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## ABSTRACT

Toxic heavy metals such as lead have been discharged into water streams due to industrialization, particularly from the stationery industry. Even though there are several ways to remove heavy metals, running the procedures is quite expensive. As a result, this research will simulate the performance of tea waste as a bio sorbent agent for removing lead ions from wastewater. The Fixed-Bed Adsorption Simulation Tool (FAST) program will create a simulation in this investigation. Furthermore, different manipulation factors such as lead ion initial concentration, contact time, and adsorbent dose were employed to evaluate its influence on the biosorption process. The results are comparable to a previous study on tea waste as a source of biosorption. According to the previous research and case study, the optimal contact duration is 60 minutes, the best metal ion concentration for adsorption is 100 mg/L, and the best adsorbent dose is 2 g. Furthermore, a comparison of the Langmuir isotherm with the Freundlich isotherm reveals that the Langmuir isotherm produces better results. Moreover, when the pseudo-first-order kinetic model is compared to the pseudo-second-order kinetic model, the pseudo-first-order yields superior results.

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# Simulation Study of Lead Removal from WasteWater by using Tea Waste as Biosorbent

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## ABSTRACT

*Toxic heavy metals such as lead have been discharged into water streams due to industrialization, particularly from the stationery industry. Even though there are several ways to remove heavy metals, running the procedures is quite expensive. As a result, this research will simulate the performance of tea waste as a bio sorbent agent for removing lead ions from wastewater. The Fixed-Bed Adsorption Simulation Tool (FAST) program will create a simulation in this investigation. Furthermore, different manipulation factors such as lead ion initial concentration, contact time, and adsorbent dose were employed to evaluate its influence on the biosorption process. The results are comparable to a previous study on tea waste as a source of biosorption. According to the previous research and case study, the optimal contact duration is 60 minutes, the best metal ion concentration for adsorption is 100 mg/L, and the best adsorbent dose is 2 g. Furthermore, a comparison of the Langmuir isotherm with the Freundlich isotherm reveals that the Langmuir isotherm produces better results. Moreover, when the pseudo-first-order kinetic model is compared to the pseudo-second-order kinetic model, the pseudo-first-order yields superior results.*

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## I. INTRODUCTION

Lead was among the first elements that mankind encountered, and it was utilised as early as 3000 B.C. Lead was used to create pipework and bath linings by the ancient Romans, and the plumber who joins and repairs pipes derives his name from

the Latin term plumbum, meaning lead. Plumbum is also the name of the surveying phrases "plumb bob" and "plumb line," as well as the chemical symbol for lead, Pb [1]. Although it can exist in numerous chemical forms, Pb does not disintegrate in the environment. Pb-containing particulate particles can travel through the air, water, and soil. In general, atmospheric deposition is the most common source of Pb in soils that are not influenced by other non-air sources (e.g., dust from deteriorating leaded paint) [26].

The WHO's method for assessing the global burden of illness is DALYS or disability-adjusted life years; they are defined as the total of years of life lost due to death and impairment due to a certain illness or condition case, lead exposure [19]. The entire disease burden due to lead is estimated to be over 9 million DALYs (disability-adjusted life years)! This DALY estimate is mostly due to mental impairment (as assessed by IQ), but it also includes elevated blood pressure (which raises the risk of ischemic heart disease), stroke, hypertensive illness, and other cardiovascular illnesses (WHO). In addition, lead poisoning was predicted to be responsible for 143,000 fatalities and 0.6 percent of the worldwide disease burden in 2004 [22].

Besides, biosorption is an effective and environmental-friendly method to treat wastewater. Metal biosorption is used to remove metal ions from aqueous streams using agricultural products [21]. A solid phase (sorbent) and a liquid phase (solvent) containing a dissolved species to be sorbed are involved in the biosorption process. Due to the sorbent's high affinity for metal ion species, the latter is attracted and bound by a complicated process comprising chemisorption, complexation, adsorption on surface and pores, ion exchange, chelation, and physical force adsorption.

There are a variety of biomaterials with different sorption capabilities. The utilisation of these materials is based on their sorption capacity as well as their reusability over time [11]. Hence, tea waste will be employed as a bio sorbent in this investigation to aid lead biosorption. Tea comes in various flavours, including green, black, and Oolong; all tea drinks are made from the same fundamental tea leaves (*Camellia sinensis* L.). Extracts from it are utilised in various drinks, health foods, nutritional supplements, and cosmetic products [10].

Furthermore, FAST is an acronym for Fixed-bed Adsorption Simulation Tool. FAST is a water treatment program that predicts the breakthrough curves of fixed-bed adsorption filters by the simulation method. [25] Various adsorbent media, such as granular activated carbon (GAC) or metal oxides, can be used depending on the pollutant to be removed in the process. Determining kinetic parameters from laboratory tests is another use. The homogeneous surface

diffusion model (HSDM) and the linear-driving force approximation may both be solved numerically with FAST (LDF). are a valuable teaching tool for water engineering and water chemistry classes because of the extensive built-in support. [25]

## II. METHODOLOGY

As previously indicated, we will compare the simulation findings to the experimental data in this simulation research. As a consequence, the experimental result from Mehrdad Cheraghi's publication "Removal of Pb (II) from Aqueous Solutions Using Waste Tea Leaves" is being compared to our simulation of Lead (Pb II ion) removal using tea waste.

Furthermore, the categorization of bio-sorbent properties is regarded as the initial technique here. Table 3 shows the characteristics of tea waste used by the experimental research, which will also be used in this simulation study.

*Table 2.1:* The characteristics of tea waste for this simulation study

Parameter	Tea Waste Values
Humid (%)	10.5
Density (g cm <sup>-3</sup> )	0.353
Dissolved material (%)	81
Solution particles total (mg l <sup>-1</sup> )	108
Organic matters (%)	85
Ash content (%)	2.85
pH <sub>ZPC</sub>	6

Many process factors such as contact duration, adsorbate concentration, and adsorbent dose were evaluated. Hence, several parameters are calculated and compared with the experimental research to obtain the values for the simulation to run. Firstly, the bed density was calculated using data from an experimental case study on Pb (II) biosorption by tea waste. The diffusion coefficient for the film is considered to be proportional to the surface area and the difference in concentration between the bulk solution and the adsorbent surface.  $k_L$  may also be calculated by fitting the simulation to experimental data. Besides, empirical correlations for the Sherwood number

are used to calculate the film diffusion coefficient  $k_L$ .

$$\frac{\partial M}{\partial t} = k_L A (c - c^*) \tag{1}$$

$$A = \pi d_p^2 \tag{2}$$

Fick's second law is used to simulate mass transport in the adsorbent grain, which is considered to be homogeneous surface diffusion—fitting the simulation to experimental data yields the surface diffusion coefficient DS.

$$\frac{\partial q}{\partial t} = D_s \left( \frac{\partial^2 q}{\partial r^2} + \frac{2}{r} \frac{\partial q}{\partial r} \right) \tag{3}$$

To investigate the kinetics of Pb (II) adsorption by tea waste, 100 ml of 100 mg/L Pb (II) solution was mixed with known quantities of each adsorbent. For Pb, the program got to run for 120

minutes. The adsorption kinetics of Pb (II) ions were studied using Lagergren's pseudo-first-order kinetics expression and pseudo-second-order rate expression equation.

Table 2.2: The overall kinetic models used in this study

Reaction Kinetic Models	Non-Linear Equation	Linear Equation	Model Parameters
pseudo-first order	$q_t = q_e (1 - e^{-k_1 t})$	$\log(q_e - q_t) = \log q_e - \left(\frac{k_1}{2.30}\right) t$	$q_e, k_1$
pseudo-second order	$q_t = \frac{q_e^2 k_2 t}{1 + q_e k_2 t}$	$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$	$q_e, k_2$

The adsorption of Pb (II) ions by tea waste particles adsorbents was studied using two Langmuir and Freundlich adsorption isotherm models. [18]

The Langmuir isotherm model can be written as follows:

$$q_e = \frac{Q_m K_L C_e}{1 + K_L C_e} \quad (4)$$

Where:

$q_e$  = the amount of lead adsorbed equilibrium (mg/g)

$Q_m$  = the maximum monolayer coverage capacity (mg/g)

$K_L$  = the Langmuir isotherm constant (L/mg)

The Freundlich Isotherm can be identified through:

$$\log q_e = \log k_F + \frac{1}{n} \log C_e \quad (5)$$

Where:

$C_e$  = The Lead ion's equilibrium concentration in the remaining solution (in mol/L)

$q_e$  = The adsorbed Lead ion's equilibrium concentration per unit of mass sorbent (in mol/g)

$k_F$  = The capacity for adsorption

$n$  = Related to the adsorption intensity (unitless)

To study the effect of contact time, the contact time is varied in the range from 30 mins, 60 mins and 90 mins. The other parameters are being held constant for this study, like the Pb (II) ion concentration in wastewater to 100 mg/L and the mass of tea waste to 2g on each run. The effect of initial bio sorbent dose on % of Pb (II) ion elimination was investigated by adjusting the bio sorbent concentration of 1g, 2g and 3g. A graph of adsorption capacity vs contact time after 120 minutes was generated. To investigate the effect of metal ion concentration on the lead removal from the wastewater using the tea waste, the

concentration of lead solution differs from 100 mg/L to 300 mg/L. The contact time is 60 min while the adsorbent dose is also kept constant to 2g for each run. To investigate the effect of metal ion concentration, the concentration of lead solution differs from 100 mg/L to 300 mg/L. The contact time is set to be as before which is 60 min while the adsorbent dose is also kept constant to 2g for each run.

### III. RESULTS AND DISCUSSION

#### 3.1 Comparison of Biosorption Isotherms with Experimental Study

In this case study, the Langmuir and Freundlich isotherms were investigated. The simulation was

done using the identical settings (2g adsorbent mass, 100mg/L Pb(II) concentration, 60 minutes contact duration) for both isotherms. Figures 3.1 and 3.2 depict simulation runs for the Langmuir and Freundlich isotherms, respectively.

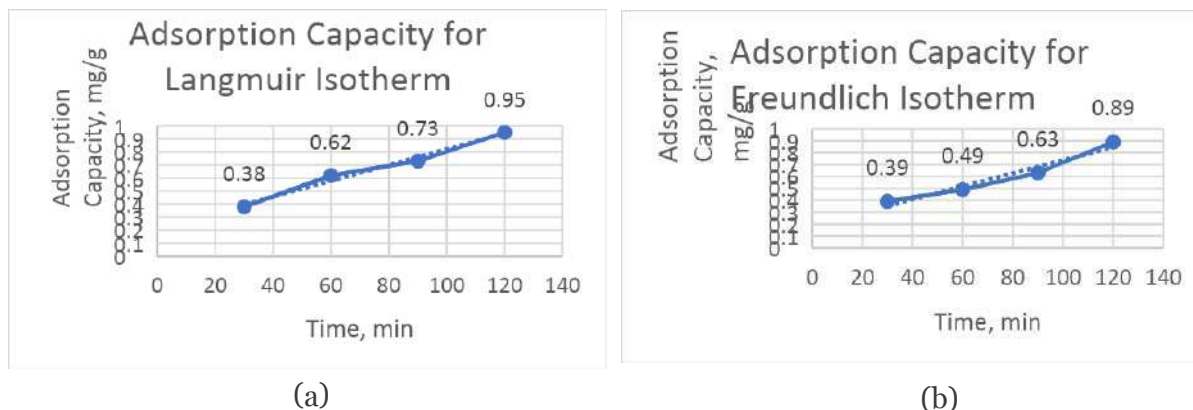


Figure 3.1 a & 3.1 b: Simulation run for the adsorption capacity for Langmuir Isotherm and Freundlich Isotherm using FAST

According to Figures 3.1 and 3.2, the Langmuir isotherm has a higher  $R^2$  value of 0.9823 than the Freundlich isotherm. Other research studies comparing Freundlich and Langmuir isotherms have also found that the Langmuir isotherm gives the greatest value of  $R^2$  correlation, suggesting that it is the best fit model to forecast the data's trendline. Consequently, it may be inferred that the Langmuir isotherm outperforms the Freundlich isotherm. As a result, the same procedure of comparing  $R^2$  is utilised to determine the most accurate isotherm for this case study.

#### 3.2 Kinetic Study on the Lead Removal

Both the pseudo-first-order and pseudo-second-order kinetic models were explored in this research. Both models were simulated using the same parameters (2g adsorbent mass, 100mg/L Pb (II) concentration, 60 minutes contact time). Simulation runs for the pseudo-first-order and pseudo-second-order kinetic models are shown in Figures 3.3a and 3.3b, respectively.



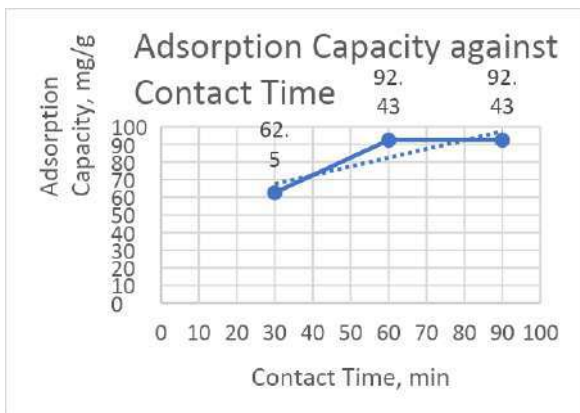
Figure 3.2a & 3.2b: Simulation run for Pseudo-first-order equation and Pseudo-second-order equation

The pseudo-second-order kinetic model has a higher and more suitable  $R^2$  value than the pseudo-first-order kinetic model. Other studies

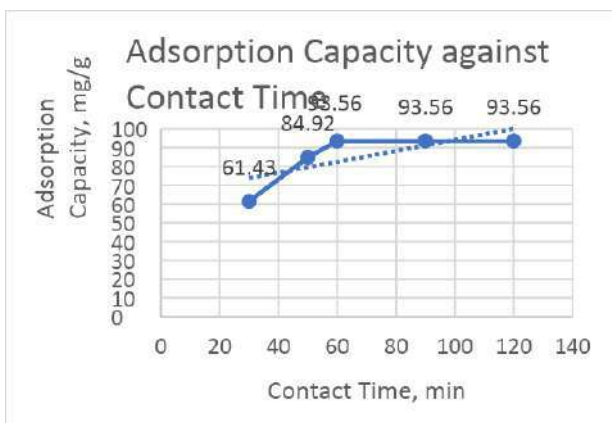
that compared pseudo-first-order and pseudo-second-order kinetic models discovered that the pseudo-second-order model had the highest  $R^2$

correlation, implying that it is the best-suited model for forecasting the data's trendline.

### 3.3 Comparison Study of Variables on Simulation Results with Experimental Results



(a)

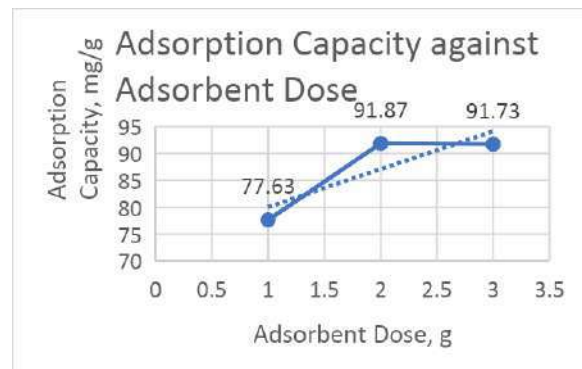


(b)

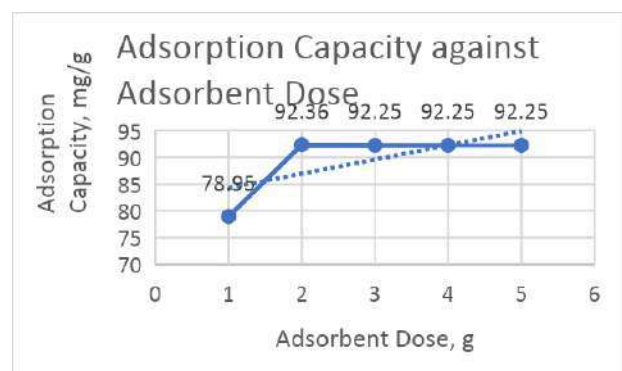
Figure 3.3 a & 3.3 b: Effect of contact time on the adsorption capacity of tea waste for simulation run and experimental research

Both the simulation and experimental values indicate a rising trend in adsorption capacity and then become static after a while, with little difference in the values. Moreover, both findings demonstrated that the best contact time for the maximum adsorption capacity of the tea waste particle occurs at the 60<sup>th</sup> minute. The adsorption rate was quick at the beginning of the contact period due to a large number of accessible adsorbent surfaces. The lower adsorption effectiveness over some time might be attributable to two factors. To begin with, occupying the sites limited the number of active surface sites available on the adsorbent. Second, owing to the repulsive effect of the deposited metal ions on the

solid and bulk phase, the remaining unoccupied surface sites were difficult to occupy.



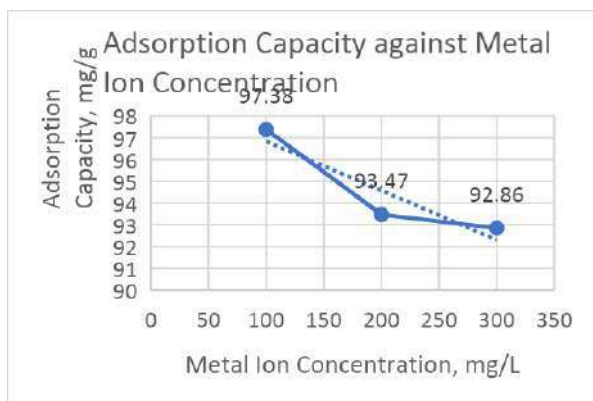
(a)



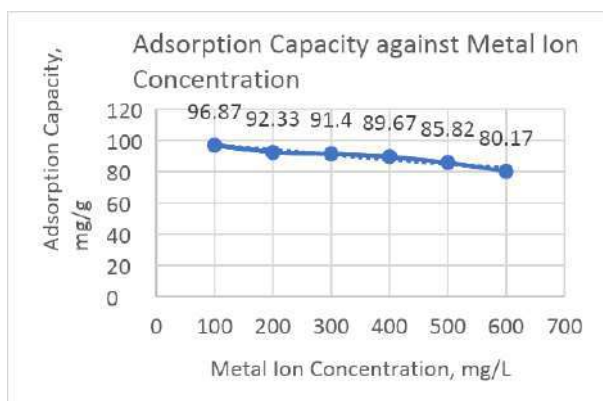
(b)

Figure 3.4 a & 3.4 b: Effect of adsorbent dose on the adsorption capacity of tea waste for simulation run and experimental research

Both simulation and experimental results show a growing trend in adsorption capacity and reduce with successive dose increments until becoming static beyond a specific dosage, with less variation in the result data. Adsorption of Pb (II) is expected to rise when the adsorbent dosage is increased. It was raising the adsorbent dosage gives more adsorption sites for a constant starting adsorbate concentration, the removal efficiency improves with increasing the adsorbent dose. Metal ion binding to tea waste's surface functional groups is another possible explanation. But beyond a certain point, increasing the amount did not influence removal effectiveness, and 2g was the optimum amount proven from both the experimental and simulation study. We discovered a similar behaviour with Zn (II) [23]. As a result, the adsorption capacity is influenced by the adsorbent mass.



(a)



(b)

Figure 3.5 a & 3.5 b: Effect of metal ion concentration on the adsorption capacity of tea waste for simulation run and experimental research

As the metal ion concentration increases, the simulated and experimental values reveal a declining trend in adsorption capacity, and the value difference is not particularly noticeable. A rise in the initial Pb (II) concentration may have increased the driving power of the concentration gradient. As a result of the restricted number of active adsorbent particle sites and the limited uptake capacity, the removal efficiency is high at low concentrations. In contrast, when the metal concentration is high, the active sites of the adsorbent particles are occupied. Hence, it can be concluded that Pb (II) concentration will influence the adsorption capacity. Furthermore, both analyses revealed that the ideal metal ion concentration for achieving maximal adsorption capacity is 100 mg/L.

#### IV. CONCLUSION

In a nutshell, the effectiveness of tea waste as a bio-sorbent for lead ion adsorption in wastewater

was investigated successfully. According to this case study, tea waste is an effective bio-sorbent for adsorbing lead in wastewater. It was found that ideal contact time for adsorption is 60 minutes. 100mg/L, 200mg/L, and 300mg/L of metal ion concentration were utilised in the investigation of Pb (II) concentration and adsorption capacity, and 100mg/L of metal ion concentration recorded the best adsorption capacity compared to other concentrations. The adsorbent doses employed in this case study were 1g, 2g, and 3g, with the 2g dosage having the best adsorption capacity. The comparison of Langmuir isotherm with Freundlich isotherm reveals that Langmuir isotherm outperforms Freundlich isotherm. Moreover, this study also proved that the pseudo-second-order kinetic model is the best fit model for this investigation compared to the pseudo-first-order kinetic model. Furthermore, in this case, study, the accuracy of the simulation data was determined. The adsorption process which was aided by the FAST program, gave accurate data. Because FAST software is specifically created to analyze adsorption processes, it was utilised in this case study to investigate the influence of contact time, metal ion concentration, and adsorbent dose on the adsorption capacity of tea waste particles in the removal of lead from the wastewater. As a result, FAST software is employed in this case study to evaluate its efficiency, and the results are favourable.

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