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Integrating Physical Chemistry and Sustainability: An Educational Study of Linear and Non-Linear Adsorption Isotherms Using Chitosan in Wastewater Remediation

Tanishka Chauhan,^a Santunu Barua^b and Alexandre H. Pinto

Sustainability Spotlight

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Tanishka Chauhan,^a Santunu Barua^b and Alexandre H. Pinto^{*a}Received 00th January 20xx,
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Water scarcity is an escalating global challenge. Addressing this issue requires not only technological solutions but also educational strategies that integrate sustainability into chemistry curricula. Herein, we report the design and implementation of a two-session undergraduate Physical Chemistry laboratory experiment focused on the adsorption of the synthetic food dye tartrazine onto chitosan, a sustainable biopolymer. The experiment contextualizes adsorption thermodynamics within wastewater remediation and the United Nations Sustainable Development Goals, particularly SDG 6 (Clean Water and Sanitation). Students investigated adsorption equilibrium by measuring tartrazine uptake over a range of initial concentrations at two temperatures (25 and 50 °C). Equilibrium data were analyzed using both linear and non-linear forms of the Temkin adsorption isotherm, enabling a critical comparison of modeling approaches commonly used in the adsorption literature. Apparent thermodynamic parameters (ΔH_{app} , ΔG_{app} , and ΔS_{app}) are derived from the temperature dependence of the Temkin isotherm constant, providing a quantitative link between experimental data and thermodynamic theory. This laboratory activity emphasizes the physical meaning and limitations of linearized models while introducing non-linear regression methods that are often underrepresented in undergraduate instruction.

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1 Introduction

Water scarcity is a prevalent environmental problem worldwide. A recent study evaluating population exposure to current and future water scarcity concluded that 55% of the global population is currently exposed to clean water scarcity at least one month per year.¹ Intending to mitigate social and environmental issues such as hunger, health, education, and clean water, among others, in 2015, the United Nations (UN) defined 17 Sustainable Development Goals.² The water scarcity issue is dealt with in the Sustainable Development Goal (SDG) 6 – Clean Water and Sanitation. One of the targets of this SDG is to increase water-use efficiency and reduce water scarcity by 2030, underscoring the need for sustainable water treatment solutions.³

A widely used water remediation technique is solid-liquid adsorption. The adsorption is based on the intermolecular interactions between the pollutant molecule (adsorbate) and functional groups on the solid surface (adsorbent), followed by some separation technique to separate the adsorbent from the liquid phase, leaving the liquid phase with a decreased pollutant concentration.⁴ In the literature, different categories of materials have been used as adsorbents, for instance, activated carbon, biomass, zeolites, metal oxides, polymers, and graphene oxide.⁵

A promising adsorbent is the biopolymer chitosan. Chitosan is derived from chitin, the second most abundant biopolymer after cellulose. Chitin is found in crustacean shells, for instance, in prawns and crabs.⁶ Some features that make chitosan a promising adsorbent are the chitin abundance and the simplicity of the deacetylation process to convert it to chitosan, biodegradability, relatively low cost, non-toxicity, low solubility in water, and the possibility to interact with dyes through different types of interactions, such as electrostatic interaction, hydrogen bonding, and π - π stacking.⁷

Synthetic dyes used in food products — notably tartrazine ($C_{16}H_9N_4Na_3O_5$), also known as FD&C Yellow 5 — are water-soluble, enter wastewater streams through manufacturing and food processing, and have been detected in effluents and

^a Manhattan University, Kakos School of Arts & Sciences, Department of Biological & Chemical Sciences, 4513 Manhattan College Parkway, New York, NY 10471

^b Manhattan University, School of Engineering, Department of Civil & Environmental Engineering, 4513 Manhattan College Parkway, New York, NY 10471

* alex.pinto@manhattan.edu.

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surface waters at $\mu\text{g/L}$ levels, underscoring their potential role as emerging aquatic contaminants.⁸ Toxicological studies further demonstrate that tartrazine exposure can cause oxidative stress, developmental, and histopathological damage in aquatic organisms, suggesting ecological risk even at relatively low concentrations.^{9,10}

Even though tartrazine is commonly detected in surface waters at $\mu\text{g/L}$ levels, reported toxicological thresholds vary depending on species and exposure duration. Acute toxicity values for aquatic organisms are generally observed in the mg/L range, whereas chronic exposure studies have reported oxidative stress, developmental alterations, and histopathological effects at lower concentration levels.^{11–13} These findings suggest that ecological risk assessment depends not only on instantaneous concentration but also on long-term exposure and environmental persistence.

The scientific literature presents some examples of chitosan application as an adsorbent for removing tartrazine from simulated wastewater. For example, Dotto et al. studied the adsorption kinetics of tartrazine adsorption onto chitosan and chitin at five different pH values.¹⁴ They concluded that the optimum adsorption happened at pH 3 due to chemical interactions between chitosan and tartrazine. However, the authors did not provide further information about which type of chemical interaction they referred to.¹⁴ Fransina et al. also studied the tartrazine adsorption kinetics onto chitosan at different pH values, unlike Dotto et al., they concluded that pH 9 was the optimum pH.¹⁵ Additionally, they studied the contrast of modeling the kinetics by using the linear and non-linear versions of the pseudo 1st order kinetics model, and concluded that the non-linear model produced a superior fit to the experimental data.¹⁵ Zhang et al. studied the adsorption isotherms of tartrazine onto chitosan at different temperatures, and modeled the adsorption based on the multilayer statistical physics method.¹⁶

Leveraging the experience of our research group in working with methods for tartrazine removal from simulated wastewater and the use of chitosan as an adsorbent to remediate simulated wastewater from synthetic dyes, we developed and implemented a two-lab session experiment applied in a Physical Chemistry Lab I course about the thermodynamic parameters of tartrazine adsorption onto chitosan.^{17,18}

The adsorption experiments were carried out at two different temperatures, 25 and 50 °C, to analyze the influence of temperature on the adsorption equilibrium. The thermodynamic parameters were derived from using the non-linear and linear versions of the Temkin isotherm. And the values obtained for the isotherm constant were later used to calculate the thermodynamic functions, such as ΔH , ΔG , and ΔS related to the adsorption process at each temperature. Then, students reflected on how this experiment fitted into the context of the 12 Green Chemistry Principles and the United Nations (UN) Sustainable Development Goals.^{2,19,20} This experiment combines concepts of Green Chemistry with Physical Chemistry, providing students with the opportunity to learn about the thermodynamic models described by non-linear

equations, which are generally overlooked in undergraduate chemistry courses in favor of linear models.

Although tartrazine has been detected in environmental waters at $\mu\text{g L}^{-1}$ levels, the concentration range selected in this study was chosen to ensure reliable spectrophotometric quantification and meaningful thermodynamic modelling within the time constraints of an undergraduate laboratory. At trace concentrations, adsorption studies often require more sensitive analytical techniques or preconcentration strategies to achieve reliable quantification.^{21–24} Furthermore, removal of contaminants at environmentally relevant $\mu\text{g L}^{-1}$ levels typically involves modified or high-surface-area adsorbents specifically engineered for trace-level uptake.²⁵ The objective of this experiment is therefore educational, to illustrate adsorption thermodynamics and model comparison, rather than to present a field-optimized remediation system.

2 Materials and Methods

2.1 Student cohort and learning objectives

This activity was developed in the Physical Chemistry Laboratory course at Manhattan University, in New York City. The cohort had a total of six undergraduate students, all of whom were either juniors or seniors. Thermodynamics is the main topic of this lab course. All the students in the cohort had either completed the Physical Chemistry I – Thermodynamics lecture course or were taking this course concurrently with the lab course. The students worked in groups of 2 students during the whole experiment.

The main focus of this experiment was to show the students how the thermodynamic functions, such as ΔH , ΔG , and ΔS could be applied in the context of an adsorption experiment. In addition to that, a second objective was to provide the students with information about how to connect thermodynamics with Green Chemistry and sustainability topics. Finally, a third objective was to compare the non-linear and the linear Temkin adsorption models, and verify whether there are differences in the results produced by each model or not.

2.2 Problem situation to be solved

Before performing the experiment, the students were required to watch a pre-lab presentation recorded by the course instructor covering topics like adsorption definition and differences between adsorption and absorption, molecular structures of the adsorbent, chitosan, and the adsorbate, tartrazine, definitions of removal percentage and adsorption capacity, definitions and examples of adsorption isotherms, and the equations representing the linear and non-linear versions of Temkin isotherm.

In order to provide a sustainability context to the experiment, the students were presented with the following problem situation to be solved:



You are the chemistry operations director in an environmental consulting and analysis company. Your company was hired by a mid-size food processing plant that discharges wastewater containing significant amounts of tartrazine (a food azo dye).

The plant is evaluating a low-cost treatment step using chitosan powder, which could be produced from local seafood waste. Your laboratory obtained a commercial chitosan powder and used it as an adsorbent in tartrazine adsorption experiments performed at 25 °C and 50 °C. Previous knowledge in your team indicates that this system is likely to follow the Temkin adsorption isotherm models. However, at this point, your team is unsure which version of the Temkin isotherm is better, the linear or the non-linearized version. From the experiments performed, your team should estimate the Temkin constants K_T , both linear and nonlinear fits, the apparent thermodynamic constants K_{app} and the apparent thermodynamic parameters ΔH_{app} , ΔG_{app} , and ΔS_{app} . These results will be used to advise the plant on the most efficient process to adopt.

2.3 Experimental Procedure:

Chitosan medium molecular weight (Sigma-Aldrich) and tartrazine (Fisher Chemicals) were used without any purification. A tartrazine stock solution with a concentration of 300 mg/L was prepared by weighing 0.0600 g of tartrazine in 200 mL of deionized water. This stock solution was used to prepare tartrazine solution samples diluted in deionized water, with 45 mL each, and initial concentrations equal 10, 20, 30, 40, and 50 mg/L. Initially, 5 mL was taken from each tube with different initial concentrations, and the UV-vis spectra of these samples were collected to monitor the intensity of the peak centered at 426 nm, which relates to the tartrazine absorption in the visible range. These samples were used to determine the initial tartrazine concentration according to the calibration curve previously prepared by the instructor, the removal percentage, and the adsorption capacity.

Then, 0.5 g of chitosan was added to each tube, and the tubes were transferred to a shaking table, which was used as a means to produce agitation and contact between the chitosan and the tartrazine solution. The shaking table speed was adjusted to 500 rpm, and the temperature was set either to 25 or 50 °C. For a period of 30 minutes, every 5 minutes, about 3 mL was withdrawn from each sample, and allowed to decant for about one hour to separate the solution from the chitosan. The supernatant of each time point for each of the samples was separated from the chitosan, and their UV-vis spectra were collected to track the intensity of the tartrazine absorption peak centered at 426 nm. Then, the tartrazine remaining concentration in solution, the removal percentage, and the adsorption capacity at each time point for each sample.

Both the experiments performed at 25 and 50 °C were carried out in duplicate. So, the students could calculate average and standard deviation values for each thermodynamic function.

2.4 Data Analysis

From the slope of the calibration curve previously prepared by the instructor (Fig. S1 from the Supporting Information file), and the tartrazine absorption intensity peak at 426 nm, firstly, the students could calculate the tartrazine remaining concentration for each time point (C_t), measured in $\text{mg}\cdot\text{L}^{-1}$, using the Eq. (1):

$$C_t = \frac{Abs_t^{426nm}}{Slope} \quad (1)$$

Where Abs_t^{426nm} is the tartrazine absorption intensity peak at 426 nm at a certain time point, and $Slope$ is the calibration curve slope, which has the $\text{L}\cdot\text{mg}^{-1}$ units.

Once the C_t had been calculated, it was possible to calculate the tartrazine removal percentage $R_t(\%)$, which measured the percentage of the tartrazine removed, in relation to the initial tartrazine concentration, for each time point of the sample collected. The $R_t(\%)$ was calculated according to Eq. (2):

$$R_t = \left(\frac{C_0 - C_t}{C_0} \right) \times 100\% \quad (2)$$

Where C_0 is the tartrazine initial concentration in solution, in $\text{mg}\cdot\text{L}^{-1}$. In this case, the C_0 , like C_t , was calculated based on the slope of the calibration curve, as shown in Eq. (1), instead of using the nominal initial concentration value.

After calculating the $R_t(\%)$, the students calculated the adsorption capacity for each time point (q_t). The adsorption capacity (q_t) measured how many mg of tartrazine could be adsorbed per gram of chitosan at each time point of the sample collected. The q_t is measured in mg of tartrazine/g of chitosan. The q_t was calculated according to Eq. (3):

$$q_t = \left(\frac{C_0 - C_t}{m} \right) \times V \quad (3)$$

Where, m = mass of chitosan used in the experiment (0.5 g), and V = volume of tartrazine used in each experiment (40 mL).

After calculating the q_t , students proceeded to the calculations related to the Temkin isotherm. The linear version of the Temkin isotherm equation could be calculated using Eq. (4):²⁶

$$q_e = q_T \times \ln(K_T) + q_T \times \ln(C_e) \quad (4)$$

Where: $q_T = (q_m RT/b)$ = adsorption capacity per unit binding energy (mg/g), q_e = equilibrium adsorption capacity (mg/g), q_m = maximum adsorption capacity (mg/g), b = empirical parameter of Temkin model related to the heat of adsorption ($\text{J}\cdot\text{mol}^{-1}$), K_T = Temkin isotherm equilibrium binding constant ($\text{L}\cdot\text{mg}^{-1}$), C_e = tartrazine remaining concentration at equilibrium ($\text{mg}\cdot\text{L}^{-1}$), R = ideal gas constant ($8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$), and T = temperature where the isotherm data was collected (K).

The equilibrium adsorption capacity (q_e) and the equilibrium tartrazine remaining concentration (C_e) were approximated as



the adsorption capacity (q_t) and tartrazine remaining concentration at $t = 30$ minutes.

To obtain the q_T and K_T , students plotted a graph of q_e vs $\ln(C_e)$, and performed the linear fit to this equation using Microsoft Excel. The slope of the linear fit was equal to the q_T . Whereas, the intercept was equal to the product $q_T \times \ln(K_T)$. So, the Temkin isotherm equilibrium binding constant (K_T) could be calculated according to Eq. (5):

$$K_T = e^{\left(\frac{\text{intercept}}{q_T}\right)} \quad (5)$$

The non-linear model of the Temkin isotherm is represented by Eq. (6):²⁶

$$q_e = q_T \times \ln(K_T C_e) \quad (6)$$

The parameters q_T and K_T were obtained from the non-linear fit of Eq. (6) by using a free graphing software called SciDavis.

The K_T values for each experimental condition, both from the linear and non-linear models, were converted to an apparent equilibrium constant (K_{app}). Then, K_{app} values were later used to calculate the apparent values for ΔH , ΔG , and ΔS . The conversion from K_T to K_{app} was necessary because the equilibrium constant (K_{app}) used for the calculation of the ΔH and the ΔG should be dimensionless, which is not the case of K_T , which has units of $L \cdot mg^{-1}$. The conversion from K_T into K_{app} was accomplished by the Eq. (7):²⁷

$$K_{app} = K_T \times C_{adsorbate}^\circ \times MW_{adsorbate} \quad (7)$$

Where: K_{app} = apparent equilibrium constant for the adsorption process (dimensionless), K_T = Temkin isotherm equilibrium binding constant ($L \cdot mg^{-1}$), $C_{adsorbate}^\circ$ = tartrazine standard molar concentration ($1 \text{ mol} \cdot L^{-1}$), $MW_{adsorbate}$ = tartrazine molar mass ($534.3 \times 10^{-3} \text{ g} \cdot \text{mol}^{-1}$).

The ΔH_{app} of the adsorption process was calculated using a two-points version of the van't Hoff equation (Eq 8a), and solving it for ΔH_{app} , as shown in Eq. (8b):

$$\ln\left(\frac{K_{app}^{TB}}{K_{app}^{TA}}\right) = \frac{\Delta H_{app}}{R} \left(\frac{1}{T_B} - \frac{1}{T_A}\right) \quad (8a)$$

$$\Delta H_{app} = \left(\ln\left(\frac{K_{app}^{323K}}{K_{app}^{298K}}\right)\right) \times \left(\frac{1}{2.69 \times 10^{-3}}\right) \quad (8b)$$

The ΔG_{app} of the adsorption process was calculated using the Eq. (9):

$$\Delta G_{app} = -RT \ln(K_{app}) \quad (9)$$

Since the R is used with units of $J \cdot \text{mol}^{-1} \cdot K^{-1}$ and the temperatures are given in K . So, the ΔG_{app} will be given in $J \cdot \text{mol}^{-1}$.

The ΔS_{app} of the adsorption process was calculated using Eq. (10). The ΔS_{app} units will be $J \cdot K^{-1}$.

$$\Delta S_{app} = \frac{\Delta H_{app} - \Delta G_{app}}{T} \quad (10)$$

The students calculated ΔH_{app} , ΔG_{app} , and ΔS_{app} using the K_T data from both the linear (Eq 5) and non-linear models (Eq 6), for 25 and 50 °C.

The thermodynamic parameters derived from adsorption isotherm constants, including the Temkin equilibrium constant, are appropriately referred to as apparent thermodynamic quantities (ΔH_{app} , ΔG_{app} , and ΔS_{app}) because the isotherm constant does not represent a true thermodynamic equilibrium constant in the rigorous sense. In adsorption systems, the equilibrium constant obtained from isotherm modelling reflects a complex combination of surface heterogeneity, adsorbate-adsorbent interactions, and non-ideal behavior rather than a well-defined standard-state equilibrium between bulk phases. Moreover, the Temkin isotherm incorporates assumptions regarding a linear decrease in adsorption energy with surface coverage, meaning that the extracted constant is an effective or averaged parameter rather than a fundamental thermodynamic quantity. Consequently, the thermodynamic functions calculated from the temperature dependence of the Temkin constant describe the overall energetic trend of the adsorption process rather than absolute thermodynamic state functions, justifying the use of the "apparent" designation.^{21,23}

3 Results and Discussions

3.1 Experimental Results

Fig. 1 (a) shows a typical set of tartrazine absorption spectra vs time in contact with chitosan. The tartrazine maximum absorption peak centered around 426 nm decreases systematically as the contact time with chitosan increases.

Although a slight decrease in absorbance is observed up to 30 min, the variation between 25 and 30 min was within experimental uncertainty ($\pm 5\%$, in average), and no statistically significant change in the removal percentage was detected beyond this time. For the purposes of this laboratory experiment, equilibrium was operationally defined as the point at which concentration changes fell within this experimental uncertainty. Therefore, equilibrium concentrations used for isotherm construction correspond to measurements obtained after 30 min of contact time. By taking the 30 minutes as the time point for isotherm constructions, it allowed us to use a condition very close to the equilibrium, according to the instrumental resolution, and still have enough time for each group to perform replicated adsorption measurements at 25 and 50 °C within the two-weeks range allotted to this experiment. More details about this result can be observed on Figs. S2 and S3 of the Supporting Information file.



Fig 1 (b) shows the picture of the aliquots collected from the tartrazine solution before any contact with chitosan ($t = 0$ min), and after 30 minutes in contact with chitosan. It is visually clear that the contact with chitosan caused the decolorization of the yellow tartrazine solution. To confirm that the tartrazine removed from the solution was adsorbed onto the chitosan surface, the chitosan powder was isolated after the end of the experiment and let to dry under mild heating on a hot plate. The chitosan powder isolated after the end of the adsorption experiment is shown along with the chitosan powder before any contact with tartrazine in Fig 1 (c). It is visually clear that the chitosan powder turned yellow after the adsorption experiment.

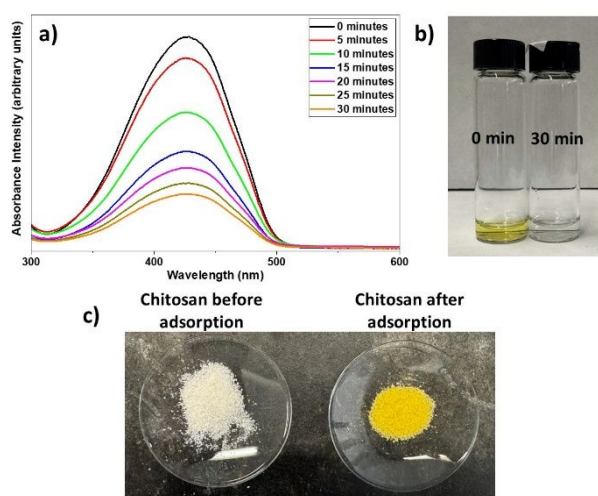


Fig 1 (a) Representative absorption spectra of tartrazine before and after contact with chitosan from time points ranging from 5 to 30 min; (b) Picture of the tartrazine solution before ($t = 0$ min, left) and after contact with chitosan ($t = 30$ min, right); (c) Picture of the chitosan powder before (left) and after (right) tartrazine adsorption.

The influence of the temperature and initial tartrazine concentration on the removal percentage was evaluated. Fig 2 shows the average tartrazine removal percentage vs the tartrazine initial concentration calculated from the results of all six trials performed by the students across the two weeks of experimental sessions, for each temperature. As an additional information, in order to show the variability presented by each experimental group, Fig. S4 from the Supporting Information file presents the removal percentage vs initial tartrazine concentration graphs for the replicate trials for each group separately.

The temperature does not have a strong influence on the tartrazine removal percentage by chitosan. In general, all experimental conditions achieved average removal percentages of around 85% after 30 minutes of contact between tartrazine and chitosan. Both adsorption temperatures had nearly identical average removal percentages from initial tartrazine concentrations ranging from 30 to 50 mg/L. Whereas, for initial concentrations between 10 and 20 mg/L, the adsorption experiments at 25 °C had slightly higher removal percentages. For both temperatures, there was a slight decrease in the

average removal percentage as the tartrazine initial concentration increased.

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Then, the students evaluated whether the type of Temkin isotherm used, linear or non-linear, had any influence on the thermodynamic parameters obtained for the adsorption experiment, as presented in Table 1 and Fig. 3.

Both the linear and non-linear versions of the Temkin isotherm satisfactorily fitted the experimental data for each temperature, with correlation factors (R^2) of around 0.96 for each isotherm. This result indicated the adequacy of both isotherm versions for the experimental data obtained.

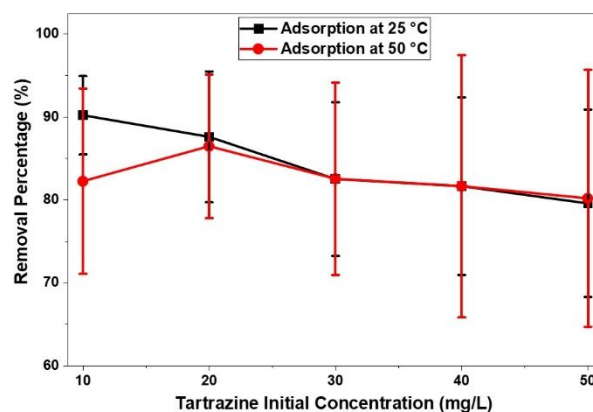


Fig 2 Tartrazine removal percentage vs the tartrazine initial concentration for the adsorption experiments performed at 25 and 50 °C.

The Temkin adsorption isotherm is particularly suited to systems in which adsorbate–adsorbent interactions lead to a progressive decrease in the heat of adsorption with increasing surface coverage. Unlike the Langmuir model, which assumes a uniform surface with identical and energetically equivalent adsorption sites, the Temkin isotherm accounts for heterogeneous adsorption energies arising from interactions between adsorbed species and from variations in surface functional groups. In the Temkin model, the adsorption energy is assumed to decrease linearly rather than exponentially as coverage increases, reflecting adsorbate–adsorbent and adsorbate–adsorbate interactions that become significant at moderate surface loadings.^{22,28} This physical framework is consistent with adsorption on biopolymeric materials such as chitosan, whose surfaces contain a distribution of chemically distinct functional groups (e.g., amine and hydroxyl groups) and whose adsorption behavior is influenced by electrostatic interactions, hydrogen bonding, and local surface heterogeneity.^{29,30} Consequently, the Temkin isotherm provides a more realistic description of the thermodynamic adsorption process for the chitosan–tartrazine system than other models such as Langmuir or Freundlich, particularly when experimental data indicate non-constant adsorption energies.³¹ Another important point to be discussed about the Temkin isotherm is about the mathematical consequences of a presence of natural logarithm function (\ln) in the equation describing the isotherms, both for the linear and the non-linear forms (vide Eq. 4 and 6, respectively). Taking the Eq. 6 as an example for this discussion, if C_e tends to zero, the $\ln(C_e)$ would



tend to the infinity with negative signal. Consequently, the Eq. 4 and 6 are physically undefined for C_e tending to zero. This inherent mathematical limitation of the Temkin isotherm can not be seen as an impeding factor for defining Temkin isotherm as an equilibrium isotherm. Instead, it should be understood that the Temkin isotherm is valid over a finite concentration range and it is derived under the assumption of moderate surface coverage. Its logarithmic form is not intended to describe the infinite dilution limit ($C_e \rightarrow 0$), and therefore its physical interpretation is restricted to the experimental concentration domain investigated.³²

Supporting information confirms that Langmuir and Freundlich isotherm models did not adequately describe the equilibrium data, reinforcing the appropriateness of the Temkin model for this system.^{22,33,34} (See Supporting Information Figures S5 and S6).

Table 1 presents the quantitative results obtained from the fittings of the linear and non-linear versions of the Temkin isotherm for the adsorption experiments at each temperature.

Table 1: K_T , q_T , R^2 , K_{app} , ΔH_{app} , ΔG_{app} , and ΔS_{app} estimated from the linear and non-linear fit for adsorption experiments performed at 25 and 50 °C.

| | Adsorption at 25 °C | |
|----------------------------|------------------------|------------------------|
| | Linear | Non-linear |
| K_T (L/mg) | 3.24 | 3.24 |
| q_T (mg/g) | 406.14 | 406.14 |
| R^2 of the fit | 0.967 | 0.967 |
| K_{app} | $1.73 \times 10^{+6}$ | $1.73 \times 10^{+6}$ |
| ΔH_{app} (J/mol) | -92.6 | -92.6 |
| ΔG_{app} (J/mol) | $-3.56 \times 10^{+4}$ | $-3.56 \times 10^{+4}$ |
| ΔS_{app} (J/mol.K) | $1.19 \times 10^{+2}$ | $1.19 \times 10^{+2}$ |

| | Adsorption at 50 °C | |
|----------------------------|------------------------|------------------------|
| | Linear | Non-linear |
| K_T (L/mg) | 2.52 | 2.52 |
| q_T (mg/g) | 381.44 | 381.44 |
| R^2 of the fit | 0.965 | 0.965 |
| K_{app} | $1.35 \times 10^{+6}$ | $1.35 \times 10^{+6}$ |
| ΔH_{app} (J/mol) | -92.6 | -92.6 |
| ΔG_{app} (J/mol) | $-3.80 \times 10^{+4}$ | $-3.80 \times 10^{+4}$ |
| ΔS_{app} (J/mol.K) | $1.17 \times 10^{+2}$ | $1.17 \times 10^{+2}$ |

For each temperature, comparing the linear and non-linear Temkin isotherm versions, Table 1 presented identical results for all the parameters calculated. This set of results is very important because it revealed that there is no loss of accuracy by using the linear version instead of the non-linear one for the tartrazine-chitosan adsorption system, in the temperature and concentration ranges studied.

In general, the adsorption literature has shown that nonlinear regression yields more accurate estimates of adsorption parameters than linearized fits, because the transformation inherent in linearization can distort the error structure and bias parameter values.³⁵ Reviews of isotherm modeling note that linearized methods, while common, can implicitly alter error assumptions and offer poorer parameter estimates, prompting a shift toward nonlinear optimization techniques.³⁶

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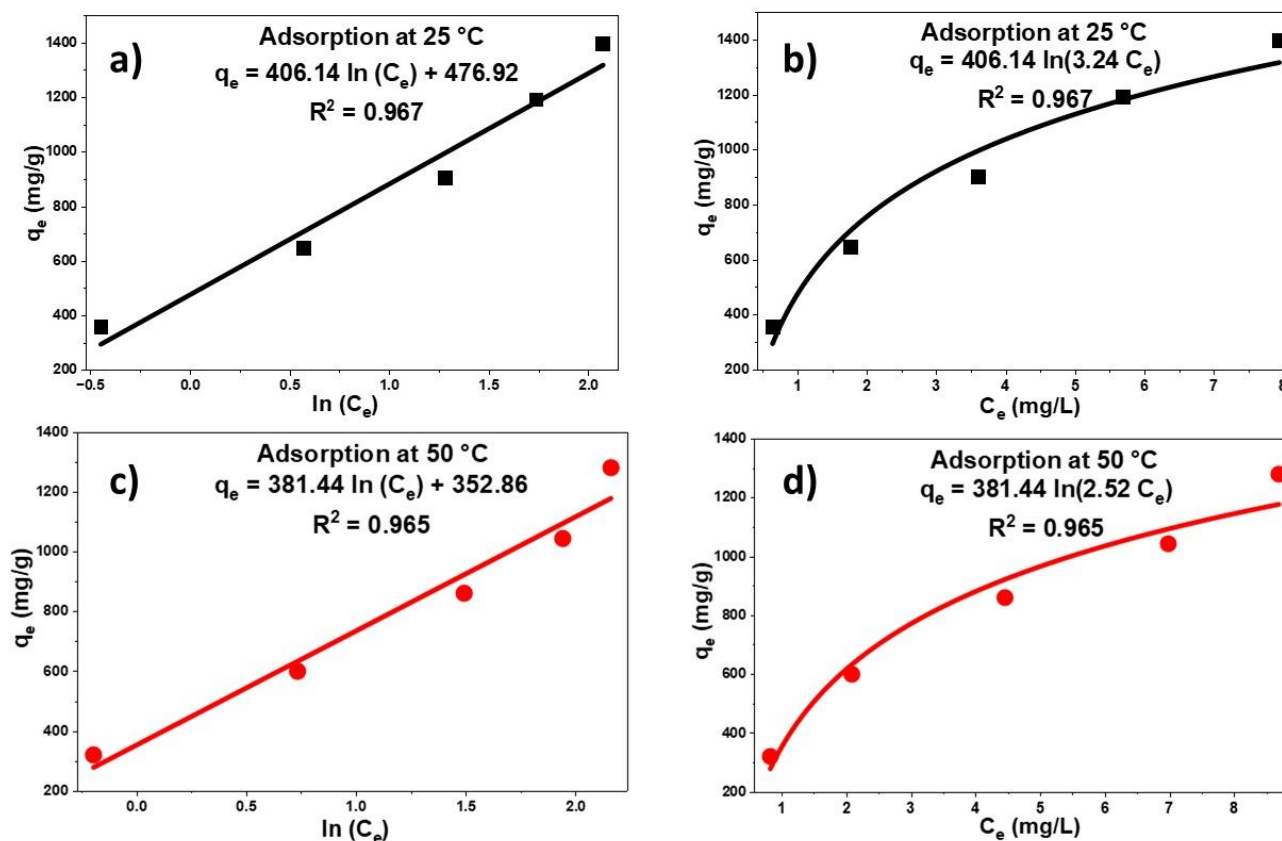


Fig 3 (a) Linear fit of the Temkin isotherm at 25 °C; (b) Non-linear fit of the Temkin isotherm at 25 °C; (c) Linear fit of the Temkin isotherm at 50 °C; (d) Non-linear fit of the Temkin isotherm at 50 °C.

However, some recent studies have reported similar numerical values for equilibrium constants and adsorption capacities from both linear and nonlinear fits, particularly when the data exhibit minimal scatter and conform closely to model assumptions.³⁷ In this study, the linear and nonlinear Temkin fits yielded effectively identical parameter values. This may be attributed to the high quality and tight alignment of the equilibrium data, such that the linear transformation did not materially distort the parameter estimates — a phenomenon observed in other adsorption systems with low experimental scatter.³⁷

A comparative analysis of the temperature influence from Table 1 revealed that the experiments performed at 25 °C had slightly higher values for K_T and q_T than the experiments performed at 50 °C. The decrease in K_T values with increasing temperature resulted in an exothermic adsorption experiment, as shown by the negative value for ΔH_{app} .

The negative ΔG°_{app} values indicate that adsorption is thermodynamically favorable under the investigated

conditions. Rather than serving to demonstrate the occurrence of adsorption, these values quantify the magnitude of the thermodynamic driving force and allow comparison of energetic favorability as a function of temperature. The reported Gibbs free energies correspond to apparent standard values (ΔG°_{app}), derived from the apparent equilibrium constant obtained from the Temkin model (Eq. 7). In adsorption systems, the definition of rigorous thermodynamic standard states for the adsorbed phase is not straightforward, and therefore these quantities should be interpreted as effective thermodynamic parameters within the experimental concentration range. In the present study, the standard state for the dissolved dye corresponds to a hypothetical 1 mol L⁻¹ ideal solution, while the adsorbed phase is treated implicitly through the isotherm constant. Because the adsorbed phase does not constitute an ideal bulk phase, the resulting thermodynamic parameters are designated as apparent quantities.



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3.2 Educational Results

The students were asked to voluntarily and anonymously answer a survey with questions about their experience after performing this two-week experiment. A total of five students from the six student's cohort answered the survey.

The survey contained a total of 12 questions where the students had to grade the affirmation made in each question with the concepts strongly disagree, disagree, neutral, agree, or strongly agree. The survey questions and their results are presented in the Table 2:

Table 2: Questions and results of the survey answered anonymously by the students regarding their impressions about the experiment

| Questions | Strongly Disagree (%) | Disagree (%) | Neutral (%) | Agree (%) | Strongly Agree (%) |
|--|-----------------------|--------------|-------------|-----------|--------------------|
| Q1. I feel confident interpreting the thermodynamic parameters ΔH , ΔG , and ΔS from experimental data | 0 | 0 | 0 | 40 | 60 |
| Q2. I can explain how temperature affects adsorption processes based on thermodynamic principles | 0 | 0 | 0 | 40 | 60 |
| Q3. I understand the purpose of using the Temkin isotherm model in this experiment | 0 | 0 | 0 | 60 | 40 |
| Q4. I can describe the difference between linear and non-linear model fitting and why the choice matters | 0 | 0 | 20 | 40 | 40 |
| Q5. I feel more confident performing non-linear curve fitting or interpreting software-generated fits | 0 | 20 | 20 | 40 | 20 |
| Q6. This activity helped me understand how chemistry contributes to real-world water | 20 | 0 | 0 | 20 | 60 |
| Q7. This experiment improved my ability to analyze experimental data using graphical and mathematical | 0 | 0 | 0 | 40 | 60 |
| Q8. This experiment activity was engaging and interesting | 0 | 0 | 0 | 60 | 40 |
| Q9. The environmental relevance of the project increased my motivation to learn | 0 | 0 | 0 | 40 | 60 |
| Q10. Connecting the experiment to real-world problems improved the learning experience | 0 | 0 | 0 | 0 | 100 |
| Q11. The sustainability focus made the chemistry feel more meaningful | 0 | 0 | 0 | 40 | 60 |
| Q12. I would recommend that future students continue to do this project | 0 | 0 | 0 | 40 | 60 |



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In general, the survey results indicated that the students had a positive experience regarding both the technical and engaging aspects of the experiment. For instance, 100% of the students answered that they agree or strongly agree that they were confident interpreting the thermodynamic data, such as ΔH , ΔG , and ΔS from the experimental data, as shown in question 1. Similar ratings were obtained for questions 2 and 3, which asked about understanding the influence of the temperature in the adsorption process and the purpose of using the Temkin isotherms in this experiment.

Some questions asked about the mathematical aspects of the experiment, more specifically about the contrast between linear and non-linear functions. For instance, question 4 asked about the ability to differentiate between the linear and non-linear and why the choice matters. Exactly, 80% of the students agreed or strongly agreed with being able to do this differentiation between the linear and non-linear versions of the function, whereas the remaining 20% answered neutral to the affirmation made in question 4. Probably, the most concerning results in this survey were described in question 5, which deals with the confidence in performing and interpreting the linear and non-linear software-based fittings. Only 60% of the respondents described to agree or strongly agree feeling confident in performing the linear and non-linear fittings. The remaining 40% were split evenly between feeling neutral or disagreeing with the stated affirmation.

The question 6 asked about context and application, if the developed activity helped the students to understand how the chemistry contributes to the real world water. In this question, 80% of the responses were divided between agreeing and strongly agreeing with this affirmation. However, 20% of the respondents said they strongly disagree with this affirmation. Unfortunately, no space for justification of the answer was provided on this question. So, it is not possible to state the definite reasons why this student disagreed that the experiment made them to better understand the real world problem. However, a possible hypothesis to that result is maybe that the student could be so concern on fulfilling the math-related aspects of the experiment that they may have missed a wider view of the experiment context and importance to water remediation.

Yet, about the mathematical aspects, in question 7, 100% of the students agreed or strongly agreed that this experiment improved their ability to analyze experimental data using mathematical and graphical models.

Regarding the engaging aspects of the experiment, 100% of the students agreed or strongly agreed that the experiment was engaging and interesting (question 8). The environmental

relevance of the project increased their motivation to learn (question 9). That to connect the experiment to real-world problems improved their learning experience (question 10), and that the sustainability focus made the chemistry feel more meaningful (question 11). Finally, 100% of the students agreed or strongly agreed that they would recommend performing this experiment for future students, as stated by the results from question 12.

3.3 Connections with Green Chemistry Principles and UN Sustainable Development Goals

One of the questions in the lab report that the students were required to turn in asked them to discuss which Green Chemistry Principles and UN Sustainable Development Goals this experiment is related to, and justify their viewpoint for every goal or principle they cited.

Regarding the 12 Green Chemistry Principles, the following principles were cited and properly justified:

Principle 1 – Waste prevention: The dye adsorption prevents its further discharge and treatment in the environment.

Principle 5 – Safer solvents and auxiliaries: Only aqueous solutions were used throughout the experiment. Avoiding the use of harmful solvents made the experiment safer to be performed in an undergraduate lab course.

Principle 6 – Design for energy efficiency: In this experiment, the adsorption proved to be more efficient at 25 °C than 50 °C. So, energy is saved if the experiment is performed at lower temperature.

Principle 7 – Use of renewable feedstocks: Chitosan is derived from chitin, a renewable biomass, aligning the adsorption process with the use of renewable feedstocks.

Principle 10 – Design for degradation: Chitosan is biodegradable, and so not environmentally persistent, like other synthetic adsorbents.

Principle 12 – Inherently safer chemicals for accident prevention: Only tartrazine aqueous solutions and chitosan were used in this experiment. The low tartrazine concentration range decreases its environmental impact. Additionally, the experimental setup used was simple, and all the experiments were performed under the instructor's supervision, decreasing the chances of accidents or any unsafe events throughout the experiment.

Regarding the UN Sustainable Development Goals, the following Goals were cited and properly justified:

Goal 6 – Clean water and sanitation: The experiment has its main motivation to remove a dye from simulated wastewater, which is in agreement with the search for methods to clean water.



Goal 12 – Responsible consumption and production: The experiment used chitosan, which can be obtained from wasted shells.

Goal 14 – Life below water: The dye contamination is a serious problem for marine organisms, as it can reduce the sunlight penetration in the water and damage the activity of the autotrophic marine organisms. So, it is imperative to decontaminate the water as proposed in this experiment. Since the students were able to identify many Green Chemistry Principles and UN Sustainable Development Goals, correlate them with the experiment, and justify these correlations, it is evident that this experiment fulfilled one of its objectives to introduce students to the Green Chemistry Principles and UN SDGs, and raise their awareness of the need to promote a more sustainable category of physical chemistry experiments.

3.4 Additional suggestions for the experiment implementation

In order to enable the implementation of this experiment by other instructors around the world, the full activity text from the student's lab manual is provided in the section S4 of the Supporting Information file. Also, the template of the Excel spreadsheet used by the students to perform the calculations is available in the repository link posted in the data availability section of the paper.

Additionally, this experiment can be adapted for courses in different levels for chemistry, chemical engineering, and environmental sciences and engineering courses. Some modifications can be made in order to fit the specific needs of the chosen course.

For instance, this experiment can be adapted as a modular laboratory activity in which students compare the performance of different adsorbent materials under identical experimental conditions. While chitosan was selected in this work because of its biodegradability and the presence of protonatable amine groups that promote electrostatic interactions with anionic dyes such as tartrazine, several other low-cost materials could be incorporated into similar instructional experiments. For example, activated carbon is one of the most widely used adsorbents for dye removal due to its high surface area and porous structure and has been extensively reported for the adsorption of tartrazine and other azo dyes from aqueous solutions.^{38,39}

In addition, cellulose-based materials derived from biomass have received increasing attention as sustainable adsorbents. For instance, wood-derived cellulose nanocrystals have been investigated as efficient adsorbents for organic dyes such as auramine O, highlighting the potential of renewable materials in water remediation applications.⁴⁰ Other inexpensive sorbents such as agricultural waste-derived carbons, clays, or biochars have also demonstrated promising adsorption capacities for food dyes and related organic pollutants.^{4,41} Incorporating such materials into the present experiment could allow instructors to design comparative studies in which different student groups evaluate distinct adsorbents and collectively analyze how factors such as surface chemistry, porosity, and functional groups influence adsorption efficiency

and equilibrium behavior. This type of comparison can reinforce fundamental concepts in adsorption thermodynamics while also highlighting the role of sustainable materials in water treatment technologies.

Regarding the mathematical treatment, the comparison between linear and non-linear models can be extended to study the different kinetics solid-liquid adsorption models, such as the pseudo first order and the pseudo second order models.⁴² So, comparisons can be made between the linear and non-linear equations of each model to reveal which one leads to more accurate results.

In summary, this experiment is very applicable on different course majors and levels, with few adaptations or no adaptations at all, according to the Instructor's needs.

4 Conclusions

The adsorption data collected by the students fit properly to the Temkin isotherm, both to the linear and non-linear versions. There were no differences in the isotherm constant and thermodynamic functions obtained from the linear and the non-linear versions of the isotherm, for a certain temperature. The adsorption process was described as exothermic, as demonstrated by the negative value estimated for ΔH_{app} , and spontaneous, as described by the negative value estimated for ΔG_{app} .

Other isotherm models, like Langmuir and Freundlich isotherms were proved to not describe the adsorption data collected, as shown in the Supporting Information file.

The students properly correlated the goals and performance of this experiment with the Green Chemistry Principles and the UN Sustainable Development Goals.

In general, the students rated positively the implementation and performance of this experiment.

Author contributions

Conceptualization – TC, AHP; Data Curation – TC, AHP; Formal Analysis – TC, SB, AHP; Methodology – TC, AHP; Project Administration – AHP; Resources – AHP; Supervision – AHP; Validation – TC, AHP; Writing original draft – AHP.

Conflicts of interest

"There are no conflicts to declare".

Data availability

Data for this article, including the Excel spreadsheet containing all the data present in the paper are available at Google Drive Folder at:

https://docs.google.com/spreadsheets/d/1_Cggz-bXMTWhMaGD-3OQ5v5CVz8x844R/edit?usp=sharing&oid=102378786712085201156&rtpof=true&sd=true



The template of the Excel file used by the students for the calculation of all the Thermodynamic parameters is available in a Google Drive Folder in the following link:

<https://docs.google.com/spreadsheets/d/13QeGCFuKWnB55N-XbPiuY-53Dvmsb1JVI/edit?usp=sharing&ouid=102378786712085201156&rtpof=true&sd=true>

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Integrating Physical Chemistry and Sustainability: An Educational Study of Linear and Non-Linear Adsorption Isotherms Using Chitosan in Wastewater Remediation

Tanishka Chauhan,^a Santunu Barua^b and Alexandre H. Pinto

Data Availability Statement

Data for this article, including the Excel spreadsheet containing all the data present in the paper are available at Google Drive Folder at https://docs.google.com/spreadsheets/d/1_Cggz-bXMtWhMaGD-3OQ5v5CVz8x844R/edit?usp=sharing&oid=102378786712085201156&rtpof=true&sd=true

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