

Adsorption of Palmitate on Calcite in Aqueous Solution: An Initial Rate and Thermodynamics Study

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ABSTRACT

This study demonstrates the importance of understanding the thermodynamic and kinetics aspects of adsorption processes considering the attention drawn towards improving the adsorptive behaviours of fatty-acids soaps onto calcite. In view of the nexus between the surface tension of solutions of fatty acid soaps, traveling microscope was used to measure the concentrations of adsorbate filtrates with which parameters for five adsorption isotherm models namely; Langmuir, Freundlich, D-R, Temkin and Elovich were employed in assessing the adsorption behaviour of sodium palmitate on calcite in aqueous solution. Despite the high correlation R^2 values of 0.9466 and 0.9732 shown by Langmuir and Freundlich isotherms respectively, the Temkin isotherm having the highest R^2 value of 0.9821 indicates an excellent fit between the experimental data, suggesting that the model accurately describes the adsorption process of palmitate on calcite. The Temkin isotherm assumes a uniform adsorption energy, implying that the adsorption process occurred with a consistent energy distribution with the A_T value of 0.205 L/mg signifying a moderate adsorption capacity and that palmitate molecules were effectively adsorbed from the solution. The b_T value (0.986 L/g) point to a strong interaction between palmitate and calcite, suggesting that the adsorption process is favorable and the adsorption process occurred with a consistent energy distribution. The initial rate increased with increase in initial concentration. The high frequency factor and the low activation energy values determined were $8.58 \times 10^6 \text{ s}^{-1}$ and 9.14 J/mol.K respectively inferring that the reaction proceeds relatively fast due to increased collision and low steric hindrance in the adsorption reaction. Palmitate therefore, is a reliable adsorbate for the concentration of calcite in mineral beneficiation and/or flotation.

Keywords: Activation energy, Gibbs free energy, surface tension, initial rate, rate constant, adsorption order, calcite

INTRODUCTION

Its specific gravity, non-toxicity, non-magnetic properties, and capacity to absorb different kinds of radiation make calcite a vital worldwide strategic mineral resource with wide-ranging uses in petrochemical, medical protection, textiles, and construction materials^[1,2]. 85–90% calcite is commonly employed as a weighting agent in drilling mud in ultra-deep drilling, especially in the rapidly expanding 10,000 m ultra-deep drilling market. Ultra-deep drilling wells have a high demand for calcite, and a sizable amount of high-density waste drilling fluids are returned to the drain^[3].

Calcite's surface adsorption in aqueous solutions is of scientific interest for purification and flotation processes, and as an anionic collector, the study of the adsorption calcite showed that the main factors influencing the surface and thermodynamic properties of surfactants are their hydrocarbon length and degree of unsaturation^[4].

In flotation procedures, palmitate, a long-chain fatty acid, is frequently employed as a collector to separate calcite from other minerals^[5]. Ineffective flotation procedures and decreased mineral recovery may result from a lack of knowledge regarding the adsorption kinetics of palmitate on calcite.

The majority of studies on the thermodynamics and kinetics of palmitate adsorption on calcite are restricted to Langmuir and freundlich isotherms, as well as pseudo first and second orders^[4,5,6]. The current study utilized more kinetic and thermodynamic models in explaining the adsorption behaviour of palmitate on calcite in aqueous solution.

At the interface between two phases, such as solid-liquid, surface tension is the energy per unit area. The behavior of adsorption in palmitate adsorption onto calcite is largely determined by surface tension. When palmitate adsorbs onto calcite, surface tension may decrease, facilitating the adsorption of more palmitate molecules^[4].

METHODOLOGY

This study utilized the method of initial concentration for determining adsorption and kinetics parameters and different adsorption and kinetics models were used to assess the adsorption behaviour of palmitate on calcite in aqueous solution.

100 gram of the mineral was washed with distilled water, crushed to powdery size and sieved in 50µm mesh after drying at 60 °C for 30 minutes and kept in a vessel for the study. From a stock solution of 11.0 g/L, 20, 40, 60 and 80 mg/L solution of sodium palmitate was prepared and the surface tension of each measured using a traveling microscope from which a calibration graph of surface tension (dyn/cm) against concentration of sodium palmitate (mg/L) was plotted.

Adsorption and Kinetics studies

1.0 gram of the mineral was added to four 250 ml Elimier flasks containing 100ml of 20, 40, 60 and 80 mg/L of pH 4.6, agitated for 30 minutes, filtered after allowed to settle and the surface tension measured to obtain the concentration of filtrate (C_e) and the adsorbed palmitate molecules ($C_o - C_e$) with which adsorption and kinetic models as seen from equation (1) to (10) are used to assess the adsorption process.

$$\text{Langmuir model} \quad \frac{C_e}{q_e} = \frac{1}{q_{max}K_L} + \frac{1}{q_{max}} C_e \quad (1)$$

$$\text{Fruendlich model} \quad \log q_e = \log K_F + \frac{1}{n} \log C_e \quad (2)$$

$$\text{Dubinin–Radushkevich model} \quad \ln q_e = \ln q_m - k_D \varepsilon^2 \quad (3)$$

$$\text{Temkin's model} \quad q_e = \frac{RT}{b_T} \log(A) + \frac{RT}{b_T} \log(C_e) \quad (4)$$

$$\text{Elovich model} \quad \ln\left(\frac{q_e}{C_e}\right) = \ln(K_e Q_0) - \left(\frac{1}{Q_0}\right) q_e \quad (5)$$

The procedure was repeated at 50 °C to determine the effect of temperature on adsorption using the Arrhenius equation and the thermodynamic variables using equation (8), (9) and (10):

$$\text{Rate,} \quad R = - \frac{d[C]}{dt} \quad (6)$$

$$\text{Rate law} \quad \text{Rate} = KC^n \text{ or } \log R = \log K + n \log C \quad (7)$$

$$\text{Arrhenius equation} \quad \log K = - \frac{E_a}{2.303RT} + \log A \quad (8)$$

$$\text{Gibb's Free Energy} \quad \Delta G^o = -RT \ln K^o \quad (9)$$

$$\text{Enthalpy and Entropy changes} \quad \Delta G^o = \Delta H^o - T \Delta S^o \quad (10)$$

RESULTS AND DISCUSSION

Table 1 presents the results with which the adsorption behaviour of palmitate as a collector was assessed.

Table 1: Adsorption Isotherm Parameters at room temperature of 29°C

Co	Ce	Co-Ce	qe	Ce/qe	logqe	logCe
20	10.938	9	906	0.0121	2.96	1.04
40	23.500	17	1650	0.0142	3.22	1.37
60	36.380	24	2362	0.0154	3.37	1.56
80	54.019	26	2598	0.0208	3.41	1.73
qe/Ce	ln(qe/Ce)	(1/Ce)	(1/Ce) + 1	$\epsilon = RT\ln((1/Ce) + 1)$	lnqe	ϵ^2
82.85	4.42	0.091	1.091	2.17	6.81	4.71
70.21	4.25	0.043	1.043	1.03	7.41	1.06
64.93	4.17	0.027	1.027	0.67	7.77	0.45
48.10	3.87	0.019	1.019	0.45	7.86	0.20

Adsorption Isotherms

In order to define how a solute interacts with an adsorbent and to maximize the utilization of the adsorbent, adsorption isotherms are a fundamental prerequisite for the design of an adsorption system^[7]. Most researchers have only utilized the Langmuir and Freundlich isotherms in explaining the adsorptive behaviour of fatty-acid soap molecules on minerals. In this study, other adsorption isotherm models such as Dubinin–Radushkevich (D–R) isotherm, Temkin and Elovich were additionally used for the assessment of the adsorptive behaviour of palmitate on calcite.

Langmuir Adsorption Isotherm

The Langmuir model can be presented by the equation below⁸.

$$\frac{C_e}{q_e} = \frac{1}{q_{max}K_L} + \frac{1}{q_{max}} C_e \quad (1)$$

Where: q_{max} is the monolayer adsorption capacity of the adsorbent, i.e. the maximum amount adsorbed; K_L is the Langmuir adsorption constant; C_e is the equilibrium palmitate concentration in the solution and q_e is the equilibrium palmitate concentration on calcite. Values of q_{max} and K_L are calculated respectively from the slope and the intercept of the plot of $\frac{C_e}{q_e}$ against C_e as shown in Figure 1.

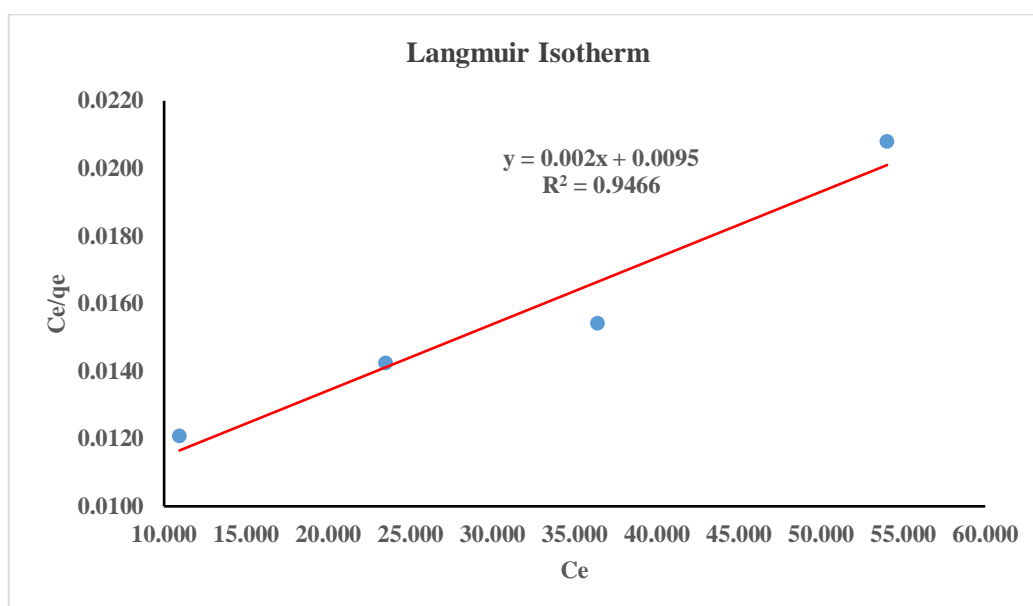


Figure 1: Langmuir adsorption isotherm

Figure 1 shows that q_{max} and K_L values are 500mg/L (5.0mgm^{-2}) and 2.1. This indicates a relatively high adsorption capacity, suggesting that significant amount of palmitate molecules were adsorbed from the solution.

Freundlich Adsorption Isotherm

Freundlich isotherm is used for modeling the adsorption on heterogeneous surfaces^[4,9,10]. The equation of the Freundlich adsorption model is expressed as:

$$\log q_e = \log K_F + \frac{1}{n} \log C_e \quad (2)$$

Where K_F is a constant related to the adsorption capacity (Freundlich constant) and $\frac{1}{n}$ is an empirical parameter related to the adsorption intensity. Values of K_F and are calculated from the slope and the intercept of the plot of $\log q_e$ vs. $\log C_e$ as shown in Figure 2.

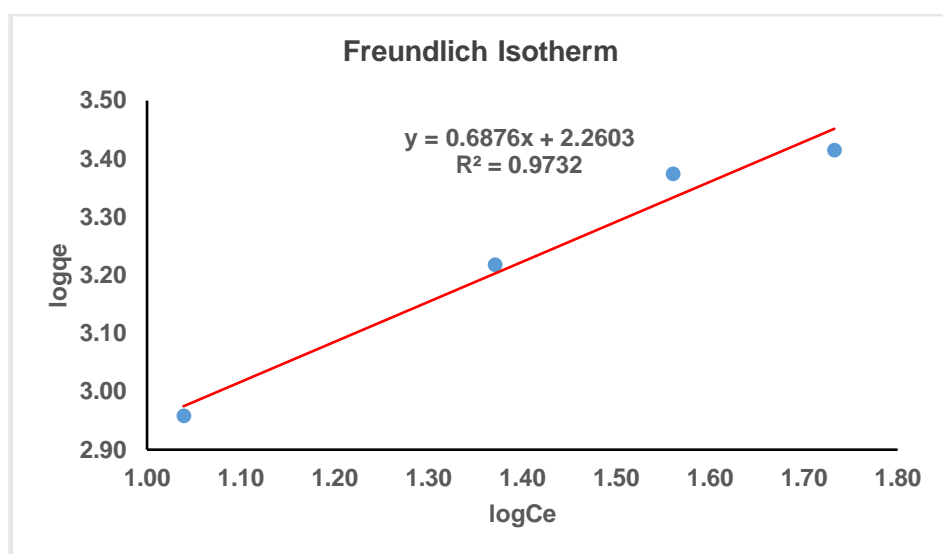


Figure 2: Freundlich Isotherm

Figure 2 presents the values of K_f and $1/n$ as 182 and 0.6876 respectively. The $1/n$ value (0.6876) is less than 1, indicating a heterogeneous surface with a variety of adsorption sites. This suggests that the adsorption process is complex and may involve multiple mechanisms^[4].

Dubinin–Radushkevich (D–R) isotherm

The physical and chemical features of soap molecules adhering to mineral surfaces cannot be adequately explained by Langmuir and Freundlich isotherms^[11]. D–R isotherm is commonly used to describe the sorption isotherms of single solute systems. The D-R isotherm is expressed as

$$\ln q_e = \ln q_m - k_D \varepsilon^2 \quad (3)$$

Where q_e is the palmitate molecules concentration (mg/L) that is adsorbed per unit mass of calcite, q_m is the D-R adsorption capacity (mg/L), k_D is the constant related with adsorption energy ($\text{mol}^2\text{kJ}/\text{J}^2$) and ε is the Polanyi potential^[10]. According to the equation (4), the Polanyi potential (ε) can be given as:

$$\varepsilon = RT \ln \left(1 + \frac{1}{C_e} \right) \quad (3a)$$

Where, R is the gas constant ($\text{kJK}^{-1} \text{mol}^{-1}$) and T is the temperature (K). The main energy of adsorption (E) is calculated by using the following formula:

$$E = \frac{1}{\sqrt{-2k_D}} \quad (3b)$$

Where, E gives information about the physical and chemical features of adsorption (Ismael *et al.*, 2016). The D–R isotherm is applied to the data obtained from the studies.

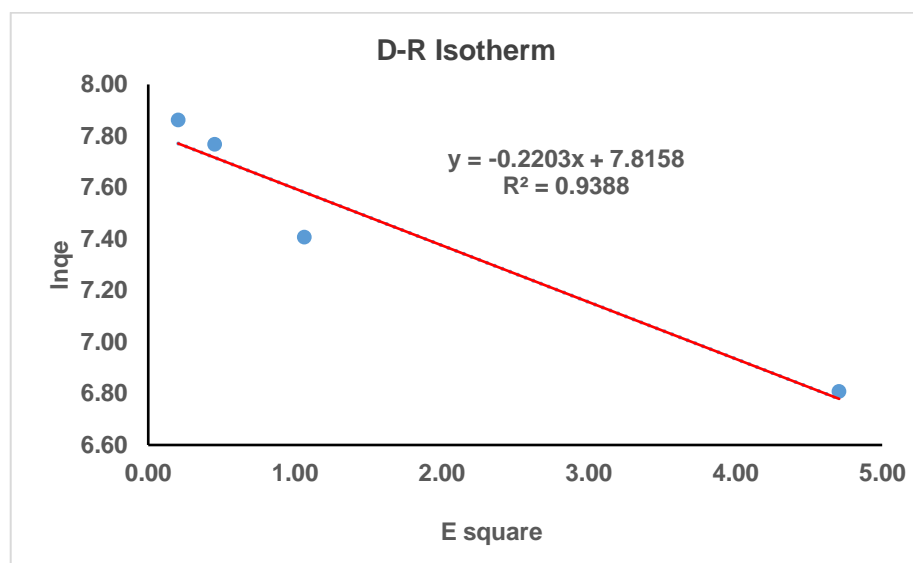


Figure 3: D-R Adsorption isotherm

As it is seen in Fig.3, the D–R plot yields a straight line. In the D–R isotherm, the values of the adsorption capacities q_m , adsorption energy constants k_D and the main adsorption energies E are calculated for palmitate adsorption onto calcite as 2.056mg/L, $0.223 \text{ mol}^2 \text{ k/J}^2$ and 1.51J respectively. These low values of adsorption energy show that the adsorption has a physical nature.

Temkin Adsorption Isotherm

The Temkin adsorption isotherm is a mathematical model that describes the adsorption of molecules onto a surface. The mathematical expression for Temkin's model is given by:

$$q_e = \text{Blog}(A) + \text{Blog}(C_e) = \frac{RT}{b_T} \log(A) + \frac{RT}{b_T} \log(C_e) \quad (4)$$

Where; A is Temkin isotherm equilibrium binding constant (L/g), C_e is equilibrium concentration (mg/L), q_e is the amount of adsorbate in the adsorbent at equilibrium (mg/g), R is universal gas constant (8.314 J/mol.K) and T is temperature (K).

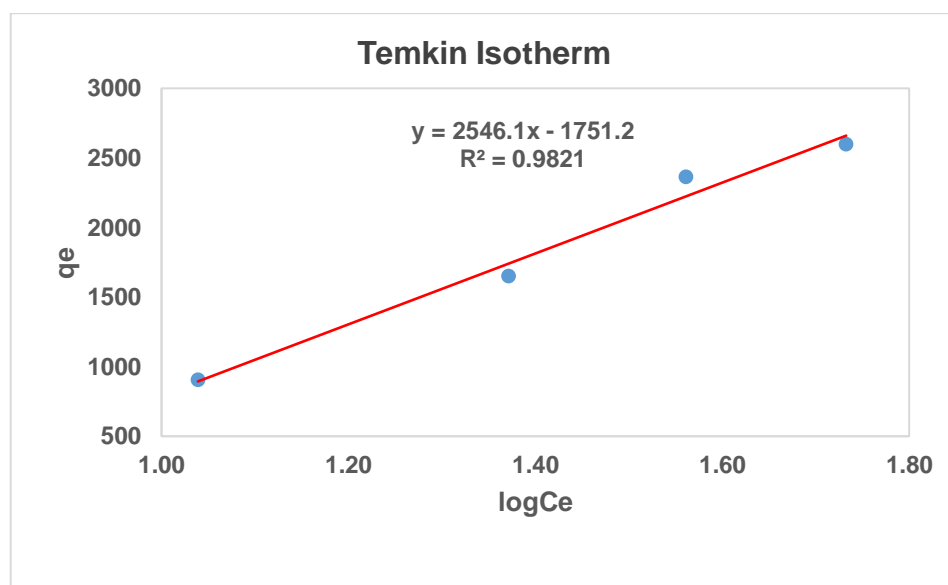


Figure 4: Temkin adsorption isotherm

Figure 4, presents a linear graph of q_e against $\log C_e$ with the values of b_T and A as 0.986 and 0.205 respectively. Since the constant b_T is positive, the adsorption process is exothermic^[12].

Elovich Adsorption Isotherm

The Elovich model is rooted in kinetic principles, suggesting that adsorption sites increase exponentially as more molecules are adsorbed, implying a multilayered adsorption process and the equation is given by:

$$\ln\left(\frac{q_e}{C_e}\right) = \ln(K_e Q_0) - \left(\frac{1}{Q_0}\right) q_e \quad (5)$$

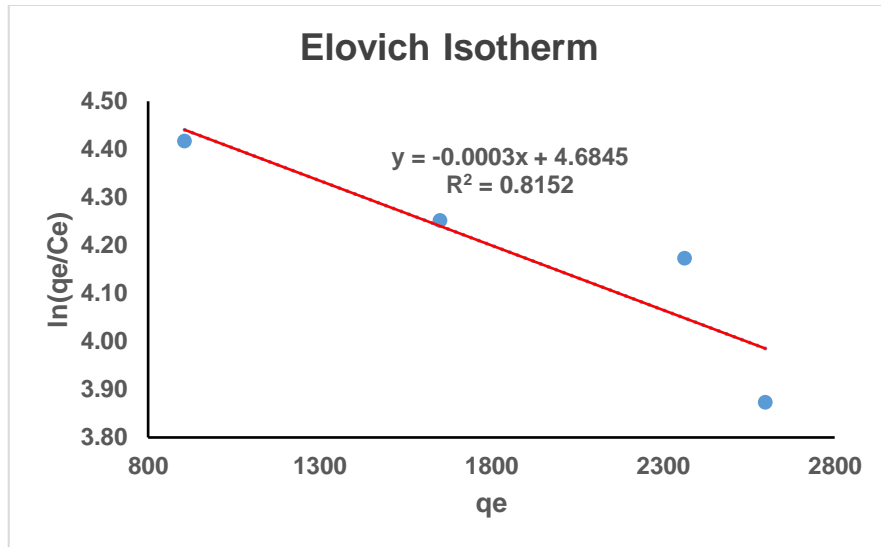


Figure 5: Elovich Adsorption isotherm

From the figure 5, the values of Q_0 and K_e are 3333 mg/g and 0.0325 min^{-1} respectively. 3333mg/g represents the maximum adsorption capacity of the adsorbent while the low value of K_e (0.0325 min^{-1}) suggests that the desorption rate is slow, indicating that the adsorbed palmitate molecules are strongly bound to the calcite surface.

Table 2. Comparison of adsorption Isotherm Parameters

Langmuir Adsorption Isotherm	R^2	$q_{max} \text{ (mg/L)}$	$K_L \text{ (l/mg)}$
	0.9466	500	2.1
Freundlich Adsorption Isotherm	R^2	$1/n$	$K_F \text{ (mg/l)}$
	0.9732	0.6876	182
Dubinin–Radushkevich (D–R) isotherm	R^2	K_D	q_m
	0.9388	$0.223 \text{ mol}^2\text{k/J}^2$	2.056 mg/L
Temkin Adsorption Isotherm	R^2	b_T	A
	0.9821	0.986	0.205
Elovich Adsorption Isotherm	R^2	K_e	Q_0
	0.8152	0.0325 min^{-1}	3333 mg/g

Strong connection between the Langmuir isotherm model and the experimental data is indicated by the high R^2 value (0.9466), which implies that the model correctly depicts the adsorption process. The q_{max} value (500 mg/L) suggests that calcite is an efficient adsorbent for palmitate and shows a reasonably high adsorption capacity of palmitate on calcite. Palmitate and calcite have a moderate affinity, as indicated by the K_L value (2.1 L/mg), which suggests that the adsorption process is advantageous but not particularly powerful. The Langmuir isotherm implies that palmitate assumes a uniform surface and forms a monolayer on the surface of calcite, which may not be the case in practice.

An excellent fit between the experimental data and the Freundlich isotherm model is indicated by the high R^2 value (0.9732), which implies that the model accurately depicts the adsorption process. The heterogeneous surface with a range of adsorption sites is indicated by the $1/n$ value (0.61876) being less than 1, and the

favorable adsorption process is indicated by the K_f value (180 mg/L), demonstrating that calcite has a high affinity for palmitate. On the surface of calcite, palmitate appears to form a multilayer, according to the Freundlich isotherm.

The high R^2 value (0.9388) suggests that the D-R isotherm model accurately represents the adsorption process of palmitate on calcite and shows a strong fit between the experimental data and the model. Palmitate molecules occupy the micropores on the surface of calcite, as suggested by the D-R isotherm, and the low K_D value (0.223 mol²/J²) suggests that the adsorption process requires little energy, indicating that calcite has a high affinity for palmitate. The moderate adsorption capacity indicated by the q_m value (2.056 mmol/g) further suggests that palmitate can adsorb onto calcite in a solution.

The Temkin isotherm model and the experimental data fit each other quite well, as indicated by the high R-Square value (0.9821), which suggests that the model correctly depicts the adsorption process of palmitate on calcite. The A_T value (0.205 L/mg) indicates a moderate adsorption capacity, indicating that calcite can effectively remove palmitate from the solution, and the Temkin isotherm assumes a uniform adsorption energy, indicating that the adsorption process proceeds with a consistent energy distribution. Strong interaction between palmitate and calcite is indicated by the b_T value (0.986 L/g), which implies that the adsorption process is advantageous.

TA satisfactory fit between the experimental data and the Elovich isotherm model is indicated by the R-Square value (0.8152), which implies that the model offers a plausible explanation of the adsorption process. A high adsorption capacity is indicated by the Q_0 value (3333 mg/g), which implies that the palmitate was successfully adsorbed on calcite from the solution. A longer contact time may be necessary for the adsorption process to attain equilibrium, as indicated by the slow adsorption rate indicated by the K_e value (0.0325 g/mg/min).

Best Fit Adsorption Isotherm

From table 2, it can be said that the adsorption isotherm that can best be used to describe palmitate adsorption on calcite is Temkin and Fruendlich isotherms having R-square values of 0.9821 and 0.9732 respectively.

Kinetic Analysis using Initial Rate-Differential analysis

Surface tension and % palmitate filtrate

Due to the variation effect of concentration change on surface tension seen in fatty-acid soap solutions, variable dimensions have been developed that allow the concentration of soap molecules to be measured using more affordable and accessible tools like contact angle and traveling microscopes.^[26] Figures 6(a) and 6(b) presents the relationship between the concentration of filtrates and contact time and the surface tension observed with contact time.

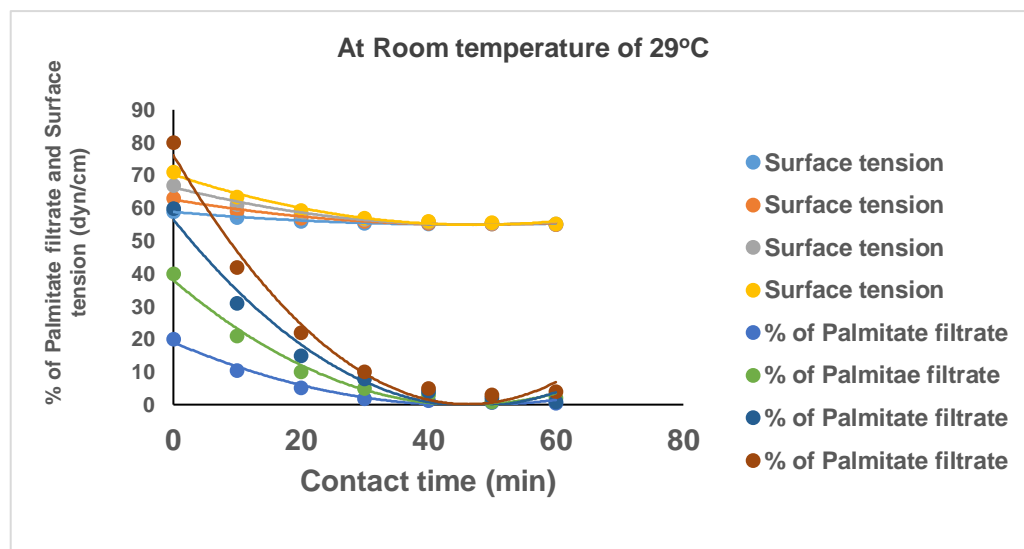


Figure 6(a): Nexus between surface tension and palmitate filtrate at 29°C

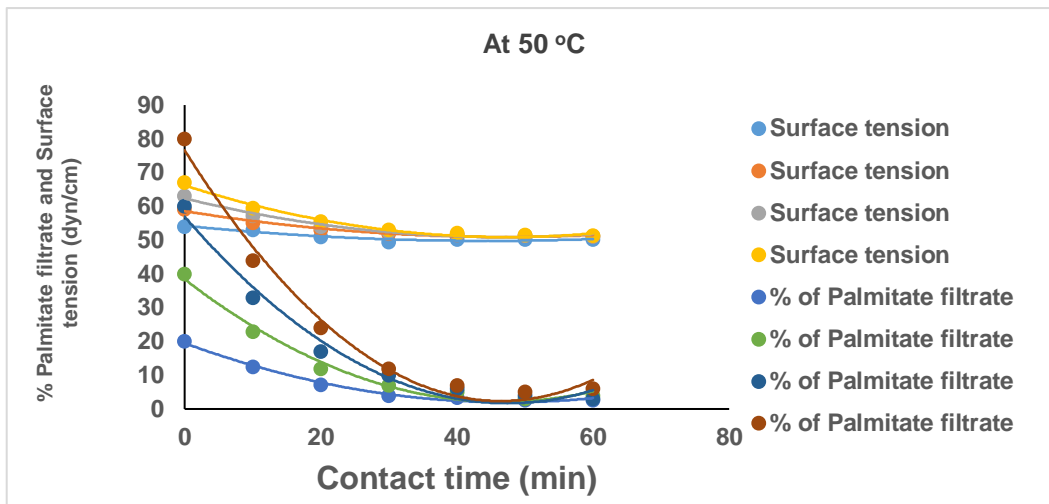


Figure 6(b): Nexus between surface tension and palmitate filtrate at 50°C

As the concentration of filtrate reduces with time, the surface tension decreases. This is because by pointing their hydrophilic heads toward the water and their hydrophobic tails toward the air, palmitate molecules, which are surfactants, lower surface tension. Surface tension falls as palmitate molecules' surfactant activity falls with decreasing concentration^[13,24,25].

Surface tension and % of palmitate adsorbed

Figures 7(a) and 7(b) present the relationship between palmitate adsorbed onto calcite with time and the effect of surface tension.

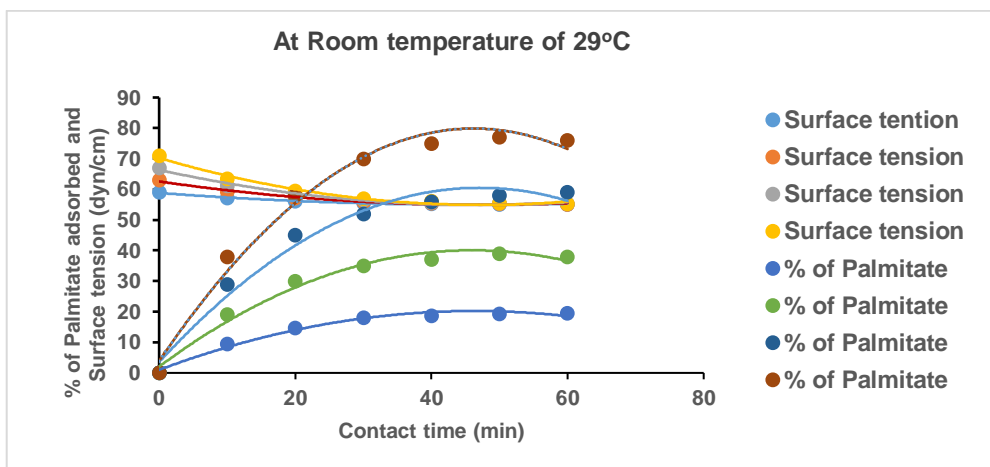


Figure 7(a): Nexus between surface tension and palmitate adsorbed at 29°C

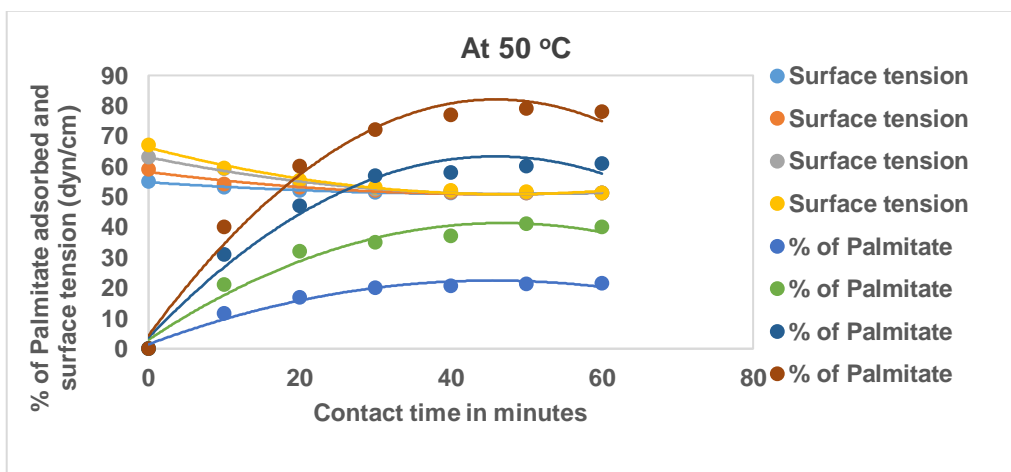


Figure 7(b): Nexus between surface tension and palmitate adsorbed at 50°C

The surface tension drops when more palmitate molecules are adsorbed onto calcite. This is due to the presence of both hydrophobic and hydrophilic areas in the palmitate molecules, which are surfactants. They align themselves so that their hydrophilic areas contact with the surrounding water and their hydrophobic regions interface with the calcite surface when they adsorb onto it.^[14]

Surface tension decreases as a result of the palmitate molecules' orientation, which lowers the interfacial energy between the water and the calcite surface.^[15] The cumulative sharp edges seen in figures 7(a) and 7(b) between 40 and 60 minutes are justified by the fact that the surface tension decreases as more palmitate molecules adsorb until a critical point is reached, after which it stays rather constant.

Determination of the Initial Rate of Palmitate adsorption on calcite

The initial rate method of differential analysis was utilized in analyzing and obtaining the kinetics parameters for the adsorption palmitate on calcite in aqueous solution and in order to obtain the initial rate of the adsorption reaction, a graph of initial concentration against contact time was plotted based on rate the rate equation^[16] expressed as:

$$\text{Rate, } R = - \frac{d[C]}{dt} \quad (6)$$

obtained from the slope of the respective graphs at 29 and 50°C respectively.

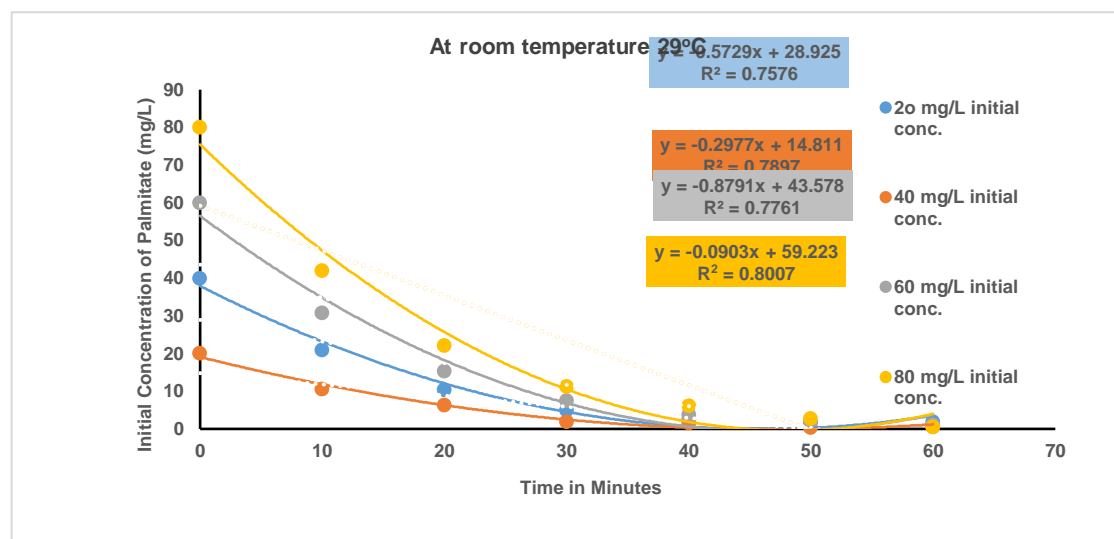


Figure 8(a): Initial concentration of palmitate with time (min) at 29°C

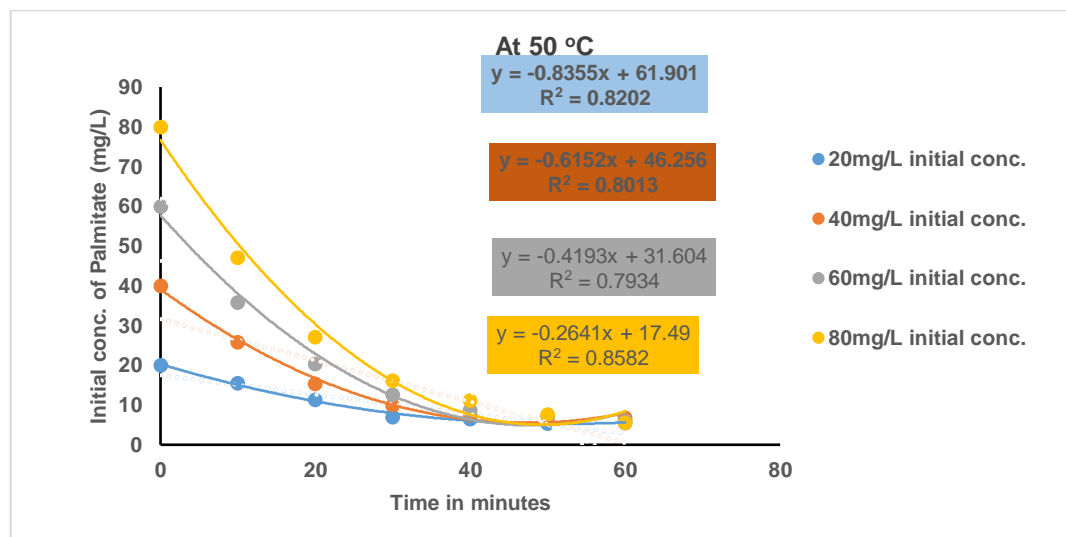


Figure 8(b): Initial concentration of palmitate with time (min) at 50°C

Table 3: Initial Rate of palmitate adsorption at 29 °C

Slope (Initial Rate, R)	Initial Concentration (C)	logC	logR
0.5729	20	1.30	-0.2419
0.2977	40	1.60	-0.5262
0.1791	60	1.78	-0.7469
0.0903	80	1.90	-1.0443

Table 4: Initial Rate of palmitate adsorption at 50 °C

Slope (Initial Rate, R)	Initial Concentration (C)	logC	logR
0.8255	20	1.3010	-0.0833
0.6152	40	1.6021	-0.2110
0.4193	60	1.7782	-0.3775
0.2641	80	1.9031	-0.5782

According to Tables 3 and 4, the initial rate rises in proportion to the initial concentration. Because more palmitate molecules are accessible for adsorption at greater initial concentrations, the initial rate is faster. Additionally, when more molecules are present, the frequency of collisions between palmitate molecules and the calcite surface rises, also increasing the initial rate.^[14,17,18]

Palmitate Adsorption Reaction Order and Rate Constant

Understanding the adsorption kinetics of palmitate onto calcite requires knowledge of the rate constant and reaction order. The rate constant indicates how quickly the adsorption process proceeds, and the reaction order explains how the adsorption rate varies with palmitate concentration.^[19]

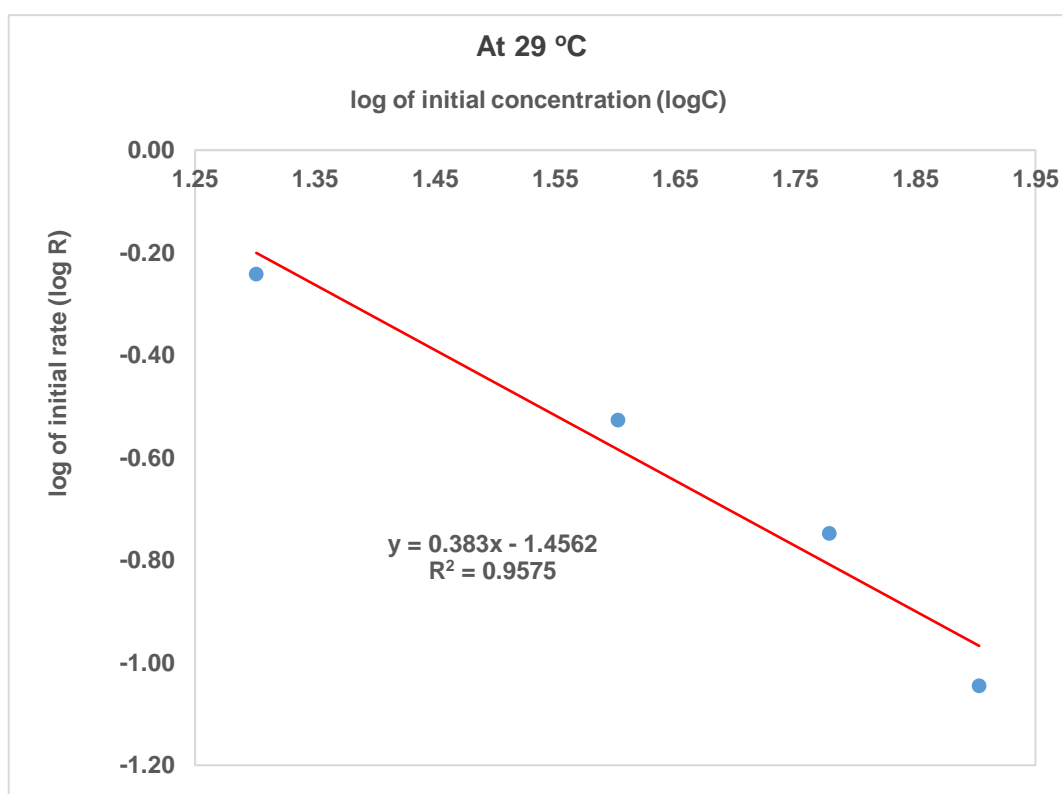


Figure 9(a): Determination of the rate constant and reaction order at room temperature

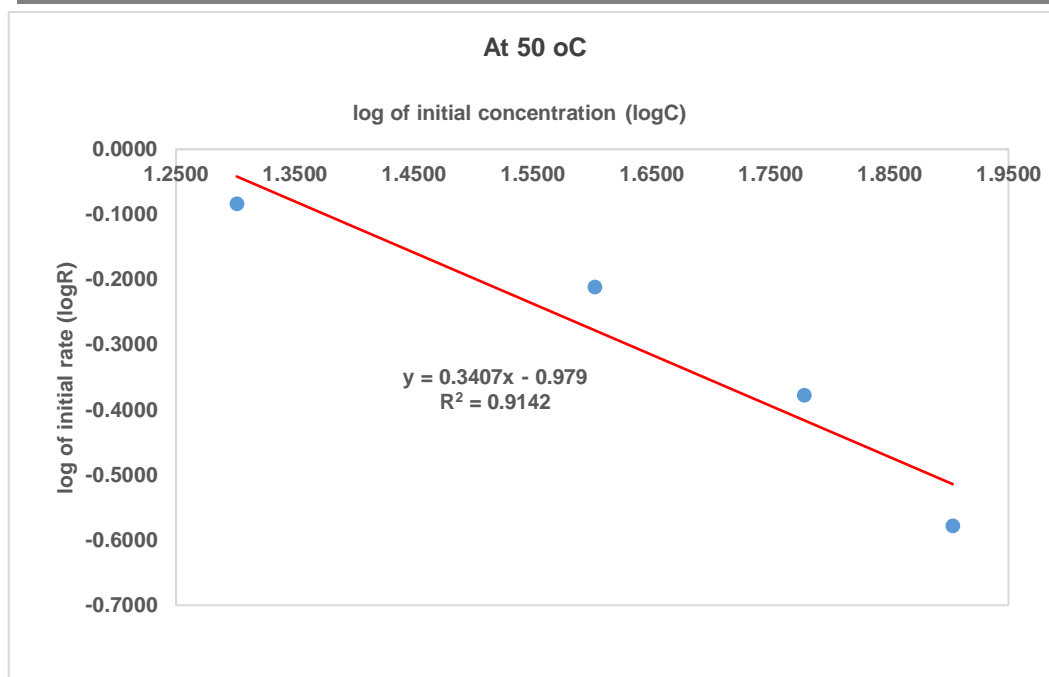


Figure 9(b): Determination of the rate constant and reaction order at 50°C

$$\log R = n \log C + \log K \quad (7)$$

When the rate equation (6) is compared to the equations on the graphs in figures 4a and 4b ($y = 0.383x - 1.4562$ & $y = 0.3407x - 0.979$), it can be said that the values of the reaction orders(n) and rate constants(R) at room temperature (29°C) are 0.3407 and 0.03498 mg/L/s and at 50°C are 0.3407 and 0.1050 mg/L/s respectively.

Palmitate adsorption reaction order

A reasonably high-order reaction is one with a reaction order larger than 2.5, which denotes a complex reaction mechanism^[11]. In addition to involving several stages, intermediates, and the adsorption of other ionic species other than palmitate ions at the calcite-water interface, the order of the adsorption of palmitate on calcite is highly dependent on the concentration of the reactant.

Palmitate adsorption rate constant

A proportionality constant that links a chemical reaction's rate to the reactant concentrations is called the rate constant. Reaction rate constant values can reveal information about the mechanism of a reaction, including the presence of intermediates, and it is well known that a greater rate constant denotes a quicker reaction rate. The rate constant for the adsorption of palmitate on calcite, as shown in figure 4, comparatively, indicates that external influences such temperature, pH modification, and agitation are necessary^[4]. In addition, Nwoko et al. confirmed that hydrogen ions disrupt the soap molecules' adsorption reaction on the mineral interface, which lowers the rate constant^[5].

Activation Energy for the Adsorption of Palmitate on Calcite

The Arrhenius equation was used to compute the value of the activation energy and the equation is given by:

$$\log K = -\frac{E_a}{2.303RT} + \log A \quad (8)$$

where K = rate constant for reaction at T ; A = constant called frequency factor for the reaction, $R = 0.008314$ J/mg·K. A plot of $\log K$ vs $\frac{1}{T}$ will give slope = $-\frac{E_a}{2.303R}$ ^[20]. From figures 4a and 4b, the values of temperatures and rate constants are presented in table 3:

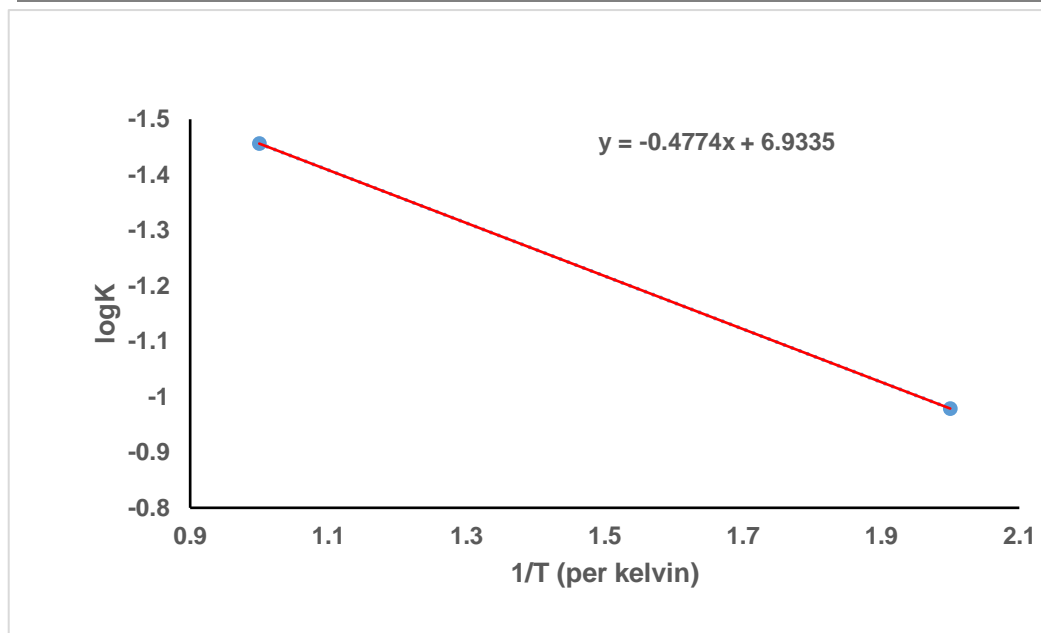


Figure 10: Graph of logK and 1/T

When the equation $\log K = -\frac{E_a}{2.303R} + \log A$ is compared to the equation $y = -0.4774x + 6.9335$ obtained from the graph in figure 5, the values of the activation energy and the frequency factor the adsorption of palmitate on calcite can be obtained from $-\frac{E_a}{2.303R} = -0.4774$ and $\log A = 6.9335$ resulting to $9.14 \times 10^{-3} \text{ J/mg.K}$ or 9.14 J/mol.K and $8.58 \times 10^6 \text{ s}^{-1}$.

Using the differential analysis method, the activation energy and frequency factor for the adsorption of oleate soap onto a Nigerian hematite in an aqueous medium were calculated between 29 and 60°C at $57.1 \text{ kJ mol}^{-1} \text{ K}^{-1}$ and $4.0 \times 10^3 \text{ liter mol}^{-1} \text{ min}^{-1}$, respectively, showing that the chemical processes are the slow, rate-determining step and that the reaction progresses relatively swiftly^[21].

In contrast to this study, which employs the initial rate method to determine the activation and frequency factor for the adsorption of palmitate soap on Nigerian calcite in aqueous solution between 29 and 50 °C, the frequency factor is higher and the activation energy obtained is lower, suggesting that there is less steric hindrance or energy barrier in the adsorption of palmitate on Nigerian calcite due to a higher degree of collision between the palmitate soap molecules and the calcite's available adsorption sites.^[4,22]

Thermodynamics Studies

An essential component of comprehending the thermodynamics of adsorption processes is the Gibbs free energy (ΔG)^[20], which was calculated using the relationship shown in equation (9) and is shown in table 6..

$$\Delta G = -RT \ln K \quad (9)$$

Table 6: Thermodynamic variables

$\Delta G = -RT \ln K$ (kJ)	Temperature (K)
-82	302
-59	323

When the Gibb's free energy equation

$$\Delta G^\circ = \Delta H^\circ - T \Delta S^\circ \quad (10)$$

is compared to the equation obtained from figure 11, $y = 1.0952x - 412.76$, then the values of ΔH° and ΔS° are -412.76 and 1.0952 respectively.

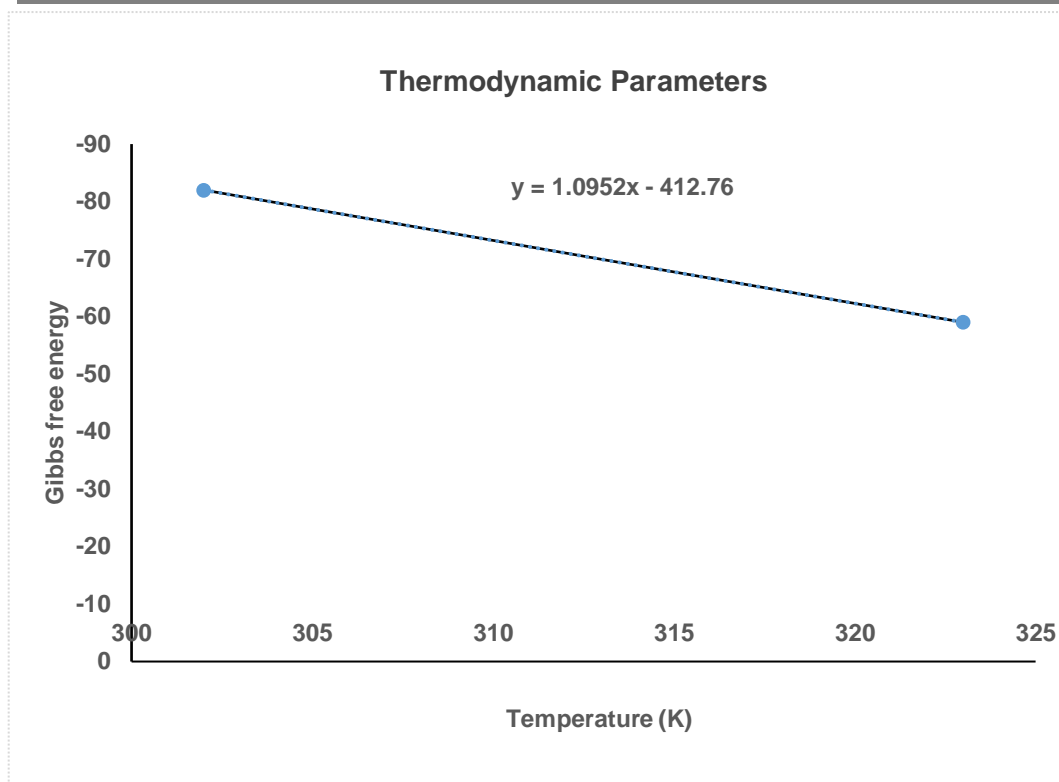


Figure 11: Determining the thermodynamic variables

An exothermic adsorption process that releases heat energy is indicated by a negative value of ΔH . The substantial negative value of ΔH indicates a persistent adsorption complex by implying significant intermolecular interactions between palmitate and calcite. The adsorption process is more disordered or unpredictable when the ΔS value is positive, indicating that the palmitate molecule or the calcite surface undergoes conformational changes.^[27]

CONCLUSION

This work highlights the significance of comprehending the kinetic and thermodynamic elements of adsorption processes. The findings demonstrate how palmitate can be adsorbed onto calcite surfaces for a range of industrial uses. Understanding the adsorption mechanisms of fatty-acid soap molecules onto mineral surfaces is significantly impacted by the findings. The findings can be applied to optimize the adsorption conditions for various industrial applications, such as flotation, detergency, and corrosion inhibition.

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APPENDIX

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Solution

SAMPLE A_20250508_152840_G01_S01_M01-Evaluation report (SAMPLE A_20250508_152840_G01_S01_M01)

General information

Analysis date	2025-05-08 15:38:36	Measurement start time	2025-05-08 15:29:35
Analyst	Default	Operator	Default
Sample name	SAMPLE A	Comment	
Measured data name	C:\WallPaper\08-05-2025B\SAMPLE A_20250508_152840_G0...	Memo	

Peak list

No.	2 θ , °	d, Å	Height, cps	FWHM, °	Int. I., cps*	Int. W., °	Asymmetry	Decay(η L/mL)	Decay(η H/mH)	Size, Å
1	26.789(14)	3.3252(17)	2909(182)	0.197(10)	654(23)	0.22(2)	2.1(7)	0.00(10)	0.6(3)	432(23)
2	28.41(5)	3.139(6)	228(39)	0.18(12)	76(10)	0.33(10)	1.3(18)	1.1(11)	1.5(10)	468(298)
3	29.653(14)	3.0102(14)	20608(499)	0.17(2)	4058(893)	0.20(5)	1.5(3)	0.19(2)	0.30(9)	503(64)
4	29.754(6)	3.0003(6)	15392(349)	0.09(2)	1549(892)	0.10(6)	1.5(3)	0.19(2)	0.30(9)	984(221)
5	36.284(15)	2.4739(10)	240(40)	0.17(4)	43(9)	0.18(7)	3(4)	0.0(8)	0.0(16)	523(129)
6	39.67(5)	2.270(3)	338(54)	0.20(3)	74(10)	0.22(6)	1.3(12)	0.0(6)	0.2(7)	442(73)
7	43.37(3)	2.0845(15)	377(64)	0.19(6)	128(9)	0.34(8)	0.6(5)	1.2(7)	1.2(5)	466(154)
8	47.71(4)	1.9045(14)	350(60)	0.28(5)	141(10)	0.40(10)	0.9(5)	1.2(5)	0.2(4)	326(63)
9	48.737(10)	1.8669(4)	606(83)	0.152(16)	136(8)	0.22(4)	1.8(4)	0.2(3)	1.5(4)	600(63)
10	54.86(5)	1.6722(15)	153(32)	0.21(10)	47(7)	0.31(11)	2(2)	1.1(9)	0.0(13)	435(204)
11	61.259(10)	1.5119(2)	1415(151)	0.151(17)	395(13)	0.28(4)	0.9(3)	1.5(2)	1.1(3)	641(74)

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Solution

No.	2 θ , °	Phase Name	Chemical Formula	Card No	Norm. I.	Profile Type	Distributi...	Degree of Orientation
1	26.789(14)	Unknown			16.12	Split pseudo-Voigt	-	-
2	28.41(5)	Unknown			1.87	Split pseudo-Voigt	-	-
3	29.653(14)	Calcite, syn: 1 0 4	Ca (C O3)	04-006-6528	100.00	Split pseudo-Voigt	-	-
4	29.754(6)	Unknown			38.18	Split pseudo-Voigt	-	-
5	36.284(15)	Calcite, syn: 1 1 0;Zincite, syn:...	Ca (C O3),Zn O	04-006-6528,01-07...	1.05	Split pseudo-Voigt	-	-
6	39.67(5)	Calcite, syn: 1 1 3	Ca (C O3)	04-006-6528	1.81	Split pseudo-Voigt	-	-
7	43.37(3)	Calcite, syn: 2 0 2;Quartz: 2 0 0	Ca (C O3),Si O2	04-006-6528,00-00...	3.15	Split pseudo-Voigt	-	-
8	47.71(4)	Calcite, syn: 0 1 8;Zincite, syn:...	Ca (C O3),Zn O	04-006-6528,01-07...	3.48	Split pseudo-Voigt	-	-
9	48.737(10)	Calcite, syn: 1 1 6	Ca (C O3)	04-006-6528	3.35	Split pseudo-Voigt	-	-
10	54.86(5)	Unknown			1.16	Split pseudo-Voigt	-	-
11	61.259(10)	Quartz: 2 1 1	Si O2	00-001-0649	9.73	Split pseudo-Voigt	-	-

No.	2 θ , °	Ring Factor	β Cluster
1	26.789(14)	-	-
2	28.41(5)	-	-
3	29.653(14)	-	-
4	29.754(6)	-	-
5	36.284(15)	-	-
6	39.67(5)	-	-
7	43.37(3)	-	-
8	47.71(4)	-	-
9	48.737(10)	-	-
10	54.86(5)	-	-
11	61.259(10)	-	-

Qualitative Analysis Results

Phase name	Formula	Figure of merit	Phase reg. detail	Space Group	DB Card Number
Calcite, syn	Ca (C O3)	1.340	S/M(PDF-4 Minerals 2025)	167 : R-3cH	04-006-6528
Zincite, syn	Zn O	2.750	S/M(PDF-4 Minerals 2025)	186 : P63mc	01-070-8070
Quartz	Si O2	3.418	S/M(PDF-4 Minerals 2025)	154 : P3221	00-001-0649

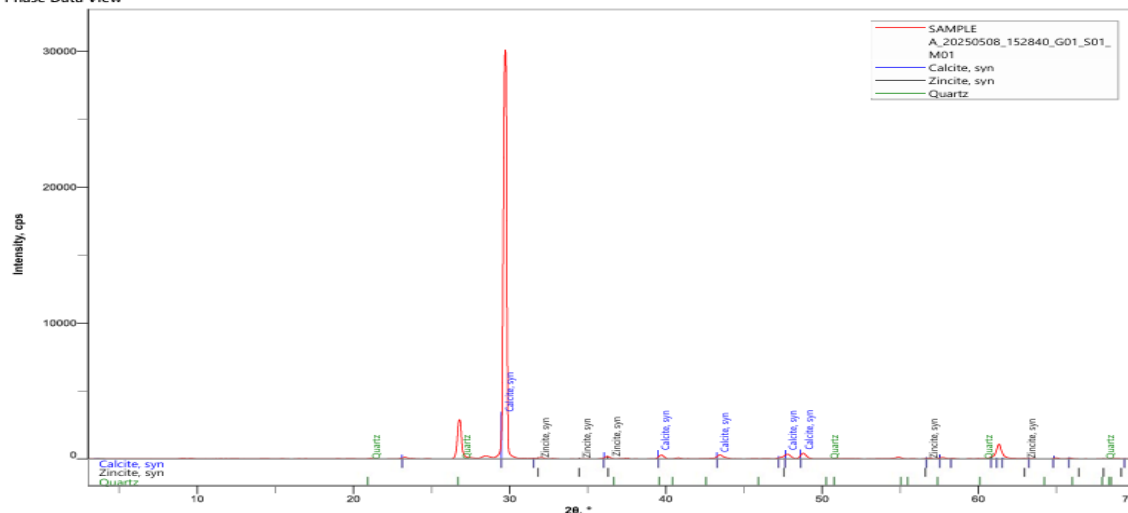
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Solution

Phase Data View



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