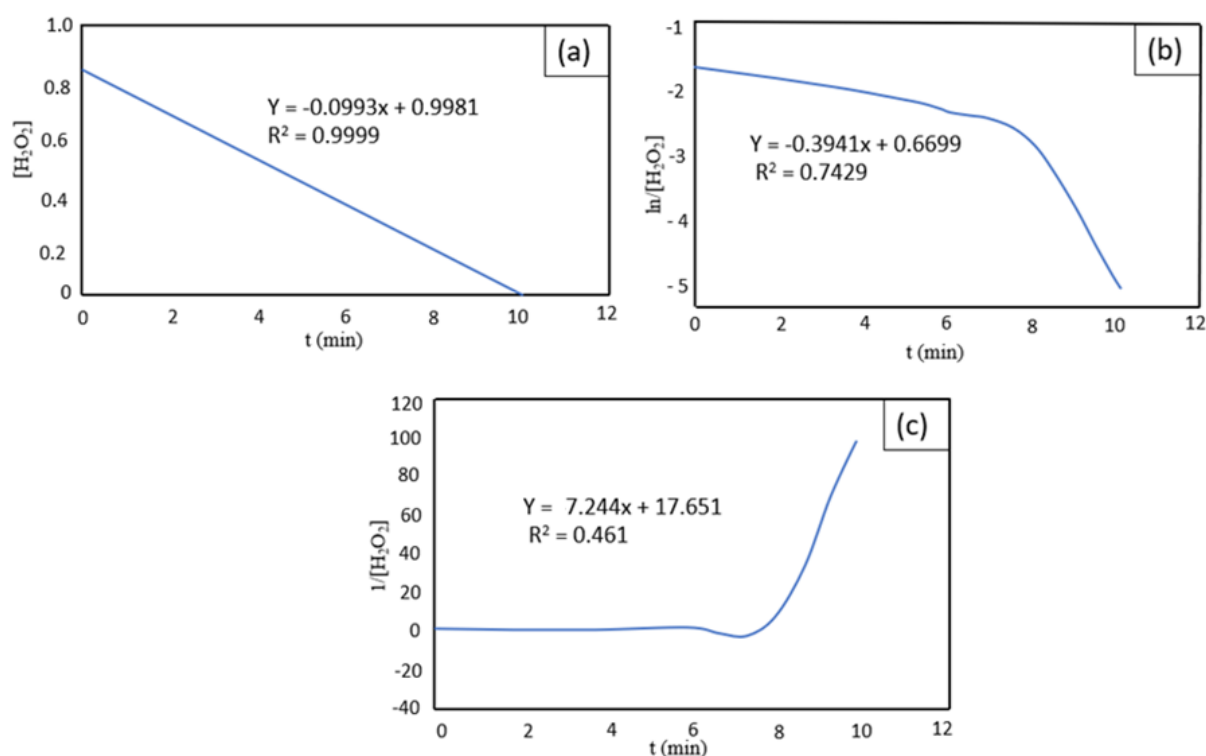
- (i) **Step 1:** Find data for the concentration of the reactant  $[\text{H}_2\text{O}_2]$  at various  $t$  (**Table 3**).
- (ii) **Step 2:** Tabulate data  $[\text{H}_2\text{O}_2]$  into  $\ln[\text{H}_2\text{O}_2]$  and  $1/[\text{H}_2\text{O}_2]$  (see **Table 4**).
- (iii) **Step 3:** Fit curves from step (ii) in **Table 4** and put a linearization curve to get slope and  $R^2$  (see **Figure 2**).

**Table 3.** Data collection of  $[\text{H}_2\text{O}_2]$  concentration against  $t$ .

$t$ (min)	$[\text{H}_2\text{O}_2]$
0	1.000
2	0.800
4	0.600
6	0.400
8	0.200
10	0.000

**Table 4.** Tabulated concentration and  $t$  dataset of  $\text{H}_2\text{O}_2$ .

$t$ (min)	$[\text{H}_2\text{O}_2]$	$\ln[\text{H}_2\text{O}_2]$	$1/[\text{H}_2\text{O}_2]$
0	1.000	0.000	1.000
2	0.800	-0.223	1.250
4	0.600	-0.510	1.666
6	0.400	-0.916	2.500
8	0.200	-0.160	5.000
10	0.100	-4.605	100.0



**Figure 2.** Data  $[\text{H}_2\text{O}_2]$  for several conditions: (a) zero order ( $[A]$  vs  $t$ ), (b) first order ( $\ln[A]$  vs  $t$ ), and (c) second order ( $1/[A]$  vs  $t$ ).



- (iv) Step 4: Compare the type of curve gained in step (iii) in **Figure 2** to the various types of curves listed in **Table 1**. **Figure 2(a)** is fit for the model **curves (a), (b), and (c)** in **Table 1**. The curve also in **Figure 2(a)** produces a straight line with  $R^2$  value  $> 0.999$  (the  $R^2$  value is greater than the other model plots). This value indicates that the reaction follows a zero-order kinetic model.
- (v) Step 5: Based on the information in **Table 2**, the curve that has been created has a predicted linearization plot as a function of  $[H_2O_2]_t$  vs  $t$  with the predicted rate equation of  $[H_2O_2]_t = [H_2O_2]_0 - kt$  and the predicted rate of  $\frac{d[H_2O_2]}{dt} = -k[H_2O_2]^0$ .
- (vi) Step 6: Taking data from **Table 2**, select from the "plotting" column to understand what curve should be made (for the x- and y-axis) for getting the  $k$  value. Following the best curve fitting from **Table 2**, we can get **Figure 2(a)** with the linearization regression of  $y = -0.0993x + 0.9981$ . Compared to **Table 2** in the " $k$ -value obtainment" column, the  $k$  value for zero order is  $-$  slope, showing the  $k$  value of 0.0993.

## 4.2. Example Case 2

A reaction following the formula (CR2) is carried out at a certain temperature.



The determination of reaction order follows:

- (i) Step 1: Collect data for the concentration of reactant A ( $[A]$ ) at various  $t$  (**Table 5**).

**Table 5.** Data collection of concentration A against  $t$ .

$t$ (min)	$[A]$
0.00	2.000
2.00	1.107
4.00	0.612
6.00	0.338
8.00	0.187
10.00	0.103

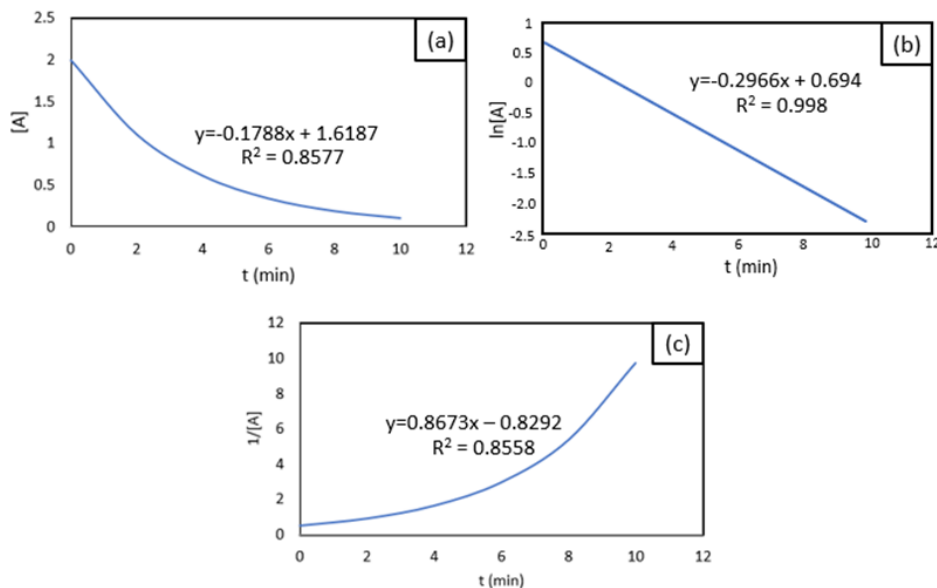
- (ii) Step 2: Tabulate data into  $\ln[A]$  and  $1/[A]$  (see **Table 6**).

**Table 6.** Tabulated concentration and  $t$  dataset of reactant A.

$t$ (min)	$[A]$	$\ln[A]$	$1/[A]$
0.00	2.000	0.693	0.500
2.00	1.107	0.102	0.903
4.00	0.612	-0.491	1.630
6.00	0.338	-1.085	2.950
8.00	0.187	-1.677	5.350
10.00	0.103	-2.273	9.710

- (iii) Step 3: Fit data (see **Figure 3**). Then, take linearization to get  $R^2$  and slope.
- (iv) Step 4: Compare curve in step (iii) to data for various types of curve images in **Table 1**. Based on the fit analysis, **Figure 3** has a good match with the curve images (m), (n), and (o) in **Table 1**. The  $R^2$  value is more than 0.90, indicating the reaction order is following the first-order model.
- (v) Step 5: Predict the reaction rate based on **Table 2**, resulting  $\frac{d[A]}{dt} = -k[A]$ .

(vi) **Step 6:** Similar to above Case 1 for getting data from **Table 2** in the “plotting” and “k-value obtainment” columns, we can get **Figure 3(b)** with the linearization of  $y = -0.2966x + 0.694$ . Thus, from the “k-value obtainment” columns in **Table 2**, the  $k$  value for the first order is – slope, showing the  $k$  value of 0.2966.



**Figure 3.** Data [A] for several conditions: (a) zero order ([A] vs  $t$ ), (b) first order ( $\ln[A]$  vs  $t$ ), and (c) second order ( $1/[A]$  vs  $t$ ).

### 4.3. Example Case 3

A  $\text{NO}_2$  decomposition reaction occurs at a temperature of  $330^\circ\text{C}$  based on the reaction equation shown by the formula in reaction (CR3).



The determination of the reaction order and the rate law expression can be determined through the following steps:

(i) **Step 1:** Take the concentration of the reactant  $\text{NO}_2$  at various  $t$  (**Table 7**).

**Table 7.** Data  $\text{NO}_2$  concentration against  $t$ .

$t$ (s)	$[\text{NO}_2]$
0	$1 \times 10^{-2}$
60	$6.83 \times 10^{-3}$
120	$5.18 \times 10^{-3}$
180	$4.18 \times 10^{-3}$
240	$3.00 \times 10^{-3}$
300	$3.01 \times 10^{-3}$
360	$2.64 \times 10^{-3}$

(ii) **Step 2:** Tabulate data into  $\ln [\text{NO}_2]$  and  $1/[\text{NO}_2]$  (**Table 8**).

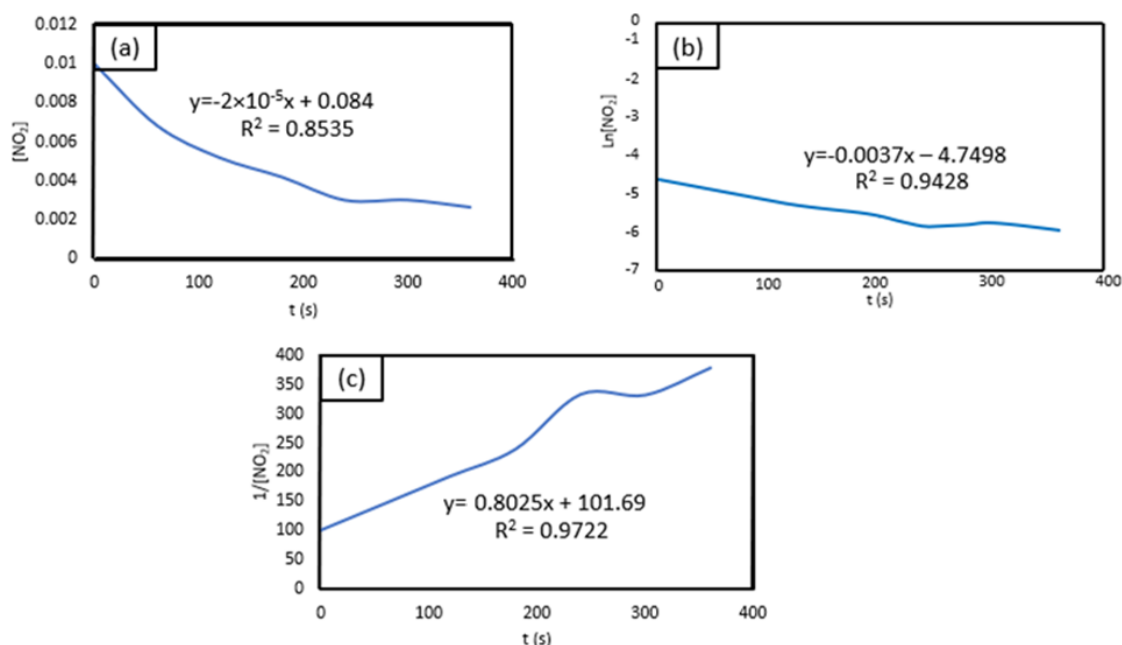
**Table 8.** Tabulated concentration and  $t$  dataset of  $\text{NO}_2$  reactant.

$t$ (s)	$[\text{NO}_2]$	$\ln[\text{NO}_2]$	$1/[\text{NO}_2]$
0	$1 \times 10^{-2}$	-4.605	100
60	$6.83 \times 10^{-3}$	-4.986	146.412
120	$5.18 \times 10^{-3}$	-5.263	193.050

**Table 8 (Continue).** Tabulated concentration and  $t$  dataset of  $\text{NO}_2$  reactant.

$t$ (s)	$[\text{NO}_2]$	$\ln[\text{NO}_2]$	$1/[\text{NO}_2]$
180	$4.18 \times 10^{-3}$	-5.477	239.234
240	$3.00 \times 10^{-3}$	-5.809	333.333
300	$3.01 \times 10^{-3}$	-5.805	332.225
360	$2.64 \times 10^{-3}$	-5.937	378.788

- (iii) **Step 3:** Using data in **Table 8** from step (ii), take a linearization curve and calculate slope and  $R^2$  (**Figure 4**).
- (iv) **Step 4:** Compare the obtained curves gained in step (iii) in **Figure 4** to **Table 1**. **Figure 4** has a good match with the **curve images (p), (q), and (r)** in **Table 1** with a straight line and  $R^2 = 0.9722$ . The reaction order follows the second-order model.
- (v) **Step 5:** Based on the information in step (iv) and compared to **Table 2**, the function of  $1/[\text{NO}_2]$  versus  $t$  correlates with  $-\frac{d[A]}{dt} = k[\text{NO}_2]^2$ .
- (vi) **Step 6:** Similar to above Case 1 for getting data from **Table 2** in the “plotting” and “k-value obtainment” columns, we can get **Figure 4(c)** with the linearization regression of  $y = +0.8025x + 101.69$ . Compared to **Table 2** in the “k-value obtainment” column, the  $k$  value for the second order is + slope, showing the  $k$  value of 0.8025.



**Figure 4.** Data  $[\text{NO}_2]$  for several conditions: (a) zero order ( $[A]$  vs  $t$ ), (b) first order ( $\ln[A]$  vs  $t$ ), and (c) second order ( $1/[A]$  vs  $t$ ).

#### 4.4. Example Case 4

The decomposition reaction of ozone in the gas phase at a certain concentration is shown by the reaction (CR4).



Based on equation (2), the following steps can be used to determine the reaction order and rate law expression.:

- (i) **Step 1:** Take data for the concentration of reactant  $[\text{O}_3]$  at various  $t$  (**Table 9**).

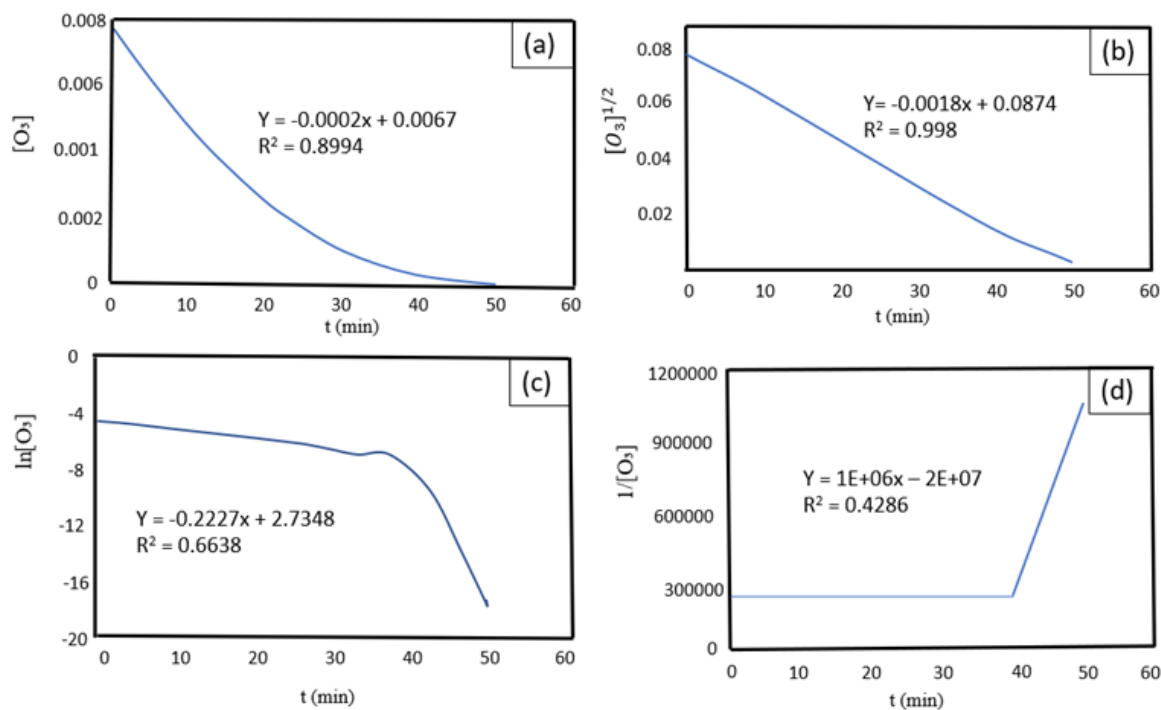
- (ii) **Step 2:** Tabulate into  $\ln[O_3]$ ,  $[O_3]^{1/2}$ , and  $1/[O_3]$  (**Table 10**).
- (iii) **Step 3:** Using data in **Table 10** from step (ii), make a linearization curve (**Figure 5**).

**Table 9.** Data collection of  $O_3$  concentration against  $t$ .

$t$ (min)	$[O_3]$
0	0.00792100
10	0.00476100
20	0.02621440
30	0.00102400
40	0.00023104
50	0.00000001

**Table 10.** Tabulated concentration and  $t$  dataset of the  $O_3$  reactant.

$t$ (min)	$[O_3]$	$[O_3]^{1/2}$	$\ln[O_3]$	$1/[O_3]$
0	0.00792100	0.0890	-4.83824	126.24669
10	0.00476100	0.0690	-5.34730	210.03991
20	0.02621440	0.0512	-5.94403	381.46973
30	0.00102400	0.0320	-6.88404	976.56250
40	0.00023104	0.0152	-8.37292	4328.2548
50	0.00000001	0.0001	-18.4207	10000000



**Figure 5.** Data  $[O_3]$  for several conditions: (a) zero order ( $[O_3]$  vs  $t$ ), (b) half-order ( $[O_3]^{1/2}$  vs  $t$ ) (c) first order ( $\ln [O_3]$  vs  $t$ ), and (d) second order ( $1/[O_3]$  vs  $t$ ).

- (iv) **Step 4:** Compare data gained from step (iii) in **Figure 5** to various types of curve images in **Table 1**. Based on the fit analysis, **Figure 5** has a good match with the **curve images (g), (h), and (i)** in **Table 1** with a straight line and has an  $R^2$  value of 0.998. This indicates that the reaction order is following the half-order model.

- (v) **Step 5:** Based on step (iv), predict the reaction model. It results  $-\frac{d[O_3]}{dt} = k[O_3]^{1/2}$ .

- (vi) **Step 6:** Similar to above Case 1 for getting data from **Table 2** in the “plotting” and “k-value obtainment” columns, we can get **Figure 5(b)** with the linearization regression of  $y = -0.0018x + 0.0874$ . Compared to **Table 2** in the “k-value obtainment” column, the  $k$  value for zero order is  $-2$  slope, showing the  $k$  value of 0.0036.

#### 4. CONCLUSION

This study provides a step-by-step guide on how to determine reaction rates and reaction orders, presenting real-world case studies to clarify the chemical process. The process for determining reaction rates and orders involves collecting experimental data, mathematical manipulation of the rate equation, and selecting the most appropriate kinetic model based on linearity and statistical parameters such as  $R^2$  and slope values. The article emphasizes the importance of curve-fitting analysis, such as plotting  $[A]$  vs  $t$ ,  $\ln[A]$  vs  $t$ , and  $1/[A]$  vs  $t$  to identify linearity patterns that match to predicted model for reaction orders. In addition, the case studies presented in the article help to strengthen the understanding of how these techniques are applied in real-world scenarios, both for simple and more complex reactions.

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#### 6. AUTHORS' NOTE

The authors declare that there is no conflict of interest regarding the publication of this article. The authors confirmed that the paper was free of plagiarism.

#### 7. REFERENCES

- Al-Basir, F., Elaiw, A. M., Kesh, D., and Roy, P. K. (2015). Optimal control of a fractional-order enzyme kinetic model. *Control and Cybernetics*, 44(4), 443-461.
- Allen, W. D. (2018). A Universal Integrated Rate Equation for Chemical Kinetics. *The Journal of Physical Chemistry A*, 122(16), 4009-4014.
- Alnasif, A., Mashruk, S., Shi, H., Alnajideen, M., Wang, P., Pugh, D., and Valera-Medina, A. (2023). Evolution of ammonia reaction mechanisms and modeling parameters: A review. *Applications in Energy and Combustion Science*, 15, 100175.
- Aquilanti, V., Coutinho, N. D., and Carvalho-Silva, V. H. (2017). Kinetics of low-temperature transitions and a reaction rate theory from non-equilibrium distributions. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 375(2092), 20160201.
- Arcus, V. L., and Mulholland, A. J. (2020). Temperature, dynamics, and enzyme-catalyzed reaction rates. *Annual Review of Biophysics*, 49(1), 163-180.
- Arndt, S., and Schomacker, R. (2022). 4.1 Chemical kinetics: A practical guide. *Catalyst*, 1(2), 6.

- Ateia, M., Alalm, M. G., Awfa, D., Johnson, M. S., and Yoshimura, C. (2020). Modeling the degradation and disinfection of water pollutants by photocatalysts and composites: A critical review. *Science of the Total Environment*, 698, 134197.
- Bhandari, S., Rangarajan, S., and Mavrikakis, M. (2020). Combining computational modeling with reaction kinetics experiments for elucidating the in-situ nature of the active site in catalysis. *Accounts of Chemical Research*, 53(9), 1893-1904.
- Blazheyevskiy, M., Serdiukova, Y., and Karpova, S. (2022). Development and validation of a simple procedure for the kinetic spectrophotometric quantitative determination of ceftriaxone using potassium Caroate. *French-Ukrainian Journal of Chemistry*, 10(1), 1-12.
- Cama, J., Metz, V., and Ganor, J. (2002). The effect of pH and temperature on kaolinite dissolution rate under acidic conditions. *Geochimica et Cosmochimica Acta*, 66(22), 3913-3926.
- Campbell, C. T. (2017). The degree of rate control: a powerful tool for catalysis research. *ACS Catalysis*, 7(4), 2770-2779.
- Dybeck, E. C., Plaisance, C. P., and Neurock, M. (2017). Generalized temporal acceleration scheme for kinetic monte carlo simulations of surface catalytic processes by scaling the rates of fast reactions. *Journal of Chemical Theory and Computation*, 13(4), 1525-1538.
- Faraji, F., Alizadeh, A., Rashchi, F., and Mostoufi, N. (2022). Kinetics of leaching: A review. *Reviews in Chemical Engineering*, 38(2), 113-148.
- Ganiyu, S. O., Sable, S., and El-Din, M. G. (2022). Advanced oxidation processes for the degradation of dissolved organics in produced water: A review of process performance, degradation kinetics and pathway. *Chemical Engineering Journal*, 429, 132492.
- Haraldsrud, A., and Odden, T. O. B. (2023). From integrated rate laws to integrating rate laws: computation as a conceptual catalyst. *Journal of Chemical Education*, 100(5), 1739-1750.
- Hu, B., and Xia, C. (2016). Factors influencing the measured surface reaction kinetics parameters. *Asia-Pacific Journal of Chemical Engineering*, 11(3), 327-337.
- Jere, S., and Mpeta, M. (2024). Enhancing learners' conceptual understanding of reaction kinetics using computer simulations—a case study approach. *Research in Science Education*, 2024, 1-25.
- Kukoc-Modun, L., Biocic, M., and Radić, N. (2021). Determination of penicillamine, tiopronin and glutathione in pharmaceutical formulations by kinetic spectrophotometry. *Acta Pharmaceutica*, 71(4), 619-630.
- Lazaridou, A., Smith, L. R., Pattison, S., Dummer, N. F., Smit, J. J., Johnston, P., and Hutchings, G. J. (2023). Recognizing the best catalyst for a reaction. *Nature Reviews Chemistry*, 7(4), 287-295.
- Leng, L., Xiong, Q., Yang, L., Li, H., Zhou, Y., Zhang, W., Jiang, S., Li, H., and Huang, H. (2021). An overview on engineering the surface area and porosity of biochar. *Science of the Total Environment*, 763, 144204.
- Li, N., Taylor, L. S., Ferruzzi, M. G., and Mauer, L. J. (2012). Kinetic study of catechin stability: Effects of pH, concentration, and temperature. *Journal of Agricultural and Food Chemistry*, 60(51), 12531-12539.

- Liao, G., Derry, M. J., Smith, A. J., Armes, S. P., and Mykhaylyk, O. O. (2024). Determination of reaction kinetics by time-resolved small-angle x-ray scattering during polymerization-induced self-assembly: Direct evidence for monomer-swollen nanoparticles. *Angewandte Chemie International Edition*, *63*(2), e202312119.
- Lin, H., Mairal, J., and Harchaoui, Z. (2018). Catalyst acceleration for first-order convex optimization: from theory to practice. *Journal of Machine Learning Research*, *18*(212), 1-54.
- Marin, G. B., Galvita, V. V., and Yablonsky, G. S. (2021). Kinetics of chemical processes: From molecular to industrial scale. *Journal of Catalysis*, *404*, 745-759.
- Marín-García, M., De Luca, M., Ragno, G., and Tauler, R. (2022). Coupling of spectrometric, chromatographic, and chemometric analysis in the investigation of the photodegradation of sulfamethoxazole. *Talanta*, *239*, 122953.
- Mavroudis, P. D., Kosmidis, K., and Macheras, P. (2019). On the unphysical hypotheses in pharmacokinetics and oral drug absorption: Time to utilize instantaneous rate coefficients instead of rate constants. *European Journal of Pharmaceutical Sciences*, *130*, 137-146.
- Mills, P. L., Quiram, D. J., AND Ryley, J. F. (2007). Microreactor technology and process miniaturization for catalytic reactions—A perspective on recent developments and emerging technologies. *Chemical Engineering Science*, *62*(24), 6992-7010.
- Motagamwala, A. H., and Dumesic, J. A. (2020). Microkinetic modeling: A tool for rational catalyst design. *Chemical Reviews*, *121*(2), 1049-1076.
- Musah, M., Azeh, Y., Mathew, J. T., Umar, M. T., Abdulhamid, Z., and Muhammad, A. I. (2022). Adsorption kinetics and isotherm models: A review. *CaJoST*, *4*(1), 20-26.
- Qu, J., Wang, Y., Tian, X., Jiang, Z., Deng, F., Tao, Y., Jiang, Q., Wang, L., and Zhang, Y. (2021). KOH-activated porous biochar with high specific surface area for adsorptive removal of chromium (VI) and naphthalene from water: Affecting factors, mechanisms and reusability exploration. *Journal of Hazardous Materials*, *401*, 123292.
- Ray, A., and Mandal, B. (2008). Kinetic rate equations in integrated form for single-step reactions involving different types of reactants. *Progress in Reaction Kinetics and Mechanism*, *33*(3), 267-281.
- Razdan, N. K., Lin, T. C., and Bhan, A. (2023). Concepts relevant for the kinetic analysis of reversible reaction systems. *Chemical Reviews*, *123*(6), 2950-3006.
- Sokolov, I. M., Klafter, J., and Blumen, A. (2002). Fractional kinetics. *Physics Today*, *55*(11), 48-54.
- Srivastava, A. (2021). Micro-level estimation of methionine using inhibitory kinetic spectrophotometric method. *Biointerface Research in Applied Chemistry*, *11*, 10654-10663.
- Tafazoli, H., Safaei, M., and Shishehbore, M. R. (2020). A new sensitive method for quantitative determination of cisplatin in biological samples by kinetic spectrophotometry. *Analytical Sciences*, *36*(10), 1217-1222.

- Taylor, C. J., Pomberger, A., Felton, K. C., Grainger, R., Barecka, M., Chamberlain, T. W., Courne, R. A., Johnson, C. N., and Lapkin, A. A. (2023). A brief introduction to chemical reaction optimization. *Chemical Reviews*, 123(6), 3089-3126.
- Walker, E. A., Ravisankar, K., and Savara, A. (2020). CheKiPEUQ intro 2: Harnessing uncertainties from data sets, Bayesian design of experiments in chemical kinetics. *ChemCatChem*, 12(21), 5401-5410.
- Wei, Z., Li, Y., Cooks, R. G., and Yan, X. (2020). Accelerated reaction kinetics in microdroplets: Overview and recent developments. *Annual Review of Physical Chemistry*, 71(1), 31-51.
- Westbrook, C., Heufer, K. A., and Wildenberg, A. (2021). Key chemical kinetic steps in reaction mechanisms for fuels from biomass: a perspective. *Energy and Fuels*, 35(19), 15339-15359.
- Zhang, Y., Wang, J., Wang, Y., and Zhao, K. (2023). In-situ real-time monitoring of chemical kinetics by an automated micro-reaction device. *Sensors and Actuators B: Chemical*, 392, 134069.