Machine Learning Based Model to Assess the Performance of Green Synthesized Iron Nano Particles for Dye Removal from Industrial Wastewater

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Abstract.
The purpose of this project is to create a machine learning predictive model that assesses the potential of green synthesized iron nanoparticles to remove dyes from industrial wastewater. The nanoparticles were prepared using an environmentally friendly green synthesis method, where plant extracts were used as reducing and capping agents, which considerably minimizes the environmental impact linked with traditional chemical synthesis processes. The prepared nanoparticles were further put to a series of experimental tests to evaluate their dye adsorption and removal performances under different physical and chemical parameters like pH, contact time, dye concentration, and dosage. The textile dye waste from industry by traditional method of dye removal was compared with ML result and found 6% variation on the result.

1 Introduction

Pollution of water, especially by industrial effluents, is a dangerous menace for environmental ecosystems and human health. The release of synthetic dyes from industries like textiles, leather, cosmetics, and paper is one of the primary causes of water pollution. These dyes, due to their stable molecular nature, are not just aesthetically displeasing but also chemically persistent and toxic, posing a risk to be carcinogenic and mutagenic human and also to aquatic bodies. Thus, their elimination from wastewater is a matter of concern in environmental engineering.[1][2][3]

Traditional dye removal methods, such as biological treatment, chemical precipitation, ion exchange, and activated carbon adsorption, tend to be inefficient, expensive, and environmentally unsustainable. The shortcomings have motivated researchers to investigate new advanced treatment technologies that are environmentally friendly and also efficient. The breakthroughs is the application of nano-materials, specifically iron nanoparticles,

owing to their high absorption surface area, active sites, and outstanding adsorption capacity. [4][5]

Nevertheless, the chemical synthesis of these nanoparticles can produce dangerous by-products that undermine environmental safety. In response, green synthesis methods have been proposed as a more environmentally friendly alternative. These processes harness plant-based materials to reduce metal ions, thus eliminating the use of toxic chemicals and enhancing biocompatibility. [6][7][8]

Concurrently, the emergence of machine learning (ML) in engineering and environmental science provides an effective tool for processing complex data, detecting underlying patterns, and making precise predictions. When coupled with nanotechnology, ML algorithms can improve the comprehension of how different parameters affect dye removal efficiency, allowing the creation of solid predictive models. This project, thus, closes the gap between sustainable nanomaterial development and smart data-driven modelling. The central aim is to prepare iron nanoparticles using green processes and use machine learning models to forecast their efficiency in decolorizing industrial wastewater. This multidisciplinary research not only promotes environmental sustainability but also facilitates the practical application of smart technologies in water treatment processes. Through intensive experimentation and data analysis, the project hopes to contribute to the creation of scalable, cost-effective, and environmentally friendly solutions for industrial wastewater management.[9][10][11][12]

Green synthesis nano particles are low-cost, non-toxic, and eco-friendly, natural caping agent, stabilizing agent, reducing agent and which can also be used to treat many types of wastewaters. Considering the above aspects, green-synthesized nanoparticles from Mangifera indica was employed to evaluate their efficiency in removing dye from textile wastewater [14][15].

2 Literature Review

Tamanna Kumari and Vineeta Shukla (2023) conducted a comparative study titled "Removal of Dye from Water using Green Synthesized Iron Nanoparticles by Different Plants Extract." The study involved synthesis of iron nanoparticles (FeNPs) through six plant extracts—Azadirachta indica (AIL), Salvadora oleoides (SOL), Syzygium cumini (SCB), Citrus limon (CLF), Prosopis cineraria (PCB), and Ocimum sanctum (OSL)—as green reducing agents. Characterization was performed using UV-Vis, FT-IR, XRD, FE-SEM, and zeta potential analysis. Photocatalytic degradation of gentian violet dye under visible light was screened in the FeNPs. Among the samples, OSL-extract-based FeNPs exhibited maximum dye removal efficiency (83%) and adsorption capacity followed by CLF (63%) and PCB (59%). Catalyst dose, dye concentration, and pH influenced photocatalytic efficiency, with maximum degradation at pH 6.0 and 50 mg catalyst load. The study highlights green synthesis as a cost-effective and sustainable route compared to chemical routes and highlights the high potential of OSL-based FeNPs in wastewater treatment.

Aynur Sahin et al. (2024) conducted research titled “An Approach for Cationic Dyes Removal from Wastewater: Green Synthesis of Iron Nanoparticles Using Prunus avium Stem Extracts.” The study focused on synthesizing iron oxide nanoparticles (FeNPs)

through a green method using sweet cherry (Prunus avium) stem extracts as a natural reducing and stabilizing agent. The FeNPs were thoroughly characterized using UV–Vis, FTIR, XRD, SEM-EDX, and DLS (Zeta Sizer), confirming particle sizes as small as 91.28 nm and successful iron oxide formation. The FeNPs were applied for adsorption of methylene blue, a cationic dye, from wastewater. Maximum removal of 67.34% was achieved after 150 minutes at pH 6 using 0.3 g of FeNPs in 20 ml of dye solution. Adsorption data best fit the Freundlich isotherm model ($R^2 = 0.9941$), indicating favorable multilayer adsorption on heterogeneous surfaces. This green method is cost-effective, eco-friendly, and shows strong promise for use in textile wastewater treatment.

Xiyao Liu et al. (2024) conducted a study titled “Green synthesis of Fe-nanoparticles using pruned tea leaf extract: Characterization and use for degradation of dyes from aqueous phase in Fenton-like systems.” This research utilized pruned tea leaf extract as a sustainable and cost-effective source to synthesize iron nanoparticles (Fe-NPs). The Fe-NPs were characterized using XRD, FTIR, XPS, UV–Vis, SEM/EDS, and TEM, confirming spherical morphology with sizes between 34–52 nm, and the presence of FeOOH, Fe_2O_3, and amorphous α-Fe. BET analysis showed a pore size of 17.9 nm and a surface area of 2.45 m^2/g. These Fe-NPs were tested for degradation of Congo Red (CR), Methylene Blue (MB), and Malachite Green (MG) under sole adsorption and Fenton-like systems. The Fenton-like system achieved over 95% degradation within 30 minutes, outperforming sole adsorption (50%). Kinetic studies showed the pseudo-second-order model best fit the reaction, while thermodynamic analysis revealed that the degradation was spontaneous and endothermic. The catalyst retained over 95% activity after five cycles, proving its reusability and practical potential for wastewater treatment.

Ahmed K. Hassan et al., (2022) conducted research titled "A Green Synthesis of Iron/Copper Nanoparticles as a Catalytic of Fenton-like Reactions for Removal of Orange G Dye." The study focuses on an eco-friendly approach using ficus leaf extracts to synthesize bimetallic iron/copper nanoparticles (G-Fe/Cu-NPs) for degrading the toxic Orange G (OG) dye in water. The nanoparticles exhibited favorable characteristics such as spherical shape (32-59 nm size), high stability, and a surface area of 4.452 m^2/g. Optimal degradation of OG dye (94.8% removal) was achieved at specific conditions: 3.52 mM H_2O_2, 1 g/L nanoparticle dose, pH 3, dye concentration of 50 mg/L, and 40°C in 30 minutes. The reaction adhered to a second-order kinetic model and was identified as endothermic, requiring 29.73 kJ/mol activation energy. This research underscores the potential of green-synthesized nanoparticles as sustainable catalysts for wastewater treatment.

Amin Barani et al. (2023) conducted a review titled "A Comprehensive Review on Catalytic Activities of Green-Synthesized Selenium Nanoparticles on Dye Removal for Wastewater Treatment." This study explores the rapid industrialization contributing to increased pollution, particularly organic dye contaminants in wastewater. Green synthesis of selenium nanoparticles (SeNPs) is spotlighted as a cost-effective, eco-friendly method for wastewater treatment. The review emphasizes SeNPs' superior catalytic, antimicrobial, and biocompatible properties, which enable efficient degradation of toxic organic dyes like methylene blue and rhodamine B through photocatalytic processes under UV or visible light. Mechanisms outlined include the production of reactive radicals (e.g., hydroxyl and superoxide) that dismantle dyes into non-toxic byproducts like CO_2 and H_2O. The findings position green SeNPs as innovative, sustainable tools for environmental remediation, with the dual benefit of minimal ecological impact and high efficiency in dye removal.

3 Materials and Methodology

3.1 General

The research work deals with the properties of green synthesized iron nano particles for dye removal from industrial wastewater and also the materials being used in the preparation of solutions. In the study, an attempt was made to check the removal efficiency of industrial waste water and properties of magnifier indica used as a removal material and also to determine the removal efficiency in Machine learning by comparing both. The methodology followed is as shown in the Figure 1.

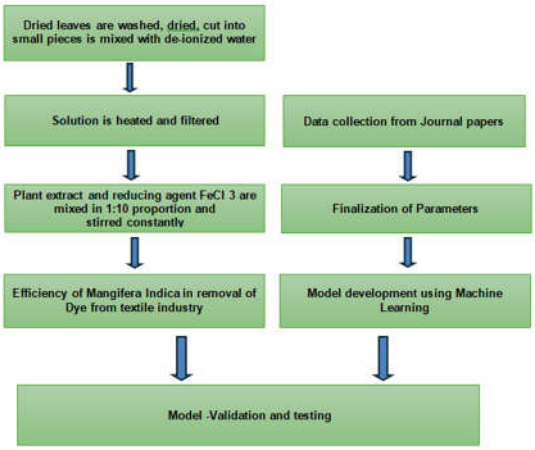

Figure 1. Methodology followed

3.2 Materials

The materials used for this research work are:

- Mango Leaves
- Rhodamine B dye
- Ferric Chloride hexahydrate
- Whatman Filter Paper
- Sodium Hydroxide
- Hydrochloric acid
- Textile industrial wastewater

3.3 Instruments required

- pH meter
- Hot air Oven
- Spectrophotometer
- Magnetic Stirrer
- Centrifuge

4 Results and Discussion

4.1 Effect of pH

pH plays a crucial role in dye decolourization as it significantly influences the reaction rates. Since the pH of a solution governs the surface charge of the catalyst, it directly affects the adsorption of dye molecules on semiconductor surfaces. To study the effect of pH on the dye degradation, the experiments were carried for pH 4, 5, 8 and 9 by keeping 1mL extract dosage constant by varying dye dosage. The highest removal was observed at pH 9 followed by pH 8. Under the condition of initial dye concentration of 4×10^{-4} mg/L, adsorbent dose of 1 mL (508.6 mg/L), and a contact time of 5 minutes percentage removal increased from 11% to 73% (Figure 1). This is due to change in the Fe_3O_4 surface which was influenced by solutions pH. Due to electrostatic attraction between Rhodamine B dye and surface charge at pH 9, removal efficiency of RB was high.

4.2 Effect of initial concentration of extract

The absorption efficiency is influenced by number of binding sites and surface area. It can be observed that, at initial dose of 1.0 mL RB removal was 72% and increased gradually till 1.5mL. Increasing in dosage helps in expansion of outer layer which helps in removal efficiency of RB (Figure 6-7). However, at higher dosages, the adsorption capacity per unit mass may decrease due to the limited availability of RB molecules relative to the large number of active sites on the iron nanoparticles.

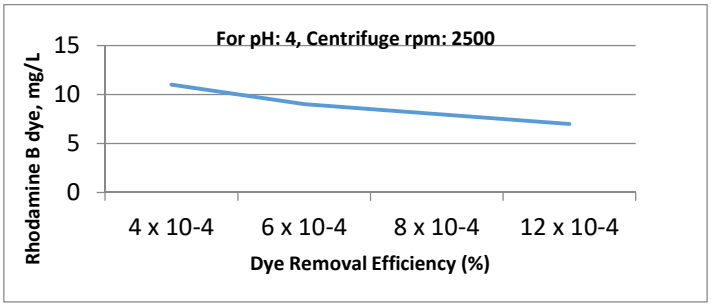

Figure 2: Removal Efficiency of Rhodamine B Dye

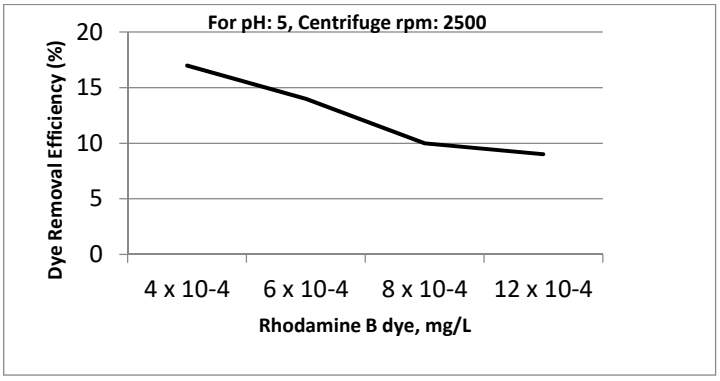

Figure 3: Removal Efficiency of Rhodamine B Dye

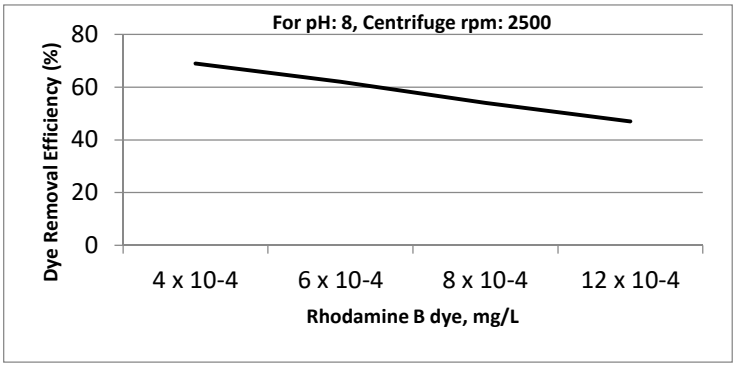

Figure 4: Removal Efficiency of Rhodamine B Dye

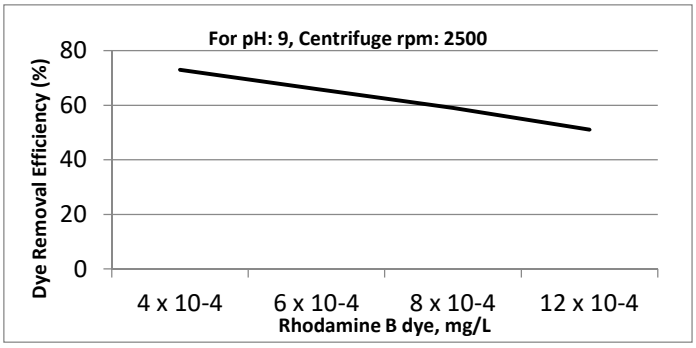

Figure 5: Removal Efficiency of Rhodamine B Dye

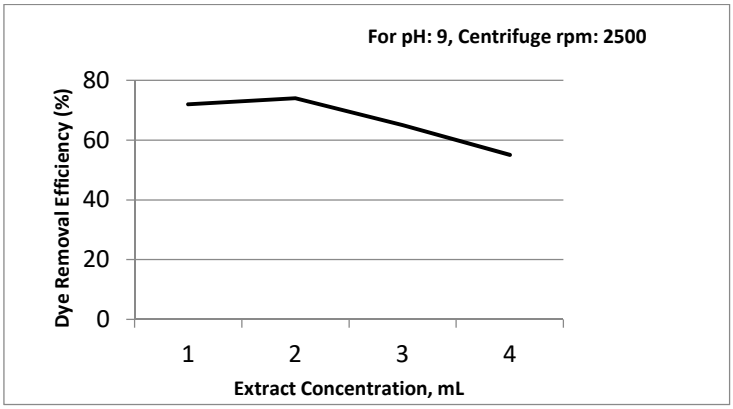

Figure 6: Removal Efficiency of Rhodamine B Dye

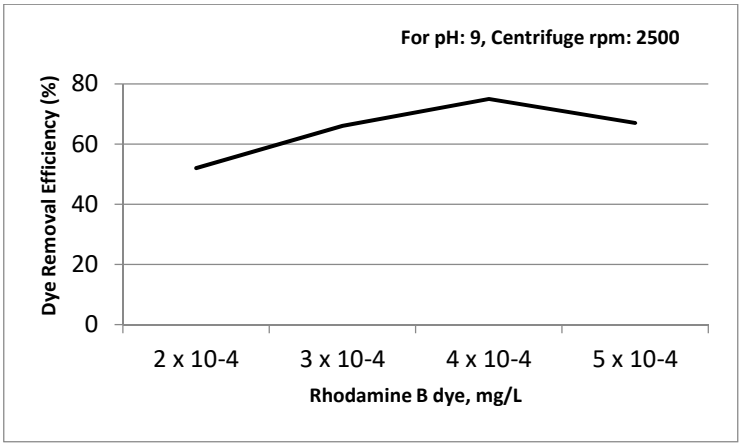

Figure 7: Removal Efficiency of Rhodamine B Dye

4.3 Machine learning

Machine learning algorithm was generated from the 50 set of data found from previous research articles. Input data includes initial concentration of dye, initial concentration of iron nanoparticle extract, time of contact, dye removal efficiency and type of leaf extract. The result generated form ML was compared with the result obtained from lab analysis.

4.4 Comparison of traditional method and ML technique for dye removal efficiency for industrial wastewater

The analysis was carried for the dye wastewater for the optimum condition and observed 63% removal efficiency. The same data was fed to ML model and found the dye removal efficiency as 57% which is 6% lesser that actual obtained (Table 1). This indicates that the ML algorithm can be used as a tool to predict the parameters like pH, concentration of extract, time of contact and percentage removal efficiency of dye.

Table 1: Comparison of traditional method and ML technique for dye removal efficiency for industrial wastewater

Particulars	pH	Extract Concentration,	Industrial wastewater, mL	Contact Time in min	Dye Removal Efficiency (%)
Experiment result	9	1 (**508.6mg/L**)	10 x 10^{-4}	15	63
	4.4	1 (**508.6mg/L**)	10 x 10^{-4}	15	32
ML model result	9	500 mg/L	10 x 10^{-4}	15	57

5 Conclusions

- The optimum conditions for maximum dye removal from the simulated sample were found to be pH 9, extract concentration of 1.5 mL, and Rhodamine B dye concentration of 4×10^{-4} mg/L
- Comparative study between traditional method and ML technique regarding removal efficiency of dye showed difference of 15% for simulated sample
- Industrial wastewater was analyzed for initial pH which observed to be 4.4 and treated for optimum condition which showed 63% removal efficiency
- Removal efficiency of industrial wastewater using ML model was observed to be 57% which was 6% slightly less than the result obtained from experiment
- Machine learning algorithm can be used efficiently to predict the optimum parameter to treat colored wastewater for industries

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