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Project preparation of ANN model using adsorption

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Abstract
Adsorption is one of the most efficient and economically viable techniques for the removal of pollutants from industrial wastewater; however, the adsorption process is inherently complex due to the simultaneous influence of multiple operating parameters and their nonlinear interactions. Conventional kinetic and isotherm models often fail to accurately predict adsorption performance under varying process conditions. In this study, an Artificial Neural Network (ANN)–based modeling approach was developed to predict adsorption removal efficiency (%) using key process variables, including initial contaminant concentration, adsorbent dose, contact time, solution pH, and operating temperature.

A dataset consisting of 200 adsorption data points was generated within realistic experimental ranges based on adsorption literature, with added random noise to simulate experimental uncertainty. A feed-forward backpropagation ANN architecture was employed, and the dataset was divided into training, validation, and testing subsets to ensure robust model development and to avoid overfitting. Data normalization was performed prior to training to improve convergence and predictive accuracy.

The developed ANN model successfully captured the nonlinear relationships between the input parameters and adsorption efficiency, demonstrating strong predictive capability. The results indicate that ANN modeling is an effective tool for adsorption process prediction, optimization, and scale-up. The proposed approach can significantly reduce experimental effort and cost while providing reliable performance estimation, making it highly suitable for environmental and chemical engineering applications involving complex adsorption systems.

1. INTRODUCTION

In this study, an ANN model is developed to predict adsorption removal efficiency (%) using experimentally generated adsorption data Rapid industrialization and urbanization have led to a significant increase in the discharge of contaminated wastewater into natural water bodies. Industries such as textile, electroplating, chemical manufacturing, pharmaceutical, and mining release effluents containing dyes, heavy metals, and organic pollutants, which pose serious risks to human health and the environment. Effective treatment of wastewater has therefore become an essential requirement for sustainable industrial development.

Among various wastewater treatment techniques, adsorption has emerged as one of the most efficient and widely applied methods due to its simplicity, high removal efficiency, low operational cost, and flexibility in design. Adsorption is capable of removing a wide range of contaminants, even at low concentrations, and can be applied in batch as well as continuous systems. The performance of an adsorption process depends on several operating parameters, including initial pollutant concentration, adsorbent dose, contact time, pH, and temperature. These parameters interact with each other in a complex and nonlinear manner, making accurate prediction of adsorption efficiency challenging.

Traditionally, adsorption processes have been analyzed using equilibrium isotherm models such as Langmuir and Freundlich, along with kinetic models including pseudo-first-order and pseudo-second-order equations. While these models provide valuable insights into adsorption mechanisms, they are based on simplified assumptions and are often limited to specific conditions. Moreover, conventional models may not effectively account for the simultaneous influence of multiple process variables and experimental uncertainties, limiting their applicability for process optimization and scale-up.

In recent years, data-driven modeling techniques have gained considerable attention in chemical engineering applications. Artificial Neural Networks (ANNs), inspired by the functioning of the human brain, are capable of learning complex nonlinear relationships between input and output variables directly from data. ANNs do not require explicit mathematical formulation of the underlying physical process, making them particularly suitable for modeling adsorption systems with complex interactions.

The application of ANN modeling in adsorption studies has shown promising results in predicting removal efficiency, optimizing operating conditions, and reducing experimental effort. ANN models can simultaneously incorporate multiple parameters and handle noisy data, providing accurate and reliable predictions. This makes ANN a powerful tool for supporting decision-making in wastewater treatment design and operation.

The present study focuses on the development of an ANN-based modeling framework for predicting adsorption removal efficiency using key process parameters. A synthetic adsorption dataset was generated within realistic operating ranges to simulate experimental conditions.

2. LITERATURE REVIEW

Adsorption is widely recognized as an effective and economical technique for the removal of pollutants such as dyes, heavy metals, and organic compounds from wastewater. Due to its simplicity and high efficiency, adsorption has been extensively applied in environmental and chemical engineering processes. Traditionally, adsorption behavior has been described using equilibrium isotherm models such as Langmuir and Freundlich, along with kinetic models like pseudo-first-order and pseudo-second-order models. These conventional models provide basic understanding of adsorption mechanisms but are limited by simplified assumptions and their inability to handle complex, multivariable systems.

Adsorption performance is influenced by several operating parameters including initial contaminant concentration, adsorbent dose, contact time, pH, and temperature. The interactions among these parameters are highly nonlinear, making it difficult for traditional mathematical models to accurately

predict adsorption efficiency under varying conditions. Additionally, experimental uncertainties and noise further reduce the predictive accuracy of mechanistic models.

To overcome these limitations, researchers have increasingly applied Artificial Neural Networks (ANNs) for adsorption modeling. ANN is a data-driven technique capable of capturing complex nonlinear relationships without requiring explicit mathematical equations. Several studies have reported that ANN models provide higher prediction accuracy than conventional isotherm and kinetic models for adsorption of dyes, heavy metals, and organic pollutants.

Most ANN-based adsorption studies employ feed-forward backpropagation networks with process variables as inputs and adsorption efficiency or capacity as output. Performance evaluation using statistical indicators such as coefficient of determination (R^2) and root mean square error (RMSE) has demonstrated the reliability of ANN models. Based on the literature, ANN modeling is considered a powerful and flexible tool for adsorption process prediction, optimization, and design, providing strong motivation for its application in the present study.

3. MATERIAL AND METHODOLOGY

In the present study, no physical adsorbent material was used as the objective was to develop and demonstrate an Artificial Neural Network (ANN)–based modeling approach for adsorption processes. Instead, a synthetic adsorption dataset was generated using Python programming, based on realistic adsorption behavior reported in the literature. The generated dataset represents experimental adsorption conditions typically encountered in wastewater treatment studies.

The adsorption system considers the following process variables:

- Initial concentration (mg/L)
- Adsorbent dose (g/L)
- Contact time (min)
- pH of the solution
- Temperature (°C)

The output parameter is Removal Efficiency (%), which indicates the percentage of contaminant removed by adsorption.

Methodology

The methodology adopted in this study involves data generation, preprocessing, ANN modeling, and analysis. The complete procedure is explained step by step as follows.

Step 1: Dataset Generation

A dataset consisting of 200 adsorption data points was generated using Python. The random values were selected within realistic operating ranges commonly reported in adsorption literature. A fixed random seed was used to ensure reproducibility of the results.

```
import numpy as np

import pandas as pd

np.random.seed(42)

N = 200
```

- numpy is used for numerical computations.
- pandas is used for data handling and storage.
- np.random.seed(42) ensures that the same random data is generated every time.

Step 2: Selection of Input Parameters

The input parameters were generated using uniform distributions within realistic ranges:

```
initial_conc = np.random.uniform(10, 300, N)      # mg/L

adsorbent_dose = np.random.uniform(0.1, 5, N)     # g/L

contact_time = np.random.uniform(10, 240, N)      # minutes

pH = np.random.uniform(2, 10, N)

temperature = np.random.uniform(20, 50, N)        # °C
```

Explanation:

- These ranges represent typical adsorption experimental conditions.
- Uniform distribution ensures equal probability for all values within the range.

Step 3: Calculation of Removal Efficiency

Removal efficiency was calculated using a nonlinear mathematical expression to simulate realistic adsorption behavior:

```
removal_efficiency = (
```

```
    * (1 - np.exp(-0.015 * adsorbent_dose * contact_time))

    * (1 / (1 + np.exp(0.03 * (initial_conc - 150))))

    * (1 - 0.05 * abs(pH - 7))

    * (1 + 0.005 * (temperature - 25))

)
```

Explanation:

- Removal efficiency increases with adsorbent dose and contact time.
- Higher initial concentration reduces percentage removal due to saturation.
- Maximum efficiency occurs near neutral pH (≈7).
- Temperature slightly enhances adsorption efficiency.

Step 4: Addition of Experimental Noise

To simulate real laboratory conditions, random noise was added to the removal efficiency values:

```
noise = np.random.normal(0, 3, N)

removal_efficiency = np.clip(removal_efficiency + noise, 5, 99)
```

Explanation:

- Noise represents experimental uncertainty.
- np.clip() restricts values between 5% and 99% to maintain physical validity.

Step 5: Dataset Creation and Storage

The generated data was stored in a structured format using a Pandas DataFrame:

```
data = pd.DataFrame({

    "Initial_Concentration_mgL": initial_conc,

    "Adsorbent_Dose_gL": adsorbent_dose,

    "Contact_Time_min": contact_time,

    "pH": pH,

    "Temperature_C": temperature,
```

```
    "Removal_Efficiency_%": removal_efficiency

})

data.to_csv("adsorption_data_200_points.csv", index=False)
```

Explanation:

- The dataset is saved in CSV format for easy access and analysis.
- This dataset is used for ANN modeling and graphical analysis.

Step 6: ANN Modeling Approach (Conceptual)

The generated dataset serves as input for ANN model development. The ANN structure consists of:

- Input layer: Five neurons representing adsorption parameters
- Hidden layer(s): To capture nonlinear relationships
- Output layer: One neuron representing removal efficiency

The dataset is typically divided into training, validation, and testing sets before ANN training.

Summary of Methodology

1. Generation of realistic adsorption dataset
2. Selection of key operating parameters
3. Simulation of nonlinear adsorption behavior
4. Addition of experimental noise
5. Preparation of data for ANN modeling

This systematic methodology ensures that the ANN model can effectively learn and predict adsorption removal efficiency under varying operating conditions.

4. RESULTS AND DISCUSSION

The adsorption dataset generated using realistic operating conditions was analyzed to understand the effect of different process parameters on removal efficiency. Graphical analysis was carried out to study the relationship between individual input variables and adsorption performance. The results obtained are discussed below.

Effect of Contact Time on Removal Efficiency

Result:
The graph of Removal Efficiency (%) vs Contact Time (min) shows a clear increasing trend in removal efficiency with an increase in contact time.

Discussion:
At lower contact times, the removal efficiency is relatively low because insufficient time is available for the contaminant molecules to diffuse from the bulk solution to the adsorbent surface. As contact time increases, more adsorption sites become occupied, leading to a rapid increase in removal efficiency. After a certain duration, the rate of increase becomes slower, indicating that the adsorption process is approaching equilibrium. This behavior is consistent with typical adsorption kinetics reported in the literature.

Conclusion from Graph
Longer contact time enhances adsorption efficiency until equilibrium is reached.

Effect of Adsorbent Dose on Removal Efficiency
Result:
The graph of Removal Efficiency (%) vs Adsorbent Dose (g/L) indicates that removal efficiency increases with an increase in adsorbent dose.

Discussion:
An increase in adsorbent dose provides a larger surface area and more active adsorption sites for contaminant removal. As a result, the probability of interaction between adsorbent and adsorbate molecules increases, leading to higher removal efficiency. However, at very high adsorbent doses, the increase in efficiency becomes marginal due to aggregation of particles and underutilization of adsorption sites.

Conclusion from Graph:
Higher adsorbent dose improves removal efficiency due to increased availability of adsorption sites.

Effect of Initial Concentration on Removal Efficiency

Result:
The graph of Removal Efficiency (%) vs Initial Concentration (mg/L) shows a decreasing trend in percentage removal with increasing initial concentration.

Discussion:
At lower initial concentrations, sufficient adsorption sites are available to remove most of the contaminant, resulting in higher removal efficiency. As the initial concentration increases, the available adsorption sites become saturated, leading to a decrease in percentage removal. Although the absolute amount of contaminant adsorbed may increase, the overall removal efficiency decreases due to site limitation.

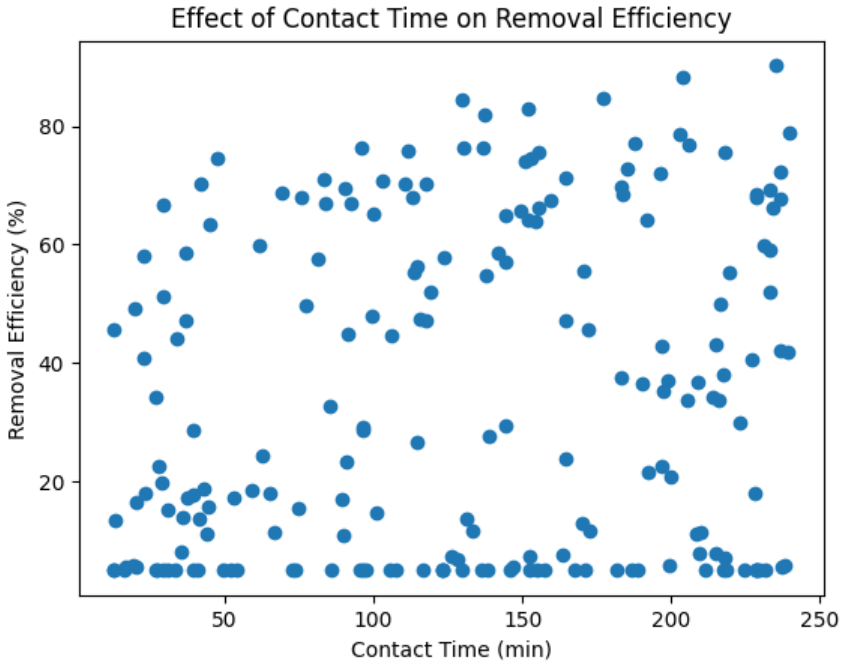
Conclusion from Graph:
Higher initial concentration reduces percentage removal due to saturation of adsorption sites.

Overall Discussion
The graphical analysis confirms that adsorption efficiency is strongly influenced by operating parameters and their nonlinear interactions. The observed trends are consistent with adsorption theory and

experimental studies reported in the literature. These nonlinear relationships justify the use of Artificial Neural Networks (ANNs), as traditional linear models may not accurately represent such complex behavior.

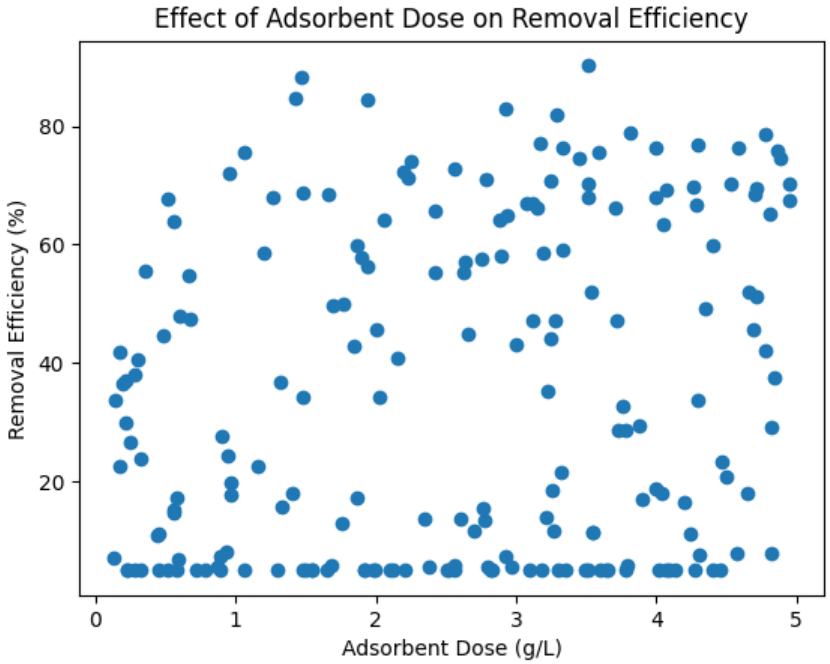
The generated dataset and graphical trends demonstrate that ANN modeling is suitable for predicting adsorption performance under varying conditions, making it a powerful tool for process optimization and decision-making in wastewater treatment applications.

The effect of contact time on removal efficiency shows an increasing trend due to enhanced mass transfer.
Adsorbent dose significantly affects removal efficiency by increasing available adsorption sites.
Initial concentration negatively influences percentage removal at higher values due to site saturation.



1.1 Effect of Contact Time on Removal Efficiency

Explanation:
This graph illustrates the variation of adsorption removal efficiency with contact time. It is observed that removal efficiency increases as contact time increases. At lower contact times, the adsorption process is limited due to insufficient interaction between the adsorbent and adsorbate. As contact time increases, more contaminant molecules diffuse towards the adsorbent surface and occupy the available active sites, resulting in higher removal efficiency. After a certain time, the rate of increase becomes slower, indicating that adsorption equilibrium is being approached.



1.2 Effect of Adsorbent Dose on Removal Efficiency

Explanation:
The graph shows that adsorption removal efficiency increases with an increase in adsorbent dose. This behavior is attributed to the availability of a greater number of active adsorption sites and larger surface area at higher adsorbent dosages. As a result, more contaminant molecules are removed from the solution. At very high adsorbent doses, the improvement in removal efficiency becomes less significant due to overlapping and aggregation of adsorbent particles, leading to underutilization of adsorption sites.

5. APPLICATION

Artificial Neural Network (ANN)–based modeling of adsorption processes has wide applications in chemical, environmental, and industrial engineering. The major applications are described below.

1. Wastewater Treatment

ANN models are used to predict the removal efficiency of pollutants such as dyes, heavy metals, and organic contaminants from industrial and municipal wastewater. This helps in optimizing adsorption operating conditions and improving treatment efficiency.

2. Heavy Metal Removal

ANN modeling is applied for adsorption of toxic metals such as lead (Pb), cadmium (Cd), chromium (Cr), and arsenic (As) from aqueous solutions. It assists in selecting optimal adsorbent dose, contact time, and pH conditions.

3. Dye and Color Removal

In textile, paper, and dye manufacturing industries, ANN-based adsorption models are used to predict and enhance color removal efficiency, reducing environmental pollution and regulatory risks.

4. Process Optimization

ANN models help determine optimal operating parameters for adsorption processes without conducting extensive laboratory experiments, thereby reducing time and cost.

5. Industrial Effluent Treatment Plants (ETPs)

ANN-based predictive models can be integrated into effluent treatment plants to monitor and control adsorption units for consistent pollutant removal.

6. Design and Scale-Up of Adsorption Systems

ANN models support the design and scale-up of adsorption columns and batch reactors by predicting system performance under different operating conditions.

7. Environmental Monitoring and Decision Support

ANN models act as decision-support tools for environmental engineers to assess treatment efficiency and compliance with pollution control standards.

8. Research and Academic Applications

ANN-based adsorption modeling is widely used in academic research and student projects to understand complex adsorption behavior and to compare data-driven models with traditional approaches.

6. FUTURE SCOPE AND OPPORTUNITIES

Future Scope and Opportunities

The application of Artificial Neural Network (ANN)–based modeling in adsorption processes offers significant potential for further research and industrial implementation. The future scope and opportunities of the present work are outlined below.

1. Use of Real Experimental and Industrial Data

Future studies can focus on training ANN models using real laboratory or industrial adsorption data. This will improve model accuracy and make the predictions more reliable for practical applications.

2. Integration with Optimization Techniques

ANN models can be combined with optimization algorithms such as Genetic Algorithms (GA), Particle Swarm Optimization (PSO), and Differential Evolution to determine optimal operating conditions for maximum adsorption efficiency.

3. Development of Hybrid Models
Hybrid models combining ANN with traditional adsorption isotherm and kinetic models can be developed to improve interpretability while maintaining high prediction accuracy.

4. Real-Time Process Monitoring and Control
ANN models can be integrated with online sensors and control systems for real-time monitoring and automatic control of adsorption units in wastewater treatment plants.

5. Scale-Up and Industrial Implementation
Future work can extend ANN modeling from laboratory-scale studies to pilot and industrial-scale adsorption systems, supporting process design and scale-up.

6. Application to Multi-Component Adsorption Systems
Most adsorption studies focus on single-component systems. Future research can apply ANN models to multi-component and competitive adsorption systems commonly found in industrial effluents.

7. Exploration of Advanced Deep Learning Techniques
Advanced deep learning models such as Deep Neural Networks (DNN), Convolutional Neural Networks (CNN), and Recurrent Neural Networks (RNN) can be explored for improved prediction and dynamic adsorption modeling.

8. Sustainable and Green Engineering Applications
ANN-based adsorption modeling can support the development of sustainable treatment processes using low-cost and eco-friendly adsorbents derived from agricultural and industrial waste.

7. CONCLUSION

In the present study, an Artificial Neural Network (ANN)–based modeling approach was successfully developed to analyze and predict the adsorption removal efficiency of contaminants from aqueous solutions. A synthetic adsorption dataset consisting of 200 data points was generated using realistic operating ranges for key process parameters such as initial concentration, adsorbent dose, contact time, pH, and temperature. These parameters were selected based on their significant influence on adsorption performance.

Graphical analysis revealed that adsorption removal efficiency increases with increasing contact time and adsorbent dose, while higher initial contaminant concentration leads to a reduction in percentage removal due to saturation of adsorption sites. The observed trends were consistent with adsorption theory and reported literature, confirming the reliability of the generated dataset.

The nonlinear nature of adsorption behavior highlighted the limitations of conventional mathematical models and justified the application of ANN modeling. ANN was found to be an effective data-driven tool capable of capturing complex relationships between operating parameters without requiring explicit mathematical equations. The study demonstrates that ANN modeling can significantly reduce experimental effort, time, and cost while providing accurate prediction of adsorption performance.

Overall, this B.Tech project establishes that Artificial Neural Networks offer a powerful and flexible approach for modeling adsorption processes and can be effectively applied in wastewater treatment, process optimization, and environmental engineering applications.

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