Supporting Information file for

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

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S1. Calibration curve for tartrazine remaining concentration determination:

The calibration curve used to convert the tartrazine absorbance intensity at 426 nm into the tartrazine remaining concentration, as shown in Eq. 1 of the main paper, was prepared by diluting a 300 mg/L tartrazine solution into aliquots with concentrations from 10 to 50 mg/L. The aliquots and data collection were carried out in duplicates. The average and standard deviation values were used in obtaining the calibration curve, which can be observed in Fig S1:

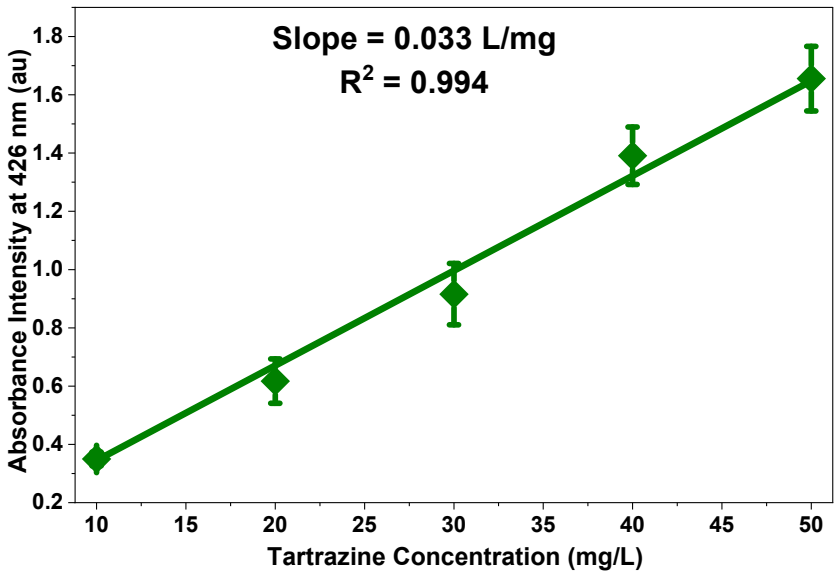

Fig S1. Calibration curve used to convert the tartrazine absorbance intensity at 426 to the tartrazine remaining concentration.

So, Eq. 1of the main paper with the slope of the calibration curve plugged will become Eq. S1:

$$C_t = \frac{Abs_t^{426nm}}{0.033} \qquad \text{Eq. S1}$$

S2. Adsorption results obtained by each group separately:

As an experiment performed by students that may be not fully familiar with all the techniques and apparatus needed, it is possible that the obtained results can present a meaningful variability.

In this regard, the first point to be to be discussed is the choice of 30 minutes as the time point to be taken as the time for the adsorption equilibrium, as shown in the Fig 1 a) of the main paper. Fig. S2 presents the actual replicated results of removal percentage vs time obtained by each group separately.

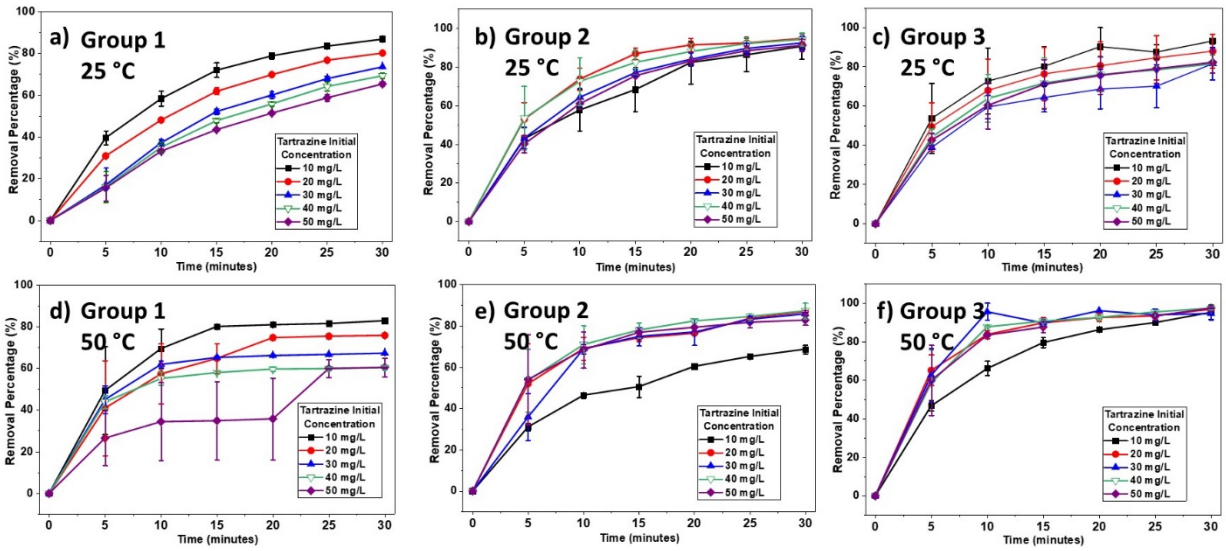

Fig. S2: Tartrazine removal percentage by chitosan for tartrazine initial concentration ranging from 10 to 50 mg/L, with a total contact time of 30 min, for adsorption experiments performed at 25 °C by different groups of students: a) Group 1, b) Group 2, c) Group 3. And for the adsorption experiments performed at 25 °C by different groups of students: d) Group 1, e) Group 2, f) Group 3.

From Fig S2, it is possible to notice that for most of the experiments, regardless the initial tartrazine concentration and temperature that tartrazine removal percentage presented a variation lower than 5% comparing the results at 25 and 30 minutes of contact time between tartrazine and chitosan.

In order to provide one more piece of evidence for the 30 minutes as an appropriate time point to analyze the attainment of the adsorption equilibrium, we performed experiments at 25 °C, and tartrazine initial concentrations equal to 10 and 20 mg/L, for a maximum contact time of 60 minutes. The results shown in Fig. S3 confirm that between 30 and 60 minutes, that there is negligible increase in the tartrazine removal percentage, for both experiments performed. The results confirm that 30 minutes is an adequate time point to consider that the adsorption equilibrium has been attained. Additionally, the 30 minutes contact time is an ideal time range allowing the students enough time to complete the replicated experiments at both temperatures within the two-classes sessions period.

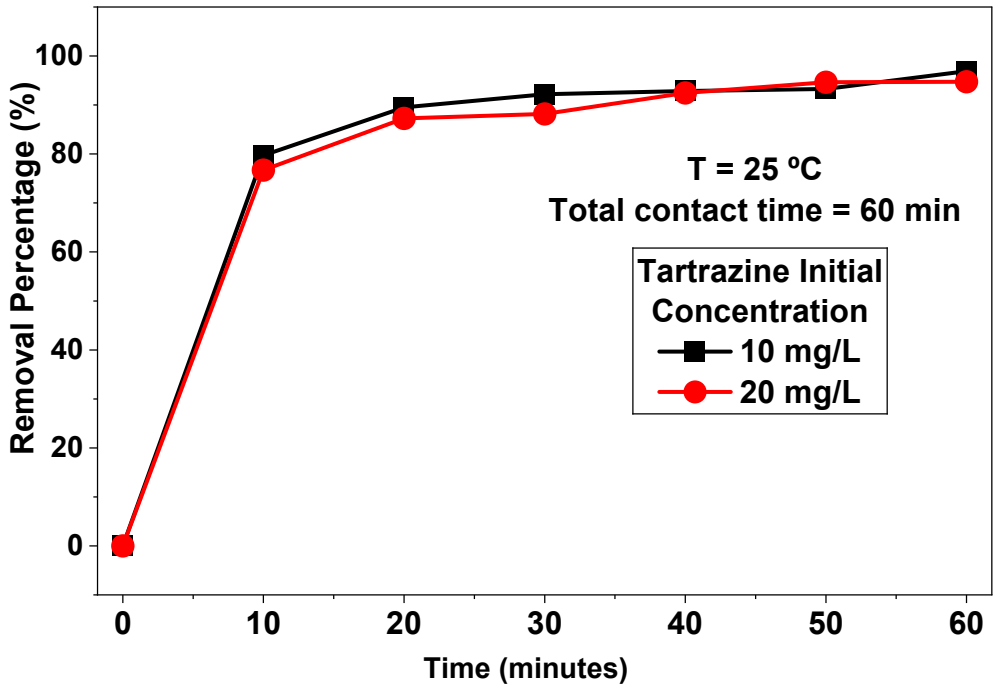

Fig S3: Tartrazine removal percentage by chitosan for tartrazine initial concentration of 10 and 20 mg/L, with a total contact time of 60 min, for adsorption experiments performed at 25 °C. These additional experiments were performed by the paper authors.

In Fig. 2 of the main paper, it was presented the average results for the tartrazine removal percentage vs tartrazine initial concentration from all the six trials obtained across the whole cohort. Then, the Fig. S4 presents the actual replicated results obtained by each group separately.

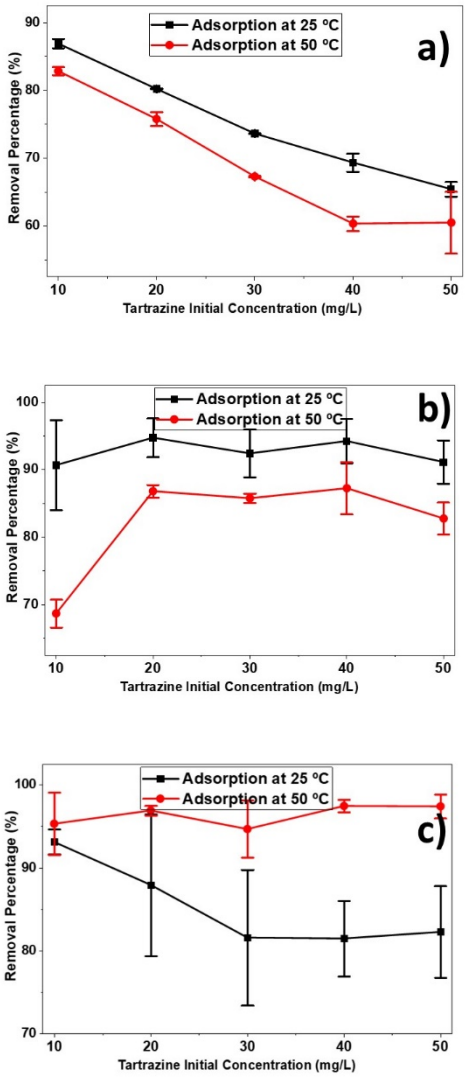

Fig S4: Tartrazine removal percentage by chitosan after 30 minutes of contact vs tartrazine initial concentration, average and standard deviation results of each group replicas, (a) Group 1, (b) Group 2, (c) Group 3.

When the data were disaggregated by group, some variability between groups became evident. In particular, Groups 1 and 2 showed slightly higher removal efficiencies at 25 °C than at 50 °C, whereas Group 3 exhibited the opposite trend. Such inter-group variability is commonly observed in instructional laboratory environments where multiple student teams independently perform the same experimental procedure. Small differences in experimental execution, such as mixing efficiency, timing during sampling, solid–liquid separation, or spectroscopic measurement—can introduce variability in adsorption measurements. Nevertheless, despite these variations, the overall magnitude of tartrazine removal remained comparable across groups, and the pooled dataset still exhibited consistent equilibrium behavior suitable for adsorption isotherm modeling. The aggregation of data from multiple groups therefore provides a representative dataset reflecting realistic experimental variability in a teaching laboratory setting while still allowing meaningful thermodynamic analysis.

S3. Application of Langmuir and Freundlich Isotherms:

In order to prove that the Temkin isotherm was the most suitable type of isotherm to describe the tartrazine adsorption onto chitosan, the data collected by the students was tried to be fitted to the linear and non-linear versions of the Langmuir and Freundlich isotherms.

Regarding the Langmuir Isotherm, its linear version can be described by the Eq. S2:

$$\frac{1}{q_e} = \frac{1}{q_m} + \frac{1}{K_L q_m C_e} \qquad \text{Eq. S2}$$

The plot corresponding to the linear Langmuir isotherm is $1/q_e$ vs $1/C_e$, with the slope yielding $1/K_L.q_m$ and intercept equal to $1/q_m$.

The non-linear version of the Langmuir isotherm can be described by the Eq. S3:

$$q_e = \frac{K_L q_m C_e}{1 + K_L C_e} \qquad \text{Eq. S3}$$

Figure S5 shows the linear and non-linear versions of the Langmuir isotherm fitted to the adsorption experiments carried out at 25 and 50 °C:

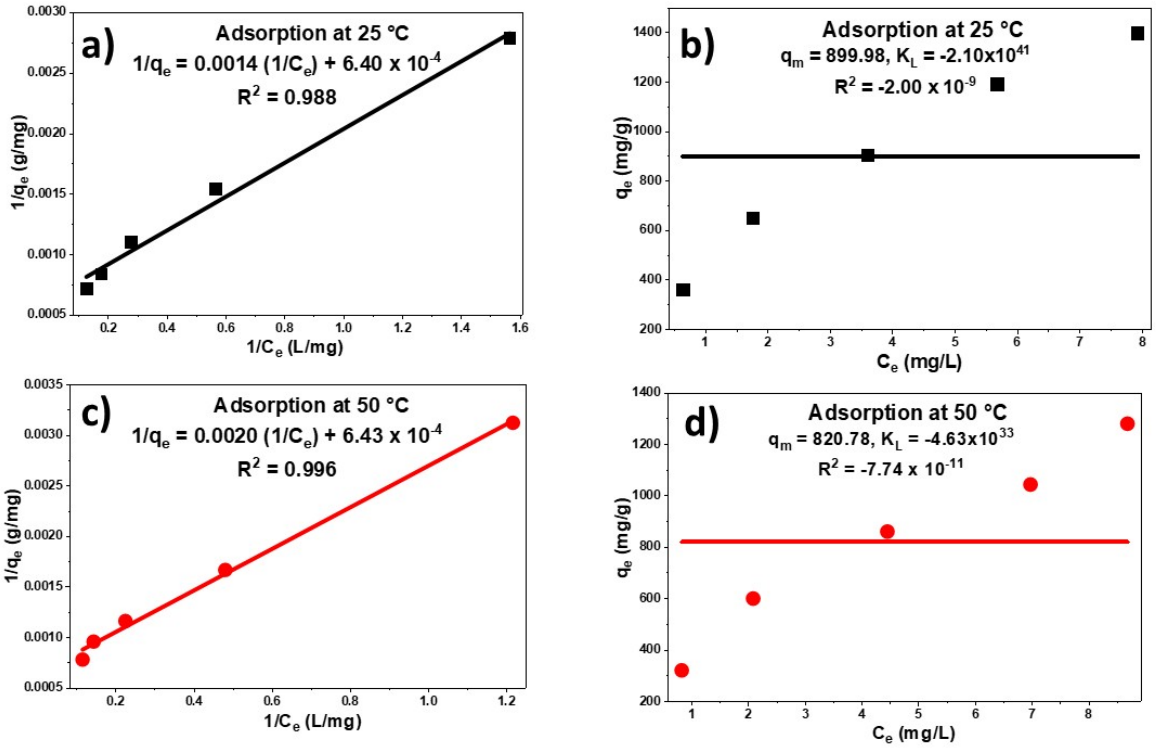

Fig S5: Langmuir isotherm fits (a) linear fit at 25 °C, (b) non-linear fit at 25 °C, (c) linear fit at 50 °C, (d) non-linear fit at 50 °C.

Regarding the Freundlich Isotherm, its linear version can be described by the Eq. S4:

$$\log\left(q_e\right) = \log\left(K_F\right) + \frac{1}{n}\log\left(C_e\right) \qquad \text{Eq. S4}$$

The plot corresponding to the linear Freundlich isotherm is log (q_e) vs log (C_e), with the slope yielding 1/n and intercept equal to log (K_F)

The non-linear version of the Freundlich isotherm can be described by the Eq. S5:

$$q_e = K_F C_e^{\left(1/n\right)} \qquad \text{Eq. S5}$$

Figure S6 shows the linear and non-linear versions of the Langmuir isotherm fitted to the adsorption experiments carried out at 25 and 50 °C:

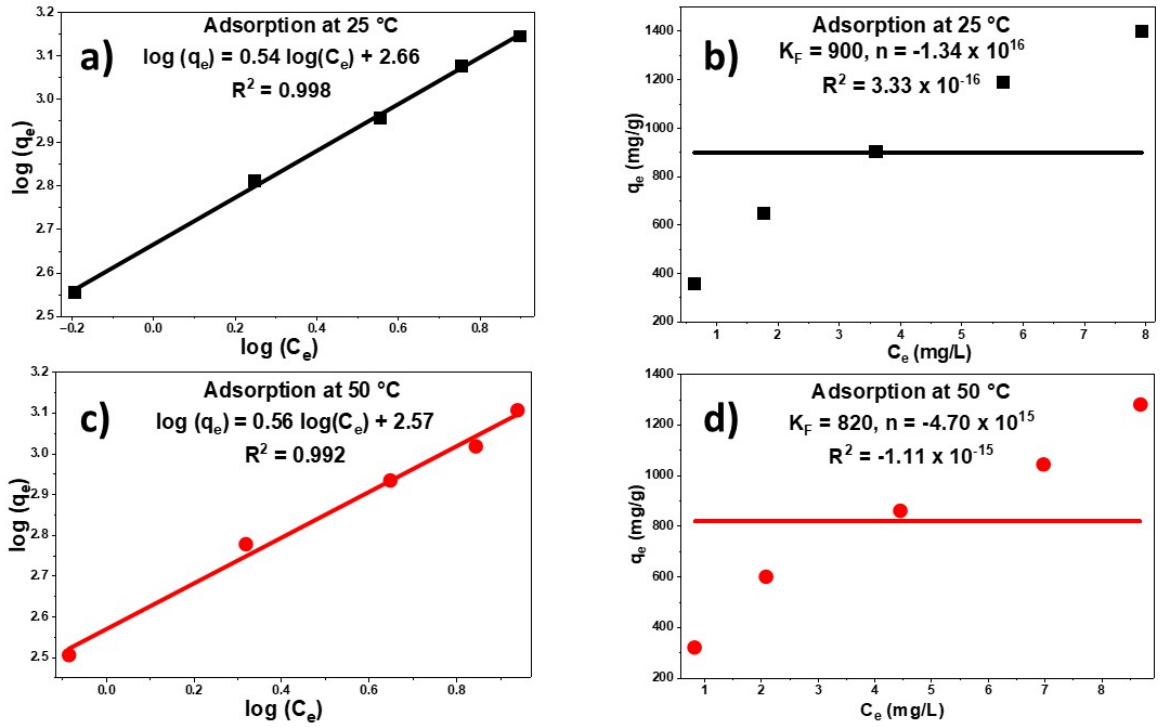

Fig S6: Freundlich isotherm fits (a) linear fit at 25 °C, (b) non-linear fit at 25 °C, (c) linear fit at 50 °C, (d) non-linear fit at 50 °C.

Table S1 presents the R^2 for the linear and non-linear fit of the Langmuir and Freundlich isotherms at 25 and 50 °C:

Table S1. R^2 values for Langmuir and Freundlich isotherm linear and non-linear fits at 25 and 50°C

	R^2 for linear fit	**R^2 for non-linear fit**
Langmuir isotherm 25 °C	0.988	-2.00×10^{-9}
Langmuir isotherm 50 °C	0.996	-7.74×10^{-11}
Freundlich isotherm 25 °C	0.998	3.33×10^{-16}
Freundlich isotherm 50 °C	0.992	-1.11×10^{-15}

The parameters obtained from the non-linearized fittings of the Langmuir and Freundlich models are shown on Table S2:

Table S2. Fitting parameters and reduced chi-square values for the Langmuir and Freundlich isotherm non-linear fits at 25 and 50°C

Temperature (°C)	Model	Parameter	Value	Standard Error
25	Langmuir	(q_m) (mg g^{-1})	899.98	276.74
		(K_L) (L mg^{-1})	not reliable*	—
		Reduced χ^2	2.30×10^5	—
50	Langmuir	(q_m) (mg g^{-1})	820.79	660.45
		(K_L) (L mg^{-1})	not reliable*	—
		Reduced χ^2	1.87×10^5	—
25	Freundlich	(K_F)	—	—
		(n)	not reliable*	—
50	Freundlich	(K_F)	820.79	193.36
		(n)	not reliable*	—

The equilibrium adsorption data for tartrazine on chitosan were analyzed using Langmuir, Freundlich, and Temkin isotherm models through nonlinear regression. Although the Langmuir and Freundlich fitting procedures formally converged, the resulting affinity parameters presented extremely large numerical values and large associated uncertainties, indicating that these parameters cannot be interpreted in a physically meaningful way. Such numerical divergence is commonly observed when adsorption models are applied to datasets with a limited number of experimental points or when the adsorption isotherm does not clearly approach saturation conditions (Foo and Hameed, 2010).

In some cases, linearized forms of adsorption equations can yield apparently good correlation coefficients. However, it is well established that linearization can distort the error structure of experimental data and artificially inflate the coefficient of determination (R^2), potentially leading to biased parameter estimates (Ho, 2004).

In nonlinear regression analysis, the reduced chi-square (χ^2_{red}) is generally considered a more informative indicator of model performance than the coefficient of determination (R^2). While R^2 measures the fraction of variance explained by the model and can be artificially affected by nonlinear transformations of the data, the χ^2_{red} directly evaluates the magnitude of the residual errors normalized by the degrees of freedom. Consequently, χ^2_{red} provides a more reliable assessment of the goodness of fit when comparing nonlinear adsorption models (Bevington and Robinson, 2003; Motulsky and Christopoulos, 2004). For this reason, nonlinear regression methods are generally recommended for determining adsorption parameters, as they preserve the original error distribution of the experimental measurements (Foo and Hameed, 2010).

The present dataset consists of five equilibrium points collected as part of an undergraduate laboratory experiment designed to introduce adsorption equilibrium concepts. While such datasets are sufficient to illustrate adsorption behavior and to estimate adsorption capacity, they may not provide enough information to reliably determine multiple fitting parameters simultaneously. Consequently, the Langmuir affinity constant (K_L) and the Freundlich heterogeneity parameter (n) could not be reliably determined through nonlinear fitting.

In contrast, the **Temkin isotherm model provided stable parameter values and a more consistent statistical description of the experimental data**. The Temkin model assumes that the heat of adsorption decreases linearly with surface coverage as a result of adsorbent–adsorbate interactions (Temkin and Pyzhev, 1940). This assumption is particularly relevant for dye adsorption systems involving electrostatic interactions and surface heterogeneity.

Tartrazine is an anionic azo dye containing sulfonate functional groups, while chitosan contains amino groups that become protonated under acidic conditions. The resulting electrostatic attraction between the negatively charged dye molecules and the positively

charged chitosan surface can produce a distribution of adsorption energies as surface coverage increases. Such behavior is consistent with the theoretical assumptions of the Temkin model and explains the improved performance of this model in describing the experimental data.

Taken together, the statistical behavior of the nonlinear regression, the physical assumptions of the adsorption models, and the chemical nature of the adsorbent–adsorbate interaction all support the conclusion that the **Temkin isotherm provides the most appropriate description of the adsorption system investigated in this study**.

References

Temkin, M. I.; Pyzhev, V. (1940). Kinetics of ammonia synthesis on promoted iron catalysts. *Acta Physicochimica URSS*, 12, 327–356.

Bevington, P. R.; Robinson, D. K. *Data Reduction and Error Analysis for the Physical Sciences*, 3rd ed.; McGraw-Hill: New York, 2003.

Motulsky, H.; Christopoulos, A. *Fitting Models to Biological Data Using Linear and Nonlinear Regression*; Oxford University Press, 2004.

Foo, K. Y.; Hameed, B. H. (2010). Insights into the modeling of adsorption isotherm systems. *Chemical Engineering Journal*, 156, 2–10.

Ho, Y. S. (2004). Selection of optimum sorption isotherm. *Carbon*, 42, 2115–2116.

S4. Lab Manual Instructions for the Experiment:

This section presents the lab manual files accessed by the students in order to perform the experiment and analyze its data.

Manhattan University

CHEM 311 Physical Chemistry Laboratory – Prof. Alex Pinto, PhD –

Fall 2025

Experiment:

Water remediation by chitosan: An experiment to teach the contrast between linear and non-linear adsorption isotherms and kinetics models

1. Introduction:

Adsorption is the process by which atoms, ions, or molecules (adsorbate) accumulate on the surface of a solid (adsorbent), forming a molecular or atomic film rather than dissolving in the

bulk phase. In solid–liquid adsorption, the solute species in a liquid phase adhere to the solid surface through physical or chemical interactions. The process depends on surface area, pore structure, temperature, and concentration of the adsorbate in solution.

Adsorption differs from absorption, in which a substance penetrates the bulk of another material. Together, both are sometimes referred to as sorption.

In practical terms, adsorption is used to remove contaminants, purify solutions, or recover valuable materials from liquids. Adsorbents such as activated carbon, zeolites, metal–organic frameworks (MOFs), and biopolymers like chitosan are widely studied for wastewater treatment, catalysis, and sensing.

An adsorption isotherm describes the relationship between the amount of adsorbate adsorbed per unit mass of adsorbent (q, mg g^{-1}) and its equilibrium concentration in solution (C_e, mg L^{-1}) at constant temperature. Isotherms help reveal the adsorption mechanism, capacity, and surface heterogeneity.

In this experiment, the adsorbate will be yellow food dye tartrazine, while the adsorbent will be the biopolymer chitosan. The isotherm described by this system is a Temkin isotherm, which is an isotherm where the heat of adsorption decreases with increasing coverage.

Most of the equations used will be used with their respective linear and non-linear version, expecting to enable some comparison of the parameters obtained through the linear and non-linear models.

2. Experimental Procedure:

2.1 Adsorption Experiments at 25 °C

Aqueous solutions of tartrazine in water, with concentrations equal to 10, 20, 30, 40, and 50 mg/L will be provided by the Instructor to the students. Each solution contains a total volume of 45 mL. Take 5 mL of each one of the solutions prepared of the solutions prepared and transfer them to glass vials labelled with the tartrazine concentration of the sample.

Then, collect the UV-vis absorption spectrum of each of these samples, recording the intensity of the absorbance peak centered at 426 nm. For these measurements, the blank should be collected with deionized water.

After that, on each conical tube containing the remaining 40 mL of each tartrazine solution, the students should add the 0.5 g of chitosan previously weighed by the Instructor. Following that, insert each tube in one of the slots of the shaking table, the shaking table speed should be adjusted to 500 rpm, and the temperature to 25 °C. Only start the shaking function after all the five samples have been inserted in the equipment.

Then, start the timer, and every 5 minutes collect 3 mL of each sample in separated 15 mL centrifuge tubes. Keep the sample collection until 30 minutes of the beginning of the experiment. Make sure you label every centrifuge tube with the concentration of the sample and the time point of the collection. After collecting each sample, let their respective centrifuge tubes standing in the tube holder to decant the chitosan, for, at least, 5 minutes.

After the collection of the 30 minutes samples, turn off the shaking table. Keep the remainder of the content of each sample until the experiment is completed.

2.2 Adsorption Experiments at 50 °C

Repeat everything as described for the experiment at 25 °C, only adjusting the shaking table temperature to 50 °C, instead of 25 °C.

3. Data Collection and Treatment

3.1 Conversion of the absorption peaks into remaining concentration in solution, the removal percentage, and the chitosan adsorption capacity (q_t):

The maximum absorption intensity at 426 nm, for all the time points from all the samples with different chitosan initial concentrations should be recorded on the appropriate column of the **Excel spreadsheet template** provided in the course page. Make sure you record the data properly for each trial at 25 °C and 50 °C experiments.

To track the progress of the adsorption experiment three important quantitative parameters should be calculated for each time point on each one of the samples, they are:

- The tartrazine remaining concentration in solution (C_t(mg/L))
- The tartrazine removal percentage (R_t(%))
- The chitosan adsorption capacity for tartrazine (q_t(mg tartrazine/g chitosan))

The tartrazine remaining concentration (C_t(mg/L)) measures how much tartrazine is left in solution at each time point of the sample collected. The C_t is measured in mg/L and it is calculated according to the Eq. (1):

$$C_t = \frac{Abs_t^{426nm}}{Calib.\ Curve\ Slope}$$ Eq. (1)

Where: Abs_t^{426nm} = intensity of the absorption peak at 426 nm on each time point t

Calib. Curve Slope = slope of the calibration curve to be provided by the Instructor

Record the C_t results on the appropriate column of the **Excel spreadsheet template** provided in the course page.

The tartrazine removal percentage (R_t(%)) measures how the percentage of the tartrazine removed, in relation to the initial tartrazine concentration, for each time point of the sample collected. The C_t is measured in mg/L and it is calculated according to the Eq. (2):

$$R_t = \left(\frac{C_0 - C_t}{C_0}\right) \times 100\% \qquad \text{Eq. (2)}$$

Where: C_0 = initial tartrazine concentration as calculated from the calibration curve

C_t = tartrazine remaining concentration on each time point as calculated on the Eq. (1)

Record the R_t(%) results on the appropriate column of the **Excel spreadsheet template** provided in the course page.

The chitosan adsorption capacity (q_t) measures how many mg of tartrazine were adsorbed per gram of chitosan on each time point of the sample collected. The q_t is measured in mg of tartrazine/g of chitosan. The q_t is calculated according to the Eq. (3):

$$q_t = \left(\frac{C_0 - C_t}{m}\right) \times V \qquad \text{Eq. (3)}$$

Where: C_0 = initial tartrazine concentration as calculated according to the calibration curve provided by the Instructor

C_t = tartrazine remaining concentration on each time point as calculated on the Eq. (1)

m = mass of chitosan used in the experiment (0.5 g)

V = volume of tartrazine used on each experiment (40 mL)

Record the R_t(%) results on the appropriate column of the **Excel spreadsheet template** provided in the course page.

3.2 Temkin Isotherm

3.2.1 Linear Model for Temkin Isotherm:

The Linear Model of the Temkin isotherm is represented by the Eq. (4 a):

$$\frac{q_e}{q_m} = \left(\frac{RT}{b}\right) \times \ln\left(K_T\right) + \left(\frac{RT}{b}\right) \times \ln\left(C_e\right) \qquad \text{Eq. (4a)}$$

The Eq. (4a) can be further simplified into the Eq. (4b):

Where: 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 ($J.mol^{-1}$)

K_T = Temkin isotherm equilibrium binding constant ($L.mg^{-1}$)

C_e = tartrazine remaining concentration at equilibrium ($mg.L^{-1}$)

R = ideal gas constant (8.314 $J.mol^{-1}.K^{-1}$)

T = temperature where the isotherm data was collected (K)

The equation (4a) can be further simplified into the equation (4b), by the following procedure starting from the equation (4a):

$$\frac{q_e}{q_m} = \left(\frac{RT}{b}\right) \times \ln\left(K_T\right) + \left(\frac{RT}{b}\right) \times \ln\left(C_e\right)$$

$$q_e = \left(\frac{q_m RT}{b}\right) \times \ln\left(K_T\right) + \left(\frac{q_m RT}{b}\right) \times \ln\left(C_e\right)$$

$$q_e = q_T \times \ln\left(K_T\right) + q_T \times \ln\left(C_e\right)$$

Eq. (4b)

Where: $q_T = (q_m RT/b)$ = adsorption capacity per unit binding energy (mg/g)

To treat the data to plot Eq. (4b), for a certain temperature, you should approximate the q_e and C_e values to those obtained at t = 30 min. So, for T = 25 °C, from the **C_t column**, copy for each different initial concentration sample. Then, paste C_t for t = 30 min, in the **column corresponding to the C_e values**, for each initial concentration sample. About the q_e values, copy the **q_t for t = 30 min**. Then, paste them into the column that lists the q_e values respective for each initial concentration sample. Then, in the following column, calculate the $\ln(C_e)$.

Finally, paste the calculated $\ln(C_e)$ values into a SciDavis spreadsheet in the X-axis, and the q_e values in the Y-axis. Plot the data from this table as a scatter graph, and perform its linear regression, take note of the slope, intercept and R^2 values provided for the linear equation.

The slope of this graph will be simply q_T ($mg.g^{-1}$), and the intercept will be equal to $q_T.\ln(K_T)$, report K_T value in the Table S4, which should be calculated according to Eq. (5):

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

Eq. (5)

For the data collected at T = 50 °C the procedure to be followed is exactly the same, except for the fact that the C_e and q_e data should be copied from their respective columns in appropriate column of the **Excel spreadsheet template** provided in the course page, and pasted into their respective columns in of the **Excel spreadsheet template** provided in the course page.

3.2.2 Non-linear Model for Temkin isotherm:

The Non-linear Model of the Temkin isotherm is represented by the Eq. (6b):

$$\frac{q_e}{q_m} = \left(\frac{RT}{b}\right) \times \ln\left(K_T C_e\right)$$ Eq. (6a)

$$q_e = q_T \times \ln\left(K_T C_e\right)$$ Eq. (6b)

For the 25 °C data, copy the **C_e** data from **C_t column for t = 30 min**, and paste them into an X-axis column of a SciDavis spreadsheet. Then, copy the **q_e** data from the **q_t column for t = 30 min** the into a Y-axis column of a SciDavis spreadsheet. Then, plot the graph of q_e vs C_e. You will notice that this graph is not linear. Then, you are going to input and fit the a non-linear version of Temkin equation in the SciDavis according the instructions provided in the Supplemental Information file.

The fitted curved will appear superposed to the data points, and in the result log window, it will automatically show the values for q_T, K_T and R^2. Take notes of all of them.

For the data collected at 50 °C, you can follow the same procedure, except for the fact that the C_e and q_e data will come from the tables for the experiments performed at 50 °C.

3.3 Thermodynamics Data:

The Temkin isotherm equilibrium binding constants (K_T) can be converted into apparent thermodynamic equilibrium constants (K_{app}), and used to calculate the apparent values for ΔH, ΔG, and ΔS. The conversion from KT to Kapp is 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 $L.mg^{-1}$. The conversion from K_T into K_{app} can be accomplished by the Eq. (7):

$$K_{app} = K_T \times C^{\circ}_{adsorbate} \times MW_{adsorbate}$$ Eq. (7)

Where: K_{app} = apparent equilibrium constant for the adsorption process (dimensionless)

K_T = Temkin isotherm equilibrium binding constant ($L.mg^{-1}$)

$C^{\circ}_{absorbate}$ = tartrazine standard molar concentration ($1\ mol.L^{-1}$)

$MW_{adsorbate}$ = tartrazine molar mass ($534.3 \times 10^{+3}\ mg.mol^{-1}$)

Convert the K_T into K_{app} for both the linear and non-linear models, both for the 25 and 50 °C, and report these results.

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

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

$$\ln\left(\frac{K_{app}^{323K}}{K_{app}^{298K}}\right) = \frac{\Delta H_{app}}{8.314}\left(\frac{1}{323} - \frac{1}{298}\right)$$

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

As the ideal gas constant R is used with units of $J.mol^{-1}.K^{-1}$, and the temperatures are given in K. So, the ΔH_{app} will be given in $J.mol^{-1}$.

Calculate the ΔH_{app} using the K_{app} data from both the linear and non-linear models and report these results.

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

$$\Delta G_{app} = -RT\ ln(K_{app}) \qquad \text{Eq. (9)}$$

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

Calculate the ΔG_{app} using the K_{app} data from both the linear and non-linear models, for 25 and 50 °C, and report these results.

The ΔS_{app} of the adsorption process can be calculated using the van't Hoff equation, as shown in the Eq. (10a and b):

$$\Delta G_{app} = \Delta H_{app} - T\,\Delta S_{app} \qquad \text{Eq. (10 a)}$$

$$\Delta S_{app} = \frac{\Delta H_{app} - \Delta G_{app}}{T} \qquad \text{Eq. (10 b)}$$

Calculate the ΔS_{app} using the ΔH_{app} and the ΔG_{app} data from both the linear and non-linear models, for 25 and 50 °C, and report these results. The ΔS_{app} units will be $J.K^{-1}$.

4. Data Analysis and Reporting:

4.1 Problem Situation:

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** produced from local seafood waste. Your laboratory obtained the 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.

Context constraints:

- The plant prefers processes that operate near ambient temperature (≤ 30 °C) to save energy.
- They want a one-paragraph recommendation for whether chitosan adsorption is appropriate and whether they should operate at ambient or elevated temperature.

4.2 Questions to be answered in your consulting report:

1) Present the average removal percentage at 25 and 50 °C for all the tartrazine initial concentration studies in a table like Table S3:

Table S3.

Tartrazine Initial Concentration (mg/L)	Average Removal Percentage after 30 min at 25 °C (%)	Average Removal Percentage after 30 min at 50 °C (%)
10		
20		
30		
40		
50		

2) What conclusions can you draw from the data presented in Table S3?

3) Derive the linear version of the Temkin isotherm (Eq 4(b)) from the non-linearized version (Eq. 6(b)). (Hint: this derivation is straightforward as long as you know the ln properties)

4) Present the Temkin isotherm graphs for the linear and non-linear models at 25 and 50 °C. Along with each graph, present the equation obtained from the linear or non-linear fit,

along with the correlation coefficient R^2. (Notice that a total of 8 graphs should be presented, considering that each experiment was performed in duplicate). Do both fits (linear and non-linear) lead to the same qualitative conclusion? Which fit would you recommend the plant rely on and why?

5) Show the average values and their respective standard deviation (avg ± std dev) for the K_T(linear and non-linearized) and q_T(linear and non-linearized) at 25 °C and 50 °C. Present the results in a Table like Table S4:

Table S4.

	Avg and std dev values at 25 °C		Avg and std dev values at 50 °C	
	K_T	q_T	K_T	q_T
Linear				
Non-linear				

6) What are the units for K_T and q_T?

7) What conclusions can you draw from the data presented in Table S4?

8) Convert the K_T into K_{app} according to the Eq. (7) of the experimental procedure and fill out their values in Table S5.

Table S5

	Avg at 25 °C	Avg at 50 °C
	K_{app}	K_{app}
Linear		
Non-linear		

a) Comment about possible differences between the K_{app} values for the same temperature between the values measured from the linear and non-linearized models.

b) For each model (linear and non-linearized) comment about how the Kapp varies with the temperature.

9) Compute the ΔG_{app} values, according to the Eq. (9) of the experimental procedure, in the Table S6:

Table S6

	Avg at 25 °C	Avg at 50 °C
	ΔG_{app}	ΔG_{app}
Linear		
Non-linear		

a) Based on the sign and magnitude of ΔG_{app} at 25 °C, is adsorption spontaneous at ambient temperature? And at 50 °C? If ΔG_{app} differs between 25 and 50 °C, what does that say about the effect of temperature? Clearly tell the units for the ΔG_{app}.

10) Using the two-point van't Hoff (Eq. 8), compute ΔH_{app} ($J \cdot mol^{-1}$) in Table S7:

Table S7

	Average at 25 °C	Average at 50 °C
	ΔH_{app}	ΔH_{app}
Linear		
Non-linear		

a) Based on ΔH_{app} sign, is adsorption exothermic or endothermic? What does that imply about whether increasing temperature will favor or disfavor adsorption?

11) Compute ΔS_{app} ($J.mol^{-1}.K^{-1}$) using Eq. (10b) in the Table S8:

Table S8

	Average at 25 °C	Average at 50 °C
	ΔS_{app}	ΔS_{app}
Linear		
Non-linear		

a) Relate the sign of ΔS_{app} to the ordering of molecules at the interface (does adsorption increase or decrease system randomness?) What is the effect of the temperature on the ΔS_{app}?

12) To visually prove to your client that this process is efficient, collect the supernatants of your samples with tartrazine initial concentration of 30 mg/L at 25 °, transfer them to glass vials and take a picture with the samples of different time points lined up. So, your client can observe the tartrazine decolorization over the contact time with chitosan.

13) Collect a sample of the chitosan powder after the experiment, dry it onto a petri dish, then put side by side a chitosan sample before and after adsorption to prove visually that the yellow dye tartrazine has adsorbed onto the chitosan surface.

14) The sustainable and environmental chemistry communities follows some guidelines in order to show they are aligned with the sustainability mindset. One of those guidelines is the **12 Principles of Green Chemistry**. Another guideline is the United Nations Sustainable Development Goals. Look for those two references and discuss to which Green Chemistry Principles and UN Sustainable Development Goals this experiment is related to, and justify your viewpoint for every goal or principle you cite. This type of information will help to show your client that your company is aware of the sustainable practices in the chemical industry.

15) Based on all the data collected and interpreted so far, write a <u>one-page double-spaced report</u> for your client. In this report, you should not simply tell the values encountered for the thermodynamic functions. You may tell them, but go beyond and discuss these values. You also have to make recommendations to your client about which process to use, at room temperature or at a higher temperature. Other factors to consider are the efficiency of the process in removing tartrazine at different initial concentrations. Also, identify at least two possible caveats of this adsorption system that your client can improve for the future.