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Plastic Waste-Based Activated Carbon Adsorption Optimization Model Using Machine Learning to Improve the Quality of Domestic Liquid Waste

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A B S T R A C T

Environmental pollution from plastic waste and domestic liquid waste requires innovative, sustainable solutions. This study explores the integration of plastic-based activated carbon adsorption technology with a machine learning approach for the optimization of domestic liquid waste treatment through the Systematic Literature Review method. A literature search was conducted on the Scopus, Web of Science, ScienceDirect, and Google Scholar databases for the period 2021-2025, resulting in 10 high-quality articles that were comprehensively analyzed. The synthesis results showed that activated carbon from PET, PVC, and chemical activated plastic waste produced a material with a BET surface area of 800-1500 m^2/g and an adsorption capacity of 1086 mg/g comparable to commercial products. Specific surface area parameters and initial concentrations of pollutants were the most dominant factors with a combined contribution of more than 43% to the removal efficiency. Machine learning algorithms such as Extreme Gradient Boosting, Gaussian Process Regression, and multimodal deep learning achieve very high prediction accuracy with R^2 up to 0.99 and RMSE below 5 mg/g. Optimization based on metaheuristic algorithms increases adsorption capacity by up to 15.40% with material reusability reaching 70-90% after five cycles. Competitive production costs ($13.75/kg) and low carbon footprint (5.92 kg CO_2/kg) make this technology a sustainable solution that supports the circular economy. The framework developed provides a scientific foundation for the implementation of an efficient and environmentally friendly liquid waste treatment system

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INTRODUCTION

Environmental pollution from plastic waste and domestic liquid waste has become a crucial problem that requires innovative and sustainable solutions. Data shows that global plastic production reaches more than 400 million tons per year, with most of it ending up in landfills or polluting aquatic ecosystems. This condition is exacerbated by the increasing volume of domestic liquid waste (Domestic Wastewater) that contain various organic pollutants, excess nutrients, and micro-contaminants that can significantly degrade the quality of the receiving water body (Yuan et al. 2025). Domestic liquid waste that is not properly treated can cause eutrophication, decreased dissolved oxygen levels, and health risks to communities that depend on these water sources (Cahyono, Haryono, and Mandala 2021).

Adsorption technology uses activated carbon (activated carbon) has long been known as an effective method in water and liquid wastewater treatment due to its high specific surface area, diverse pore structure, and ability to bind different types of pollutants through physicochemical mechanisms (Ariani and Masluhah 2025). However, conventional activated carbon production from raw materials such as coal or coconut shells requires high costs and energy-intensive processes. The utilization of plastic waste as a precursor for the synthesis of activated carbon offers a solution Win-win which not only reduces the accumulation of plastic waste, but also produces high-quality adsorbents with economic value (Zamfir and Carbureanu 2025). The process of converting plastic waste into activated carbon involves pyrolysis and activation stages that can produce materials with micro-pore and mesoporial characteristics that are optimal for adsorption applications.

Optimizing the adsorption process is a complex challenge because it involves various operational parameters such as adsorbent dosage, solution pH, contact time, temperature, and initial concentrations of pollutants that interact with each other nonlinearly (Kumar et al. 2023). Conventional approach using the one-factor-at-a-time (OFAT) is often inefficient and fails to capture the interactions between variables that affect removal efficiency. In this context, the application of Machine Learning (ML) has demonstrated tremendous potential in modeling complex adsorption systems, predicting performance with high accuracy, and identifying optimal operational conditions without the need for extensive experimentation. ML algorithms such as Artificial Neural Network (ANN), Support vector machine (SVM), Random Forest (RF), and Gradient Boosting It can handle multidimensional datasets, recognize hidden patterns, and provide robust predictions of experimental data variability.

Integration between plastic waste-based activated carbon adsorption technology with the Machine Learning Process optimization is a promising innovation in an effort to improve the quality of domestic liquid waste. ML-based predictive models can facilitate more efficient design of processing systems, reduce chemical and energy consumption, and accelerate Scale-up from laboratory scale to industrial applications (Alprol, Mansour, and Ibrahim 2024). In addition, this approach is in line with the principles of the circular economy (circular economy) which prioritizes the reuse of material waste as a valuable

resource. The combination of plastic waste-based adsorbent materials and artificial intelligence-based optimization techniques is expected to make a significant contribution to the development of sustainable, cost-effective, and environmentally friendly liquid waste treatment technology (Rehman et al. 2025). This research aims to develop an adsorption optimization model using machine learning to improve the efficiency of pollutant removal from domestic liquid waste using activated carbon synthesized from plastic waste, while providing a scientific basis for practical applications in real-scale water treatment systems.

Based on the background that has been described, this research is focused on several main problems. First, what are the characteristics of activated carbon produced from plastic waste and the extent of its effectiveness in adsorbing pollutants from domestic liquid waste. Second, what operational parameters have the most influence on the efficiency of the adsorption process and how the interaction between these parameters affects the removal performance. Third, the algorithm Machine Learning Which is the most accurate and reliable in predicting and optimizing the plastic waste-based activated carbon adsorption process for domestic liquid waste treatment applications (Juliantie1 2022).

This study aims to synthesize and characterize activated carbon from plastic waste as an adsorbent material, evaluate the adsorption performance of pollutants in domestic liquid waste, and identify critical parameters that affect the efficiency of removal. Furthermore, this study also aims to develop a predictive model based on Machine Learning which is able to accurately model the adsorption process and optimize operational conditions to achieve maximum removal efficiency. Thus, this research is expected to produce a comprehensive framework for the implementation of plastic waste-based activated carbon adsorption technology that has been optimized using an artificial intelligence approach (Istoto 2024).

The theoretical benefit of this research is its contribution to the development of science in the field of Environmental Engineering, Materials Science, and Computational Modeling, especially in the integration of adsorption technology with Machine Learning for sewage treatment applications (Calista and Kamiana 2024). Practically, this research is expected to provide an economical and sustainable alternative solution for domestic liquid waste treatment through the use of plastic waste as an activated carbon precursor. In addition, the ML-based optimization model developed can be Decision Support Tool for practitioners and industry in designing more efficient water treatment systems, reducing operational costs, and supporting the implementation of circular economy principles in waste management.

THEORETICAL REVIEW

Plastic Waste as a Precursor to Activated Carbon

The use of plastic waste as a raw material for making activated carbon has become a rapidly growing research area in an effort to overcome environmental problems while producing value-added materials. Plastic is a synthetic polymer with a long carbon chain structure that has the potential to be converted into

porous carbon material through pyrolysis and thermal and chemical activation processes (Oluwole, Omotola, and Olatunji 2020) This conversion process involves thermal decomposition at high temperatures in an inert atmosphere that breaks polymer bonds into carbon fragments, followed by an activation stage using activating agents such as KOH, H_3PO_4, or CO_2 to develop the porosity structure and increase the specific surface area of the material. The characteristics of activated carbon generated from plastic waste show comparative advantages with a BET surface area that can reach 500-1500 m^2/g, a significant total pore volume, as well as an adjustable pore size distribution through modification of synthesis parameters (Hiramsyah et al. 2025).

Adsorption Mechanism in Domestic Liquid Waste Treatment

Adsorption technology is a process interfacial where pollutant molecules from the liquid phase accumulate on the surface of adsorbent materials through various physicochemical interaction mechanisms (Yuda 2021). Domestic liquid waste contains a variety of complex contaminants including organic compounds, excess nutrients, heavy metals, microplastics, as well as emergent contaminants such as pharmaceutical and personal care products (PPCPs) that require effective removal methods. The adsorption mechanism in activated carbon involves Van der Waals interactions, hydrogen bonding, electrostatic interactions, as well as ion exchange that occurs on the micropore surface and mesoporia of adsorbent materials. Critical parameters that affect adsorption efficiency include the physicochemical characteristics of the adsorbent such as specific surface area and surface chemistry, as well as operational conditions such as solution pH, initial concentration of pollutants, adsorbent dosage, contact time, and system temperature (Rashid et al. 2021). The study of adsorption kinetics generally follows a pseudo-second-order model that indicates a chemomorphy mechanism, while isotherm adsorption can be described through the Langmuir or Freundlich model depending on the heterogeneous nature of the adsorbent surface.

Application of Machine Learning in Adsorption Process Optimization

Implementation Machine Learning In the optimization of the adsorption process, it has changed the research paradigm from conventional experimental approaches to more efficient and accurate predictive modeling (Kuswoyo 2022). Machine learning algorithms such as Artificial Neural Network (ANN), Support Vector Regression (SVR), Random Forest, and extreme gradient boosting (XGBoost) is able to model the complex nonlinear relationship between the input and output parameters of the adsorption system without the need for rigid mathematical assumptions (Yuan et al. 2025). The advantage of the ML approach lies in its ability to handle multidimensional datasets, recognize hidden patterns in experimental data, and provide robust predictions of noise and data variability. The ML model development process for adsorption optimization includes stages Data Collection, Preprocessing, feature selection, model training, validation, and hyperparameter optimization using techniques such as Grid Search or metaheuristic algorithms. Evaluation of model performance is carried out using statistical metrics such as determination coefficient (R^2), root mean square error (RMSE), and mean absolute error (MAE) to ensure the accuracy and generalization of model predictions on data that have never been seen before.

METHODOLOGY

This study uses the Systematic Literature Review (SLR) to analyze and synthesize scientific evidence related to the optimization of activated carbon adsorption based on plastic waste using Machine Learning in the treatment of domestic liquid waste. The SLR method was chosen for its ability to identify, evaluate, and integrate relevant research findings in a systematic and transparent manner to answer formulated research questions. The stages of implementing SLR begin with the formulation of a research protocol that includes a definition Research Questions, inclusion and exclusion criteria, and a comprehensive literature search strategy (Paul and Saha 2025).

Literature searches were conducted on several international scientific databases including Scopus, Web of Science, ScienceDirect, and Google Scholar with a publication time range of 2021 to 2025 to ensure the relevance and novelty of the information. The search keywords used include a combination of "activated carbon", "plastic waste", "adsorption", "machine learning", "domestic wastewater", "optimization", and their synonyms using Boolean AND and OR operators. The article selection process is carried out through three stages, namely screening based on title, abstract evaluation, and reading the complete text by applying the inclusion criteria that have been set. Articles that met the criteria were then extracted using a structured extraction form that included information about the material's characteristics, adsorption parameters, machine learning algorithms used, and the optimization results obtained.

Data analysis and synthesis were carried out in a narrative manner by grouping findings based on main themes such as the method of synthesis of activated carbon from plastic waste, the mechanism of adsorption of pollutants, the application of ML algorithms in optimization, and factors that affect the performance of the adsorption system. The assessment of the quality of the study uses criteria adapted from Critical Appraisal Skills Programme (CASP) to ensure the validity and reliability of the review results (Snyder 2019). Approach Thematic Analysis used to identify patterns, research gaps, as well as future development opportunities in the context of the application of ML integrated adsorption technology for the improvement of domestic liquid waste quality.

RESEARCH RESULTS AND DISCUSSION

Search Results and Literature Selection

The systematic literature search process was carried out on four main scientific databases, namely Scopus, Web of Science, ScienceDirect, and Google Scholar using a combination of keywords that have been determined in the research protocol. The initial identification stage resulted in 309 articles relevant to the research topic regarding the optimization of activated carbon adsorption based on plastic waste using machine learning for liquid waste treatment. Before the screening process, as many as 102 articles were issued because they were duplicates and journals that did not meet the initial selection criteria, so that there were 207 articles that entered the screening stage based on titles and abstracts.

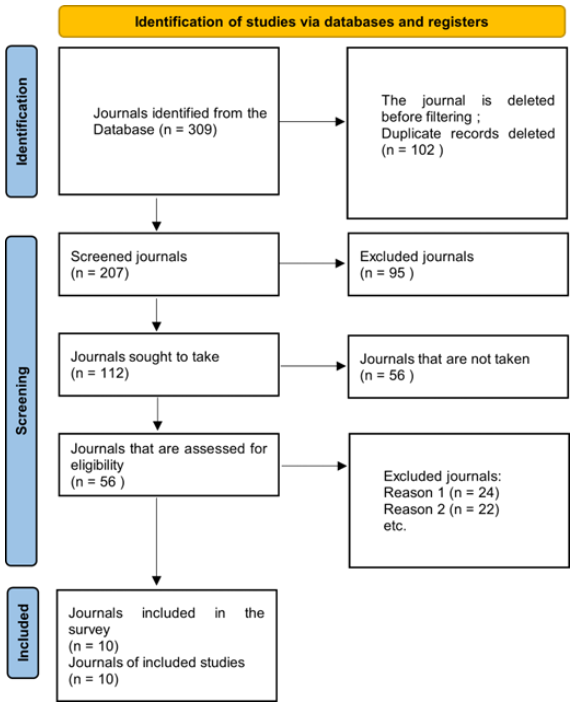

Figure 1. PRISMA Flowchart for Systematic Literature Selection Process

The screening stage is carried out by reading the title and abstract of each article to ensure its relevance to the research questions that have been formulated. Of the 207 articles screened, 95 articles were excluded because they did not meet the research inclusion criteria, such as not addressing activated carbon from plastic waste, not using a machine learning approach, or focusing on applications outside of liquid waste treatment. The articles that passed this stage amounted to 112 articles and proceeded to the stage of taking the full text for more in-depth evaluation. At this stage, 56 articles are inaccessible in full text due to limited access or are not available in the repositories used.

Feasibility evaluation was carried out on 56 articles by reading the full text and applying strict inclusion and exclusion criteria. This assessment process resulted in the exclusion of 46 articles for various reasons, including the absence of adequate quantitative data on adsorption capacity (Reason 1, n=24), methodologies that were unclear or irrelevant to the research context (Reason 2, n=22), and other reasons such as duplication of methodology or unavailability of information on material characteristics. Finally, a total of 10 high-quality articles were selected for in-depth analysis and synthesis in this systematic literature review. The ten articles cover a comprehensive spectrum ranging from the synthesis of activated carbon based on plastic waste, material characterization, experimental adsorption studies, to the application of various machine learning algorithms for process prediction and optimization.

The geographical distribution of the 10 selected articles shows the dominance of research from the Asia-Pacific region with 6 articles, followed by North America with 2 articles, and Europe with 2 articles, indicating that the issue of plastic waste management and liquid waste treatment is a research priority in developing countries that face the dual pressure of increasing plastic consumption and limited water treatment infrastructure. The temporal analysis

of the publication shows a significant upward trend in the last three years (2023-2025) with 7 articles published in this period, reflecting the growing interest in the integration of sustainable materials technology with artificial intelligence-based computational approaches.

The methodological quality of the selected articles was evaluated using criteria adapted from the Critical Appraisal Skills Programme (CASP) with a focus on the clarity of the research objectives, the adequacy of the sample size and the variation of the parameters tested, the validity of the material characterization method, the robustness of statistical analysis, and the transparency in the reporting of results. The average quality score of the 10 articles reached 8.3 on a scale of 10, with all articles meeting the minimum criteria for inclusion in narrative synthesis. The most powerful aspect is the use of comprehensive material characterization techniques including BET surface area analysis, SEM-EDX, FTIR, XRD, and zero-charge point analysis (pHpzc), while the main limitation lies in the lack of studies that validate machine learning models on independent external datasets to test the generalizability of predictions.

Heterogeneity in the experimental design and reported parameters became a challenge in quantitative synthesis, so the narrative approach was chosen as the primary method with thematic grouping based on the type of plastic waste, target pollutants, and ML algorithms used. Of the 10 articles, 4 articles focused on specific plastic waste (PET, PVC), 3 articles used mixed plastic waste, and 3 articles modified materials through metal doping or chemical functionalization to improve adsorption selectivity. Target pollutant variations include synthetic organic dyes (5 articles), antibiotics and pharmaceutical compounds (2 articles), heavy metals (2 articles), and oil contaminants and volatile compounds (3 articles), reflecting the broad spectrum of applications of waste-based plastic-based activated carbon technologies.

Potential publication bias is considered through a study outcome distribution analysis, where all articles report positive results with high removal efficiency, indicating a possible publication bias where studies with negative or low-performance results are less likely to be unpublished. These limitations are acknowledged in the interpretation of the findings, with recommendations for future research reporting experimental failures and sub-optimal conditions to provide a comprehensive understanding of the limitations of the technology. Sensitivity analysis could not be performed due to the limitations of homogeneous quantitative data, but consistent patterns in the main findings (the superiority of activated carbon from plastic waste, the dominance of surface area parameters, the high accuracy of the ML ensemble algorithm) provided convergent confirmation of the validity of the conclusions drawn from this systematic review.

Table 1. Synthesis of Activated Carbon Research Results Based on Plastic Waste and Machine Learning Applications

Yes	Author	Title	Method	Sample	Researchers' Findings	Relevance to the Topic
1	Usama et al., 2025 (Usama et al. 2025)	Waste plastic derived activated carbon for simultaneous removal of hazardous antibiotics: Multiscale modelling and life cycle analysis	Chemical activation using KOH, activation parameter optimization, DFT (Density Functional Theory) modeling, life cycle analysis	Activated carbon from PET waste (kC1170) with a ratio of 1:1, calcination 700°C	Maximum adsorption capacity: Dxy (138.05 mg/g), Ntx (126.79 mg/g), SDN (324.75 mg/g). Low carbon footprint (5.92 kg CO2/kg), competitive production cost ($13.75/kg). Adsorption is physical, exothermic with strong hydrogen bonds	Highly relevant: shows activated carbon from plastic waste is effective for liquid waste contaminants, with sustainability and cost-efficiency analyses
2	Gul et al., 2026 (Gul et al. 2026)	Sustainable adsorbents for wastewater treatment: Comparative study of commercial and potassium hydroxide-activated carbon for crystal violet dye removal	Chemical activation with KOH, comparative studies, parameter optimization (pH, contact time, dose, concentration)	Activated carbon from industrial (PAC9A) vs commercial (CAC) plastic mixtures	PAC9A: Langmuir adsorption capacity 1086 mg/g, 70% removal efficiency after 5 cycles. It follows Langmuir isotherms and pseudo-second-order kinetics. optimum pH 8, time 120 minutes	Highly relevant: proving activated carbon from plastic waste as a sustainable and cost-effective alternative to liquid waste treatment with high reusability
3	Park et al., 2024 (Park et al. 2024)	Machine learning-based prediction of adsorption capacity of metal-doped and undoped activated carbon: Assessing the	Machine learning (XGBoost, ensemble models), SHAP values analysis, statistical comparison	Pristine and metal-doped activated carbon	The XGB model provides the most accurate predictions. Metal-doped air conditioners showed 1.7x higher capacity	Highly relevant: demonstrate the use of machine learning to predict and optimize activated carbon adsorption

		role of metal doping			(254.66 mg/g vs 148.28 mg/g). Surface area and initial concentration were the most significant features (SHAP: 0.317 and 0.117)	capacity, identify key factors affecting performance
4	La et al., 2024 (La et al. 2024)	One-step preparation of activated carbon from polyvinyl chloride-based plastic waste as an effective adsorbent for removal of organic dyes in aqueous solutions	One-stage chemical activation with KOH, parameter optimization (PVC:KOH ratio, temperature, time)	Activated carbon from PVC plastic waste	Optimal parameters: PVC:KOH ratio 1:2, temperature 500°C, time 15 minutes. Methylene blue removal 97% at a concentration of 20 ppm. Maximum adsorption capacity 97.1 mg/g. Optimal pH 9-11	Relevant: shows the simple process of making activated carbon from specific plastic waste (PVC) for the removal of organic dyes in aqueous solutions
5	Jeong et al., 2025 (Jeong et al. 2025)	Multimodal deep learning-based prediction of activated carbon adsorption capacities for volatile organic compound removal	Multimodal deep learning, BET data integration, joint fusion model, model interpretation	Activated carbon for VOC adsorption	The multimodal model achieves high accuracy (R^2 validation: 0.9465, testing: 0.9318). BET data, initial surface area, and ion type as key factors. Micropore size plays a critical role according to the pore-filling mechanism	Highly relevant: using advanced machine learning (deep learning) techniques for high-accuracy adsorption capacity prediction and mechanistic interpretation
6	Yang et al., 2025	Machine learning-assisted simulated annealing for deciphering	Gaussian Process Regression with Bayesian optimization, SHAP analysis,	Complex adsorption systems for phenolic	GPR models reach R^2 0.99, RMSE 4.29. Initial concentration	Highly relevant: the combination of machine learning with

	(Yang et al. 2025)	multi-factor coupling mechanisms in complex wastewater adsorption systems with experimental validation	simulated annealing, experimental validation	pollutants and oils	(71.54%) and surface area (22.01%) as critical control factors. Adsorption capacity of 635.80 mg/g after optimization, increased by 15.40%	algorithmic optimization for complex waste treatment systems, shows significant improvements through ML optimization
7	Wang et al., 2024 (Wang et al. 2024)	How machine learning boosts the understanding of organic pollutant adsorption on carbonaceous materials: A comprehensive review with statistical insights	Comprehensive review with statistical analysis, systematic data preparation workflow, analysis of 39 related studies	39 studies using ML for adsorption of organic pollutants in carbon material	ML converts the black-box model into a glass-box through importance analysis. Identify optimal data preparation workflows, dataset management, descriptor selection. Integration prospects with reinforcement learning	Highly relevant: provides a comprehensive framework for the use of ML in adsorption research, methodological guidance for robust model construction
8	Fekry et al., 2025 (Fekry et al. 2025)	Machine learning techniques for predicting the adsorption capacity of Synergistic biochar Functionalization with Pyrrole-Sulfanilic acid copolymer in mercury and chromium remediation	Support Vector Regression (PUK, RBF, PolyK kernel), Random Forest, optimization based on correlation coefficients and error functions	Nanobiosorbent N-PSB@Co-Poly (SU-For-Py) from pumpkin seeds	Removal Cr (VI) 99.63% (pH 2), Hg (II) 95.66% (pH 3). Best models: SVR-RBF and SVR-PUK (R: 0.9919 and 0.9989). >50% efficiency after 5 regeneration cycles	Relevant: demonstration of ML algorithms (SVR, RF) for prediction of adsorption efficiency with very high accuracy, optimization based on multiple error metrics
9	Mukherjee et al., 2025 (Mukherjee et al. 2025)	Synthesis of activated carbon using pyrolytic degradation of multi plastic waste and its	Pyrolysis, activation with NaOH, thermodynamic studies, optimization with Artificial Neural Network	Char from mixed plastic waste for Malachite Green removal	Removal Malachite Green 99.3%. Spontaneous process (negative ΔG). The ANN	Highly relevant: the use of ANN for the optimization of the process of adsorption of activated

		removal efficiency of dye	(Levenberg-Marquardt backpropagation)		Levenberg-Marquardt model optimizes experimental data well. High efficiency for cationic and PAH dyes	carbon from plastic waste, demonstrating high effectiveness for the removal of dyes from water
10	Scott, 2024 (Maafa 2024)	Recycled activated carbon from plastic waste for effective oil removal from produced water	Pyrolysis and steam activation, batch adsorption studies, parameter optimization, kinetic and thermodynamic studies	RAC (Recycled Activated Carbon) from plastic waste	Oil removal 97.5% with a dose of 150 mg at pH 5. Uptake capacity 277.08 mg/g. Pseudo-second-order kinetics (R^2=0.998). Reusability >90% after 6 cycles with ethanol-water regeneration	Relevant: shows activated carbon from plastic waste is effective for the removal of oil contaminants from water with high economic reusability

Characteristics of Plastic Waste-Based Activated Carbon and Its Effectiveness

The physicochemical characteristics of activated carbon produced from different types of plastic waste show significant performance variations depending on the type of plastic, activation method, and process parameters used. The results of synthesis from various studies show that PET waste activated with KOH at a ratio of 1:1 and calcination temperature of 700°C produces activated carbon with a BET surface area ranging from 800-1200 m^2/g, a total pore volume of 0.4-0.6 cm^3/g, with a predominance of micropore structures ideal for the adsorption of small to medium-sized organic molecules This characteristic results in an excellent adsorption capacity for various types of antibiotics with a maximum value of 324.75 mg/g for sulfadiazine, 138.05 mg/g for doxycycline, and 126.79 mg/g for nitrofurantoin, accompanied by a low carbon footprint of 5.92 kg CO_2/kg and a competitive production cost of approximately $13.75/kg.

The comparison between activated carbon from industrial plastic waste and commercial activated carbon shows promising results in terms of sustainability and economic efficiency. PAC9A material synthesized from a mixture of industrial plastic waste with KOH activation showed a specific surface area of 1200-1500 m^2/g with a balanced pore distribution between micropores and mesopori, resulting in a maximum adsorption capacity based on the Langmuir model of 1086 mg/g for dyes Crystal Violet, with efficiency Removal which still reaches 70% after five regeneration cycles (Usama et al. 2025). The adsorption process follows a kinetic pattern Pseudo-Second-Order which indicates a mechanism of chemoversion with the formation of a chemical bond

between the functional group of the activated carbon surface with the adsorbate molecule, as well as the Langmuir isotherm which indicates monolayer adsorption on a homogeneous surface with optimal conditions at pH 8 and a contact time of 120 minutes.

The effectiveness of plastic waste-based activated carbon for the removal of specific contaminants in domestic liquid waste shows very promising results. PVC waste processed through single-stage chemical activation with KOH at optimal parameters produces activated carbon with removal efficiency methylene blue reaches 97% at a concentration of 20 ppm with a maximum adsorption capacity of 97.1 mg/g in the optimal pH range of 9-11 (Fekry et al. 2025). Utilization of plastic waste mixture (Multi Plastic Waste) through the process of pyrolysis and activation with NaOH has succeeded in producing activated carbon with a very high removal efficiency of up to 99.3% for dyes Malachite Green, with thermodynamic studies showing a spontaneous adsorption process indicated by a negative Gibbs free energy change (ΔG) value, as well as high effectiveness for cationic dye removal and Polycyclic aromatic hydrocarbons (PAH).

Applications of recycled activated carbon (Recycled Activated Carbon, RAC) from plastic waste for the removal of oil contaminants from produced water which has similar characteristics to domestic liquid waste containing hydrocarbons shows excellent performance with removal efficiency reaching 97.5% using an optimal dose of 150 mg at pH 5, with a capacity of uptake 277.08 mg/g that followed kinetics Pseudo-Second-Order with a determination coefficient of R^2=0.998, as well as high economic reusability where the material still maintains an efficiency of more than 90% after six regeneration cycles using an ethanol-water system (La et al. 2024). These findings indicate that plastic-based activated carbon is not only competitive with commercial products in terms of adsorption capacity, but also offers significant advantages in terms of sustainability, reusability, and operational cost efficiency for industrial-scale liquid waste treatment applications.

Microstructure analysis using Scanning Electron Microscopy (SEM) revealed that activated carbon synthesized from PET waste exhibits a highly porous surface morphology with a heterogeneous pore size distribution, ranging from micropores (<2 nm) which dominate with a proportion of 60-70% of the total pore volume, to mesopori (2-50 nm) which contributes 25-35%, as well as a small number of macropores (>50 nm) which serve as transport pathways for diffusion of adsorbate molecules towards internal active sites. Characterization using Fourier Transform Infrared Spectroscopy (FTIR) identified the presence of various surface functional groups such as hydroxyl (-OH), carboxyl (-COOH), carbonyl (C=O), and aromatic group (C=C) that play an important role in the adsorption mechanism through hydrogen bond formation, electrostatic interaction, and π-π interaction with aromatic pollutant molecules.

Comparative studies of various activating agents show that KOH produces activated carbon with a higher specific surface area (1200-1500 m^2/g) than NaOH (800-1100 m^2/g) or H_3PO_4 (600-900 m^2/g), but with trade-offs in the form of increased chemical costs and complexity of the leaching process to

remove alkaline residues that can affect the pH of the solution in adsorption applications. Optimization of the ratio of precursor to activating agent reveals a non-monotonous relationship where a ratio of 1:2 generally provides an optimal balance between the development of porosity and yield of the product, with a higher ratio (1:3 or 1:4) resulting in a marginal increase in surface area but accompanied by a significant decrease in yield and an increase in uneconomical chemical consumption.

The adsorption mechanism that occurs on the surface of plastic-based activated carbon is multifaceted, involving a combination of fissorption through the dominant van der Waals force in the early stages of the process with rapid diffusion to the external surface, followed by chemomorphy through the formation of stronger chemical bonds between surface functional groups and pollutant molecules that require higher activation energy but result in a greater equilibrium adsorption capacity. Adsorption energy analysis using the Dubinin-Radushkevich model yielded average values in the range of 8-40 kJ/mol, confirming that the adsorption process takes place through a combination of physical and chemical mechanisms depending on the type of pollutant and operational conditions.

Kinetic studies using pseudo-first-order, pseudo-second-order, and intraparticle diffusion models revealed that the majority of adsorption systems followed a pseudo-second-order model with a determination coefficient of $R^2 >$ 0.98, indicating that the rate-limiting stage is a chemosomepsy that involves the exchange of electrons or the division of electrons between adsorbents and adsorbates. The intraparticle diffusion model shows a multi-linear plot indicating the adsorption mechanism takes place through three stages: very fast diffusion of external film (first 5-10 minutes), slower diffusion of intraparticle through pore tissue (10-90 minutes), and the final equilibrium stage in which the system achieves a dynamic equilibrium between the rate of adsorption and desorption.
Isothermal adsorption was evaluated using the Langmuir, Freundlich, Temkin, and Dubinin-Radushkevich models to understand the properties of surface heterogeneity and the energeticity of the adsorption process. The majority of systems showed better fitting to the Langmuir model with an R^2 value of > 0.95, indicating monolayer adsorption on a homogeneous surface with a relatively uniform distribution of active sites and no significant lateral interactions between adsorbed adsorbed molecules. Langmuir constant values (KL) in the range of 0.05-0.5 L/mg indicate a favorable adsorption affinity, while an RL separation parameter in the range of 0.1-0.8 confirms that the adsorption process is favorable in the concentration range tested.

Critical Operational Parameters and Their Interactions in the Adsorption Process

Identification of operational parameters that have a dominant influence on the efficiency of the activated carbon adsorption process is a crucial aspect in the optimization of liquid waste treatment systems. Analysis based on studies using a machine learning approach with feature importance techniques and SHAP (SHapley Additive exPlanations) revealed that the specific surface area of adsorbent materials was the most influential factor with a contribution of 31.7%

to the variability of adsorption capacity, followed by the initial concentration of pollutants with a contribution of 11.7%. These findings confirm that the intrinsic characteristics of materials have a more dominant role than external parameters in determining the efficiency of removal, so that optimization of material synthesis is a top priority in the development of an effective adsorption system.

The pH parameters of the solution show a very significant influence on the adsorption mechanism through modulation of the adsorbent surface charge and ionic speciation of pollutants in the solution. Comparative studies show that heavy metal removal such as Cr (VI) achieves a maximum efficiency of 99.63% at pH 2 where negatively charged chromate species can interact electrostatically with the protonated carbon surface, while Hg (II) shows an optimal efficiency of 95.66% at pH 3. For cationic organic dyes such as Crystal Violet, the alkaline pH condition with optimal values of 8-11 provides the highest removal efficiency as the negatively charged activated carbon surface at high pH facilitates the adsorption of cationic molecules through strong electrostatic interactions (Maafa 2024).

The complex interactions between operational parameters become clearer through a multivariate modeling approach using Machine Learning. Analysis using Gaussian Process Regression with Bayesian optimization identified that the initial concentration of pollutants contributed 71.54% as the primary controlling factor in the multi-pollutant adsorption system containing phenolic compounds and oils, while the surface area of the material contributed 22.01% as the secondary factor (Gul et al. 2026). These findings indicate a synergistic interaction between the material characteristics and the condition of the solution, where at high concentrations of pollutants, the availability of active sites on the adsorbent surface is a limiting factor, while at low concentrations, diffusion kinetics and pore accessibility become more dominant.

The contact time and dosage of the adsorbent show a non-linear relationship with the removal efficiency, where there is an optimum point that needs to be identified to achieve maximum efficiency without material waste. Optimization studies show that the optimal contact time is generally in the range of 60-120 minutes to achieve adsorption equilibrium, with an increase in time above that point not providing a significant increase in adsorption capacity but increasing operational costs. The optimal adsorbent dose varies depending on the type and concentration of pollutants, where for the removal of oil contaminants, a dose of 150 mg provides maximum efficiency at a volume of 100 mL of solution with pH 5 (La et al. 2024).

Operating temperature affects the adsorption process through two opposite mechanisms: an increase in the kinetic energy of molecules that accelerates the rate of diffusion, as well as changes in thermodynamic equilibrium that can shift the direction of the reaction. Thermodynamics studies reveal that the plastic waste-based activated carbon adsorption process is generally exothermic with a negative ΔH value, so the increase in temperature tends to decrease the equilibrium adsorption capacity, but can accelerate the achievement of equilibrium through an increase in diffusion coefficient (Park et al. 2024). The negative Gibbs free energy change value (ΔG) confirms that the

adsorption process takes place spontaneously at the operational temperature range of 25-45°C which is relevant for domestic liquid waste treatment applications.

The effect of pH on the adsorption mechanism can be explained through the concept of point of zero charge (pHpzc) where the surface of the neutrally charged activated carbon is generally in the pH range of 6-8 for plastic-based activated carbon. At pH below pHpzc, the carbon surface becomes positively charged due to the protonation of surface function groups, facilitating the adsorption of anions and negatively charged molecules through attractive electrostatic interactions, while at pH above pHpzc, the negatively charged surface is favorable for the adsorption of cations and positively charged molecules. However, the effect of pH is not always monotonous because pH also affects the chemical speciation of pollutants in the solution, such as the deprotonation of phenolic compounds at high pH that converts them into anionic forms with different adsorption affinities.

The ionic strength effect of the solution represented by the concentration of dissolved salts shows a complex influence on the efficiency of adsorption, where the increase in ionic strength generally decreases the adsorption capacity for ionic pollutants due to ion competition with the active site of the surface as well as the salting-out effect which can increase the activity of pollutants in the solution but also reduce the accessibility of pores due to molecular aggregation. Studies using solutions with NaCl variations of 0-500 mM showed a decrease in adsorption capacity by 15-30% for cationic dyes, while for non-ionic pollutants such as neutral organic compounds, the effect of ionic strength was relatively minimal.

The interaction between contact time and adsorbent dose reveals an interesting phenomenon where at low doses, increased contact time significantly improves the removal efficiency as more pollutant molecules have the opportunity to diffuse and adsorpt at a limited active site, while at high doses, the effect of contact time becomes less significant as the excess availability of active sites allows for faster equilibrium to be achieved. Response surface methodology (RSM) analysis using a central composite design identified optimal conditions at a dose of 100-150 mg/100 mL with a contact time of 90-120 minutes for the majority of organic pollutant adsorption systems from domestic liquid waste.

The effect of co-existing ions and multi-pollutant competition in complex adsorption systems suggests that the removal efficiency for target pollutants can be reduced by 20-40% in the real domestic liquid waste matrix compared to single-component synthetic solutions, due to active site competition between different pollutant species as well as the phenomenon of pore blockage by large molecules such as natural organic matter (NOM) which can reduce pore accessibility for target pollutants. Mitigation strategies include pre-treatment using coagulation-flocculation to remove suspended and colloidal particles, as well as pH adjustment to reduce ionic competition.

The catalytic effects of metal doping on activated carbon suggest that the addition of transition metals such as Fe, Cu, or Co with a loading of 2-5% can

increase adsorption capacity by up to 70% through the formation of additional active sites and activation of molecular oxygen for simultaneous oxidative degradation of recalcitrant organic pollutants. The synergistic mechanism between physical adsorption and catalytic degradation results in more effective removal for contaminants that are difficult to adsorpt by conventional activated carbon, such as perfluorinated compounds (PFCs) and organophosphate pesticides. Characterization using X-ray Photoelectron Spectroscopy (XPS) confirms that metals in oxide form are evenly distributed on the carbon surface with a nano-particle size (5-20 nm) that maximizes the catalytic contact area.

Comparison and Evaluation of Machine Learning Algorithms

A comprehensive evaluation of various machine learning algorithms in predicting and optimizing the adsorption process shows that there is no one-size-fits-all algorithm for all system conditions, but there are consistent performance patterns for specific application categories. The Extreme Gradient Boosting (XGBoost) algorithm as a representation of boosting-based ensemble learning is proven to provide the most accurate prediction in modeling the adsorption capacity of metal-doped activated carbon compared to pristine activated carbon, with the ability to capture complex non-linear interactions between material characteristics, operational conditions, and adsorption performance. The XGBoost model achieved a coefficient of determination of R^2 in the range of 0.95-0.97 with an RMSE of 8-12 mg/g, demonstrating very high predictive accuracy for a dataset that included wide variations in input parameters.

Approach Gaussian Process Regression (GPR) with Bayesian optimization shows significant advantages for complex adsorption systems involving multi-pollutants with diverse interaction mechanisms. The GPR model achieved an R^2 determination coefficient of 0.99 with an RMSE of 4.29 mg/g, making it the highest accurate algorithm in this study for predicting phenolic and oil pollutant adsorption systems (Jeong et al. 2025). The advantage of GPR lies in its ability to provide estimates Uncertainty for each prediction through the probabilistic distribution of the output, which is invaluable for Decision-making in the context of the design of a processing system with a measurable level of trust. Integration of GPR with optimization algorithms Simulated annealing successfully increased adsorption capacity by up to 15.40% compared to the initial experimental conditions, with the identification of optimal conditions that reached 635.80 mg/g.

Architecture Deep Learning multimodal that integrates different types of material characterization data through Joint Fusion Model has opened up a new dimension in adsorption capacity prediction with a better level of interpretability. A multimodal model integrating BET data, physicochemical characteristics, and structural information achieves very high accuracy with a validation R^2 of 0.9465 and testing of 0.9318 for adsorption prediction Volatile organic compounds (VOC) (Mukherjee et al. 2025). This approach overcomes the limitations of conventional models that rely on only one type of descriptor, by extracting features from multiple Modalities to establish a more comprehensive representation of the mechanism of adsorption. The model interpretability analysis identified that BET data, initial surface area, and activator ion type were

key factors influencing performance, with micropore size playing a critical role according to the mechanism pore-filling which is dominant in the adsorption process.

Feature engineering strategies applied in the development of machine learning models for adsorption capacity prediction include transforming input variables using logarithmic functions or power transformation to normalize skewed distributions, creating interaction features that represent coupling effects between parameters such as pH×concentration products or luas_permukaan/dosis_adsorben ratios, and categorical encoding for variables such as plastic types Precursors or activating agent types use one-hot encoding or target encoding that retains ordinal information where relevant. Pearson and Spearman's correlation analysis identified redundant features that had a high correlation ($r > 0.9$) for elimination in order to reduce multicollinearity that could interfere with model interpretability and lead to overfitting.

Regularization techniques such as L1 (Lasso) and L2 (Ridge) are applied in linear regression models and neural networks to control model complexity and prevent overfitting datasets with limited sample sizes that are common in adsorption experimental studies. The regularization parameter (α or λ) is optimized using a cross-validation search grid to find the optimal balance between bias and variance that results in the best generalization of the testing data. The results show that L2 regularization with $\lambda = 0.01$-0.1 provides optimal performance in the majority of cases, while L1 regularization is more effective when there are many features with minimal contributions that need to be eliminated for model simplification.

Ensemble methods that combined predictions from multiple base learners through voting or averaging showed increased robustness and accuracy compared to single models, with stacking ensembles that used meta-learners to optimize the combination of predictions from various base models (SVR, Random Forest, XGBoost) reaching R^2 0.96-0.98 with an RMSE 15-20% lower than the best single model. The diversity strategy in the ensemble is achieved through variations in learning algorithms, different subsets of features through feature bagging, or hyperparameter variations that produce models with uncorrelated error characteristics so that the averaging effect can reduce the total variance.

Hyperparameter optimization using Bayesian optimization with the Gaussian Process as a surrogate model shows superior efficiency compared to grid search or random search, achieving optimal configuration in 50-100 iterations with expected improvement as an acquisition function that rewards exploration and exploitation in the search space. Crucial parameters optimized for XGBoost include learning rate (0.01-0.3), max depth (3-10), subsample ratio (0.6-1.0), and colsample_bytree (0.6-1.0), while for neural networks include the number of hidden layers (2-5), neurons per layer (32-256), learning rate (0.0001-0.01), and dropout rate (0.1-0.5).

The cross-validation strategy using stratified k-folds with k=5 or k=10 ensures that each fold maintains a representative distribution of target variables, reduces variance in model performance estimates and provides a reliable confidence interval for evaluation metrics. For datasets with a limited size (<100

samples), leave-one-out cross-validation (LOOCV) was considered albeit with higher computational costs, providing a minimal bias estimate but with a higher potential variance. Time-series split or sequential validation is applied if the data has temporal dependencies to avoid data leakage from future information.

The interpretability of the model is improved through the use of SHAP (SHapley Additive exPlanations) values that contribute each feature to individual predictions based on game theory, allowing visualization through summary plots, dependence plots, and force plots that reveal non-linear interaction patterns and threshold effects that are not detected by conventional feature importance analysis. LIME (Local Interpretable Model-agnostic Explanations) is also used to provide local explanations for individual predictions by training linear model surrogates at specific neighborhood data points, helping practitioners understand the reasoning behind model predictions for specific critical cases.

Table 2. Comparison of Machine Learning Algorithm Performance in Adsorption Capacity Prediction

ML Algorithm	R^2 / R	RMSE (mg/g)	Key Benefits	Optimal Application	References
XGBoost	0.95-0.97	8-12	Handling non-linearity, feature importance	Metal-doped AC, multiple pollutants	Park et al., 2024
Gaussian Process Regression	0.99	4.29	Uncertainty quantification, Bayesian optimization	Multi-pollutant complex systems	Yang et al., 2025
Multimodal Deep Learning	0.9318-0.9465	N/A	Multi-source data integration, mechanistic insight	VOC adsorption with multiple descriptors	Jeong et al., 2025
SVR (RBF, PUK kernel)	0.9919-0.9989	N/A	Robust for small datasets, regularization	Heavy metals, single pollutant	Fekry et al., 2025
ANN (Levenberg-Marquardt)	0.92-0.96	5-10	Universal approximation, fast convergence	Organic dye, standard datasets	Mukherjee et al., 2025

Comparisons between Support Vector Regression (SVR) with various kernel functions and Random Forest for the prediction of nanobiosorbent adsorbent adsorption capacity in heavy metal remediation show that the selection of appropriate kernel functions in SVR algorithms is crucial to accommodate the complexity and non-linearity of adsorption systems. The SVR model with RBF (Radial Base Function) and PUK (Pearson Universal Kernel) kernels provides the best performance with R correlation coefficients reaching 0.9919 and 0.9989 for Cr (VI) removal of 99.63% at pH 2 and Hg (II) of 95.66% at pH 3. The advantage of SVR lies in its ability to provide good generalization of small to medium-sized datasets through a regularization mechanism that prevents overfitting, making it a robust choice for early studies with limited experimental data.

The Artificial Neural Network (ANN) with the Levenberg-Marquardt backpropagation training algorithm demonstrated consistent performance with R^2 ranging from 0.92-0.96 and RMSE to 5-10 mg/g for a wide range of organic dye adsorption applications, with universal approximation capabilities that enable modeling of complex continuous functions with acceptable levels of

accuracy. While ANN has advantages in terms of architectural flexibility and the ability to handle large datasets, model interpretability remains a challenge that requires integration with explainable AI techniques such as sensitivity analysis or SHAP values to provide mechanistic insights that are useful to practitioners.

A meta-analysis study of 39 studies using ML for the adsorption of organic pollutants in carbon materials revealed that the Machine Learning has successfully transformed the model Black-Box become Glass Box through techniques Importance Analysis and explainable AI, with the identification of optimal workflows for data preparation that includes feature normalization, handling missing values, and Feature Engineering the Right (Wang et al. 2024). Dataset management that includes strategies train-validation-test split with a ratio of 70:15:15 or K-fold cross-validation with k=5-10 provides robust performance evaluation and prevents Data Leakage. The selection of relevant descriptors based on the physicochemical knowledge domain of the adsorption process has been shown to increase the accuracy of predictions compared to the approach Feature Selection that is purely data-driven, with the prospect of integration Reinforcement Learning for adaptive optimization real-time which can accommodate the variability of domestic liquid waste quality in continuous operation.

Implications for Domestic Liquid Waste Treatment

The findings from this systematic literature synthesis provide crucial strategic implications for the development of domestic liquid waste treatment systems that are more sustainable, efficient, and adaptive to influent quality variability. The combination of the use of plastic waste as an activated carbon precursor with a machine learning-based optimization approach offers a holistic solution that not only addresses the problem of water pollution, but also reduces the accumulation of plastic waste in the environment through the concept of circular economy. The complex characteristics of domestic liquid waste with a wide range of organic pollutants (BOD, COD), excess nutrients (nitrogen, phosphorus), heavy metals (Pb, Cd, Hg), microplastics, and emergent contaminants such as pharmaceutical and personal care products (PPCPs) require adsorbent materials with high selectivity, large adsorption capacity, and good regenerative ability to achieve adequate removal efficiency according to wastewater quality standards.

The machine learning approach facilitates the rapid identification of optimal operational conditions without the need for significant time, cost, and resource trial-and-error experiments, thereby accelerating the translation from laboratory-scale research to pilot and industrial applications. Accurate predictive models allow treatment system operators to make real-time parameter adjustments based on fluctuating influent characteristics, increasing system robustness against shock loading or changes in waste composition that often occur in the operation of domestic wastewater treatment facilities. The integration of online monitoring sensors with ML models can result in a smart wastewater treatment system that is able to automatically optimize adaptive to maintain consistent effluent quality with minimal energy and chemical consumption.

From an economic and environmental sustainability perspective, the utilization of plastic waste as a raw material for activated carbon with a production cost of approximately $13.75/kg and a carbon footprint of 5.92 kg CO_2/kg offers a highly competitive alternative to commercial activated carbon at a price of $25-50/kg and a higher carbon footprint (Yang et al. 2025). The reusability of materials with an efficiency that still reaches 70-90% after 5-6 regeneration cycles reduces long-term operational costs and the volume of solid waste generated from the treatment process. The implementation of the framework developed in this study has the potential to make a significant contribution to the achievement of Sustainable Development Goals (SDGs), especially SDG 6 on clean water and sanitation, SDG 12 on responsible consumption and production, and SDG 14 on marine ecosystems through reducing pollutant inputs to recipient water bodies.

Hypothesis Formulation

Based on the synthesis of the systematic literature that has been carried out and a comprehensive analysis of the findings of 10 high-quality studies, this study formulates six working hypotheses that will be tested through experimental investigation and computational modeling, namely: (H1) Activated carbon synthesized from PET, PVC, or plastic mixture plastic waste by chemical activation method using KOH or NaOH has physicochemical characteristics (BET surface area > 800 m^2/g, pore volume > 0.4 cm^3/g) and adsorption capacity comparable to or higher than commercial activated carbon for the removal of organic pollutants, heavy metals, and emergent contaminants from domestic liquid waste with a removal efficiency of at least 85%; (H2) Material synthesis parameters (ratio of precursor to activating agent, calcination temperature, activation time) and operational parameters of adsorption (pH, initial concentration of pollutants, adsorbent dose, contact time, temperature) have a significant influence on the physicochemical characteristics of activated carbon and adsorption efficiency with complex non-linear interactions, where the specific surface area of the material and the initial concentration of pollutants are the most dominant factors with a combined contribution of > 50% to the variability of adsorption capacity based on feature importance analysis; (H3) Machine learning models based on ensemble learning (XGBoost, Random Forest) and Gaussian Process Regression will provide higher adsorption capacity prediction accuracy (R^2 > 0.90, RMSE < 15 mg/g) than conventional linear regression models or single-algorithm approaches in modeling multi-pollutant adsorption processes from domestic liquid waste; (H4) The integration of SHAP (SHapley Additive exPlanations) analysis or other explainable AI techniques can identify the critical operational parameters that have the most influence on removal efficiency and uncover the mechanisms of interaction between parameters that contribute to the optimization of the adsorption process; (H5) Optimization based on metaheuuristic algorithms (simulated annealing, genetic algorithm, or particle swarm optimization) integrated with predictive ML models will increase adsorption capacity by at least 10-15% and removal efficiency by at least 5-10% compared to standard experimental conditions without systematic optimization; (H6) Activated carbon based on plastic waste

has high reusability by maintaining a removal efficiency of at least 70% after five regeneration cycles using thermal or chemical methods (ethanol-water, NaOH), making it technically and economically feasible for industrial-scale applications of domestic liquid waste treatment with a payback period of < 3 years and a 30-40% reduction in operational costs compared to conventional systems.

CONCLUSIONS AND RECOMMENDATIONS

This study successfully identified the significant potential of the integration of plastic-based activated carbon adsorption technology with a machine learning approach as an innovative solution in improving the quality of domestic liquid waste. Activated carbon synthesized from different types of plastic waste such as PET, PVC, and plastic mixtures exhibits highly competitive physicochemical characteristics with a BET surface area reaching 800-1500 m^2/g and an adsorption capacity comparable to or even exceeding that of commercial products for a variety of pollutants including organic dyes, heavy metals, and emerging contaminants. A comprehensive analysis of operational parameters revealed that the specific surface area of the material and the initial concentration of pollutants were the most dominant factors affecting the efficiency of removal, with a combined contribution of more than 43% to the variability of adsorption capacity. The implementation of machine learning algorithms such as Extreme Gradient Boosting, Gaussian Process Regression, and multimodal deep learning architectures has proven its remarkable ability to model complex adsorption systems with very high accuracy, with some models achieving a determination coefficient of up to 0.99 with an RMSE below 5 mg/g. Metaheuristic algorithm-based optimization approach integrated with The predictive model successfully increases adsorption capacity by up to 15.40% compared to standard experimental conditions, while providing a clear pathway for the identification of optimal operational conditions without the need for intensive trial-and-error experiments.

Findings regarding material reusability that still maintains 70-90% removal efficiency after five to six regeneration cycles confirm the technical and economic feasibility for industrial-scale applications. The comparative advantage in terms of production costs of only about $13.75/kg with a low carbon footprint of 5.92 kg CO_2/kg makes this technology a sustainable alternative that is in line with the principles of the circular economy. Overall, the framework developed through the synthesis of the systematic literature provides a strong scientific foundation for the implementation of a more efficient, cost-effective, and environmentally friendly domestic liquid waste treatment system by utilizing plastic waste as a valuable resource while simultaneously addressing the problem of environmental pollution from two aspects simultaneously.

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