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Review Article

Artificial Intelligence (AI) in Adsorption Process of Heavy Metals: A Systematic Review

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Abstract

Artificial Intelligence (AI) has emerged as a transformative approach for predicting and optimizing adsorption processes in heavy metal removal, a critical aspect of water treatment plant (WTP) operations. This systematic review provides a comprehensive analysis of AI techniques that enhance adsorption performance, with a focus on machine learning (ML) models and metaheuristic algorithms. Advanced AI models, including neural networks and support vector machines, are utilized to analyze extensive datasets of adsorption parameters, improving prediction accuracy and operational efficiency. Meanwhile, metaheuristic algorithms, such as Genetic Algorithms (GAs) and Simulated Annealing (SA), effectively identify optimal parameter configurations for the adsorption process. The integration of AI facilitates real-time monitoring, predictive maintenance, and adaptive adjustments of process parameters, enabling continuous performance improvements. Additionally, AI-driven methods reveal critical adsorption features, allowing for precise control and improved resource efficiency. This review also highlights the synergy between AI and traditional adsorption models, such as Langmuir and Freundlich isotherms, proposing innovative approaches to enhance adsorption kinetics and thermodynamics. This review paper compiles 49 research articles covering the most recent developments in the field between 2019 and 2024. By demonstrating the structured application of AI, this review emphasizes its potential in achieving sustainable, adaptive, and reliable water quality management. Future research should focus on developing more advanced AI-driven

systems to broaden their applicability across diverse adsorption scenarios and pollutant types. This work underscores the pivotal role of AI in advancing adsorption technologies, paving the way for smarter, more sustainable water treatment solutions.

Keywords: Artificial Intelligence; Adsorption; Heavy Metal Removal; Machine Learning; Metaheuristic Algorithms

INTRODUCTION

Artificial Intelligence (AI) has emerged as a transformative force optimizing and enhancing the efficiency of Water Treatment Plants (WTPs) [1]. These plants play a critical role in ensuring the availability of clean and safe drinking water. AI applications in WTPs encompass a range of functions, from real-time monitoring to predictive maintenance. Machine learning algorithms can analyze vast amounts of data collected from sensors and water quality monitoring devices, enabling early detection of anomalies or potential issues [1]. Additionally, AI-powered control systems can dynamically adjust water treatment processes based on changing environmental conditions, ensuring optimal resource utilization. Predictive analytics help WTPs forecast equipment failures, allowing for proactive maintenance and minimizing downtime. Through the integration of AI, Water Treatment Plants can achieve higher levels of automation, improve energy efficiency, and ultimately contribute to the reliable delivery of high-quality water to communities [2].

Within water treatment plants (WTPs), the optimization of intricate processes relies heavily on metaheuristics and machine learning algorithms [3,4]. The application of metaheuristics, such as genetic algorithms (Gas) and simulated annealing (SA), is essential in tackling optimization issues related to water treatment. These techniques aim to identify the most efficient parameter configurations for processes like coagulation, flocculation, and filtration. Additionally, the quality control facet of WTPs is notably enhanced by the substantial contribution of machine learning techniques [3-5]. Smart control systems powered by AI enhance the overall operational efficiency of WTPs by automating decision-making processes. These systems can dynamically adjust chemical dosages, control the flow rate, and optimize the usage of resources based on real-time conditions. In the realm of quality control, AI facilitates early detection of contaminants, ensuring that water meets stringent quality standards. This advanced technology transforms WTPs into intelligent and adaptive systems, capable of providing consistently high-quality water while maximizing resource utilization and minimizing environmental impact [6].

Implementing AI models in WTPs involves a systematic approach to ensure effective integration and performance. The first step is data collection, where sensors and monitoring devices capture real-time information on water quality parameters, flow rates, and equipment statuses. The collected data is then pre-processed to remove noise and inconsistencies, making it suitable for analysis. Next, comes the model development phase, where AI algorithms such as machine learning or metahueristics are selected based on the

specific objectives, such as optimizing treatment processes or enhancing quality control. Training the model involves using historical data to enable it to recognize patterns and make predictions. After successful training, the model is tested with new data to validate its accuracy and effectiveness. Once validated, the AI model is integrated into the control systems of the WTP, allowing it to continuously analyze incoming data and make real-time adjustments to optimize operations. Regular monitoring and updates are crucial to ensure the model's continued performance and adaptation to changing conditions. This structured approach ensures a seamless and reliable implementation of AI models in Water Treatment Plants, contributing to enhanced efficiency and water quality [7-9].

In the following schematic plan (Figure 1), the stepwise implementation of AI models in WTPs is delineated, providing a visual representation of the process. The initial phase involves the deployment of sensors and monitoring devices to collect real-time data on various parameters crucial for water treatment, including water quality metrics, flow rates, and equipment statuses. This raw data undergoes pre-processing, where noise and inconsistencies are meticulously removed, ensuring the information's reliability. The subsequent stage encompasses model development, wherein appropriate AI algorithms, be it machine learning or metahueristics, are chosen based on the specific goals of the WTP, such as optimizing treatment processes or refining quality control measures [10]. The research at hand, however, centers specifically on the adsorption of heavy metals in WTPs. This focus signifies the targeted application of AI in addressing the critical issue of heavy metal contamination. The chosen AI models are trained using historical data related to heavy metal concentrations, allowing them to learn patterns and correlations crucial for predicting and optimizing adsorption processes. Once the models are successfully trained, they undergo rigorous testing with new data to validate their accuracy and effectiveness in real-world scenarios [11]. Upon successful validation, the AI models are seamlessly integrated into the control systems of the WTP, forming an intelligent framework capable of continuous analysis and real-time decision-making. This integration empowers the WTP to dynamically adjust treatment processes, optimize resource utilization, and enhance the overall efficiency of heavy metal removal. Regular monitoring and updates ensure the model's adaptability to changing conditions and guarantee sustained performance over time. This structured and comprehensive approach not only ensures the successful implementation of AI models in WTPs but also highlights their potential to address specific challenges, such as heavy metal adsorption, contributing to improved water quality and plant operational excellence [12].

At the outset, this review provides an introduction to contextualize the study's relevance and scope. The second section delves into the framework of the review, offering a detailed discussion of the state of the art in the field. This includes a scientometric analysis to provide a quantitative overview of existing research trends and to identify gaps and opportunities for future studies. The review concludes with a synthesis of insights and

reflections, summarizing key findings and outlining directions for advancing the field further.

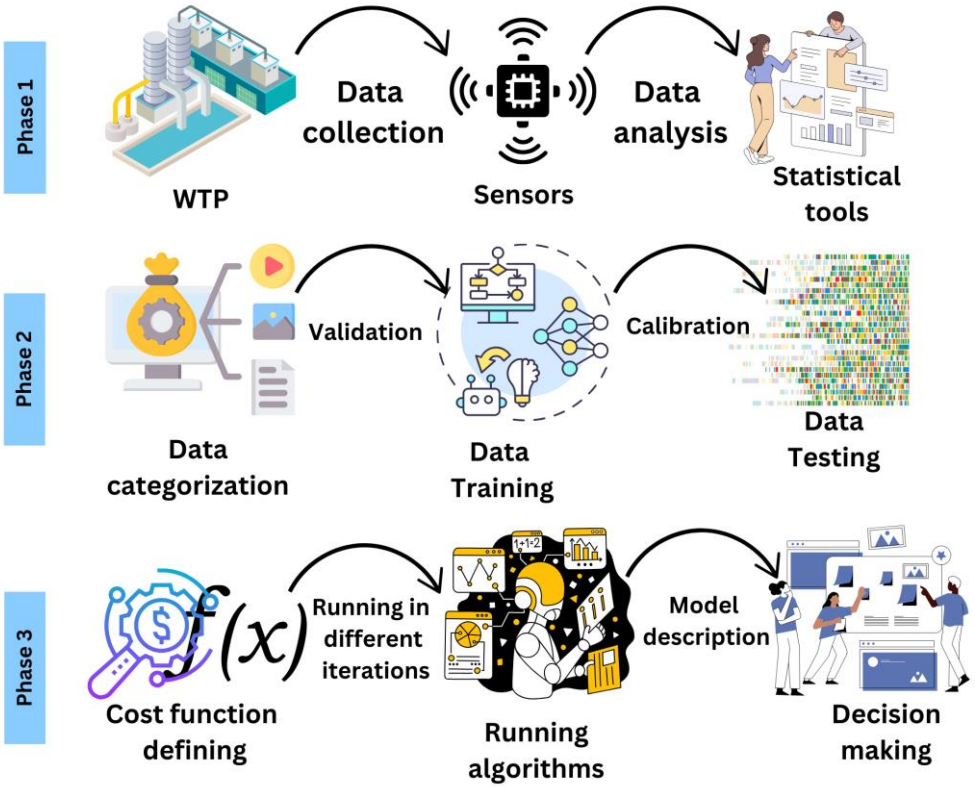


Figure 1. Schematic plan of AI applications in WTPs in the present review.

Review framework

Adsorption processes play a pivotal role in various industrial applications, such as wastewater treatment, gas purification, and material separation. The efficient operation of adsorption systems requires a comprehensive understanding and optimization of kinetic, isothermal, thermodynamic, and performance features. Traditional approaches often struggle to address the complexity and non-linearity inherent in these processes, leading to suboptimal system performance [13]. The motivation for the present research stems from the need to overcome these challenges by integrating cutting-edge technologies, specifically machine learning and metaheuristics, into the design of a Decision Support System (DSS). Machine learning computations offer a data-driven approach for accurate estimation of kinetic, isothermal specifications, thermodynamics, and adsorption performance features. The utilization of these computational techniques allows for the modeling of intricate relationships and patterns within the data, enhancing the precision of predictions and system understanding [14]. Furthermore, the incorporation of metaheuristics in the DSS provides a robust framework for implementing intelligent decision-making models. Metaheuristic algorithms excel in solving complex optimization

problems, allowing for the efficient identification of optimal operating conditions for adsorption processes. By leveraging the power of machine learning and metaheuristics synergistically, the DSS aims to enhance the overall performance, reliability, and sustainability of adsorption systems [15]. The outcomes of this research have the potential to revolutionize the field of adsorption processes by offering a versatile and adaptive decision support tool. This tool not only contributes to a deeper theoretical understanding of the underlying processes but also provides practical solutions for optimizing the operation of adsorption systems across various industrial domains. Ultimately, the integration of advanced computational techniques in this study aims to pave the way for more efficient and environmentally sustainable adsorption processes in the future [13,14].

In the domain of WTPs, the fusion of machine learning with mathematical models plays a crucial role in enhancing water quality control. This integration involves the utilization of mathematical expressions to formulate and apply machine learning algorithms for effective water quality prediction and monitoring. The present review delves into the mathematical aspects of the machine learning applications in water quality control [13-15].

One key aspect is the definition of the objective function, denoted as f(x;θ), which encapsulates the goal of predicting water quality. For instance, in a machine learning model such as a neural network, the objective function may take the form of the mean squared error (Equation 1) [16-20].

$$f(x;\theta)=\frac{1}{N}\sum_{i=1}^{N}(M(xi,\theta)-yi)^2 \quad (1)$$

Here, x represents input features, θ denotes model parameters, and N is the number of training samples.

The subsequent step involves training the machine learning model by minimizing the objective function. In a supervised learning scenario, this optimization process adjusts model parameters (θ) to minimize the prediction error (Equation 2).

$$\mathrm{Min}_{\theta}\ \frac{1}{N}\sum_{i=1}^{N}(M(xi.\theta)-yi)^2 \quad (2)$$

Following successful training, the model is applied for real-time water quality monitoring. The prediction of water quality (y^) based on the trained model and actual observed values (y) is expressed as Equation 3.

$$y\hat{}=M(x,\theta) \quad (3)$$

To assess the model's performance, mathematical metrics like Mean Absolute Error (MAE) or Root Mean Squared Error (RMSE) are employed in Equations 4 and 5, respectively.

$$MAE=\frac{1}{N}\sum_{i=1}^{N}|M(\mathbf{xi},\boldsymbol{\theta})-yi| \quad (4)$$

$$RMSE=\sqrt{\frac{1}{N}\sum_{i=1}^{N}(M(xi,\theta)-yi)^2} \quad (5)$$

Crucially, continuous monitoring and adaptation strategies are implemented through mathematical expressions. Dynamic adjustments to model parameters (θ) to adapt to changing water conditions can be expressed as Equation 6.

$$\theta_{new}=\theta_{old}-\alpha\nabla f(x;\theta) \quad (6)$$

where α represents the learning rate.

Within the domain of adsorption processes, the intricate interplay between adsorbate molecules and a solid surface finds mathematical expression through the application of ML. ML serves as a potent tool for modeling and optimizing adsorption, facilitating robust predictions and understanding of adsorbent behavior. The essential structure of ML computations in adsorption processes involves as per Table 1 [20]. The conceptual model of machine learning application in adsorption of heavy metals from water resources is demonstrated in Figure 2. According to the scheme, it can be concluded that in this effort, the initial data are gathered from experimental analysis and then a smart model will be developed for online operation of the process.

Table 1. The structure of machine learning computations in adsorption process of water resources [16-20].

Stage	Description
Feature Selection	Define the features (Mass of adsorbent, Contact Time, pH) as input variables characterizing the adsorption system. These features encompass the mass of adsorbent, contact time, and pH, which play a crucial role in determining the adsorption process. The meticulous selection of features is imperative for constructing an accurate ML model.
Data Collection and Preprocessing	Collect high-quality data (Removal Performance, adsorbent, Contact Time, and pH) essential for ML model training. The dataset, formed through experimental or simulated data, undergoes preprocessing steps, including data cleaning, normalization, and dimensionality reduction. These steps aim to enhance dataset quality and facilitate effective model training.
Model Selection	Employ diverse ML algorithms, such as Support Vector Machines (SVM), Decision Trees, Random Forests, or Neural Networks, to model adsorption processes. The choice of the model depends on the nature of the data and the specific objectives of the adsorption study.
Training and Validation	Represent the selected model with the mathematical equation: Removal Performance=a0+a1·Madsorbent+a2 ·Contact Time+a3·pH

	Where Removal Performance signifies the efficiency of adsorption, and a_0,a_1,a_2,a_3 are coefficients associated with the selected features. Train the model using the prepared dataset and validate its performance to ensure generalization capabilities. The dataset is commonly divided into training and testing sets to assess the model's accuracy on new, unseen data.
Model Evaluation and Optimization	Evaluate the ML model's performance using metrics such as mean absolute error, root mean square error, or correlation coefficients. If the model falls short of satisfactory performance, employ optimization techniques to fine-tune model parameters, enhancing predictive accuracy.

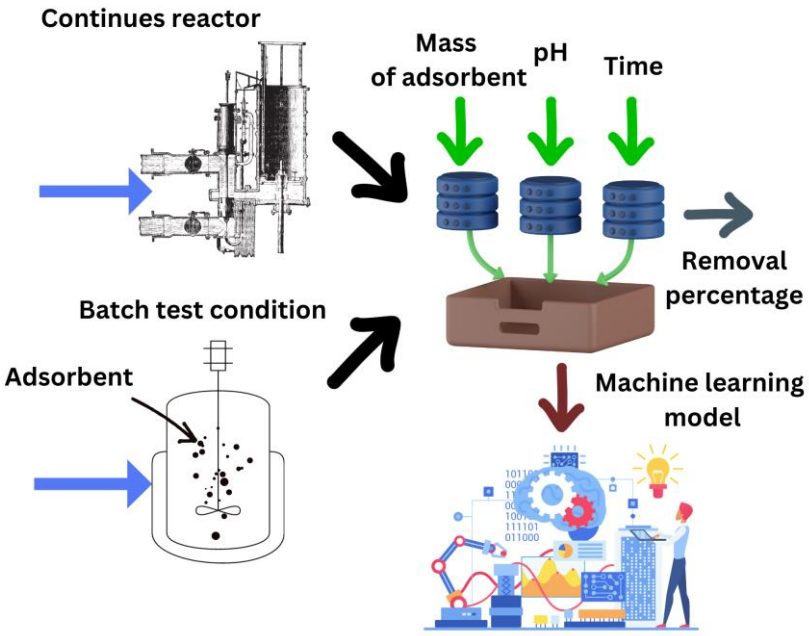


Figure 2. Framework of machine learning computations in decontamination of heavy metals from water resources.

In the second phase of AI modeling specifically tailored for WTPs, with a focus on the adsorption process, metaheuristic algorithms will be a pivotal component in the ongoing review analysis. The utilization of metaheuristics, such as the Genetic Algorithm, stands as a key strategy to optimize the operation of the adsorption process. This strategic application of the Genetic Algorithm, detailed in Table 2, will enable the system to efficiently explore the complex solution space, ultimately leading to the identification of optimal or near-optimal configurations for the adsorption process within the WTP. The Genetic Algorithm, inspired by the principles of natural selection and genetics, will iteratively generate potential solutions, evaluate them based on defined criteria within mathematical models, and refine these solutions over successive generations. This

approach aims to enhance the efficiency and effectiveness of the adsorption process, ensuring that the WTP operates at peak performance, achieves optimal resource utilization, and meets desired water treatment objectives. The incorporation of metaheuristic algorithms in this phase underscores the commitment to leveraging advanced AI techniques for the continuous improvement of water treatment processes [21-25].

Table 2. Metaheuristic Framework for Enhanced Adsorption Process Optimization in Water Treatment Plants [23-25].

Example	Stage	Description
Genetic Algorithm (GA)	Algorithm Overview	1. Consider a population of potential adsorption configurations, where each configuration represents a set of parameters such as adsorbent mass, contact time, and pH. 2. The genetic algorithm evolves this population through generations by applying selection, crossover, and mutation operators. 3. The objective function f(X) evaluates the performance of each configuration in terms of removal efficiency or another relevant metric.
	Mathematical Expressions	1. Let Xi represent an individual configuration in the population, where i is the individual index. 2. The population at generation t is Pt={X1,X2,...,XN}, with N being the population size. 3. The fitness of an individual, determined by the adsorption efficiency, is denoted as F(X). The key genetic operations can be expressed mathematically, such as: Selection: Pt′=Select(Pt) Crossover: Pt″=Crossover(Pt′) Mutation: Pt+1=Mutate(Pt″)
Simulated Annealing (SA)	Algorithm Overview	1.Imagine a current adsorption configuration X and its neighboring configuration X′ obtained by perturbing the parameters. 2.SA probabilistically accepts or rejects X′ based on the Metropolis acceptance criterion, allowing exploration of the solution space.

		3.The temperature parameter T decreases over time, controlling the probability of accepting worse solutions.
	Mathematical Expressions	1.Let X represent the current adsorption configuration, X′ a neighboring configuration, and Δf the change in removal efficiency. 2.The probability of accepting X′ is given by: P(accept)=exp(−T/Δf) 3.The temperature T decreases according to a cooling schedule.

In the framework of WTPs and adsorption, these mathematical expressions capture the essence of how Genetic Algorithms and Simulated Annealing can be applied to optimize adsorption configurations by iteratively exploring the solution space and refining solutions based on their performance [26].

The primary objective of this study is to implement a metaheuristic algorithm as part of a sophisticated online management and control system for water treatment plants, specifically focusing on the adsorption method (Figure 3). The incorporation of metaheuristic algorithms is essential for advancing the intelligent optimization capabilities of water treatment processes. By integrating these algorithms into the control system, the study aims to enhance the efficiency and responsiveness of water treatment plants, ensuring a smarter and more adaptive approach to the adsorption method. The implementation of metaheuristic algorithms represents a forward-looking strategy to address the dynamic and complex nature of water treatment operations, contributing to improved process performance, resource utilization, and overall operational effectiveness. This research aligns with the broader goal of leveraging advanced technologies for the sustainable and optimal management of water treatment facilities [27].

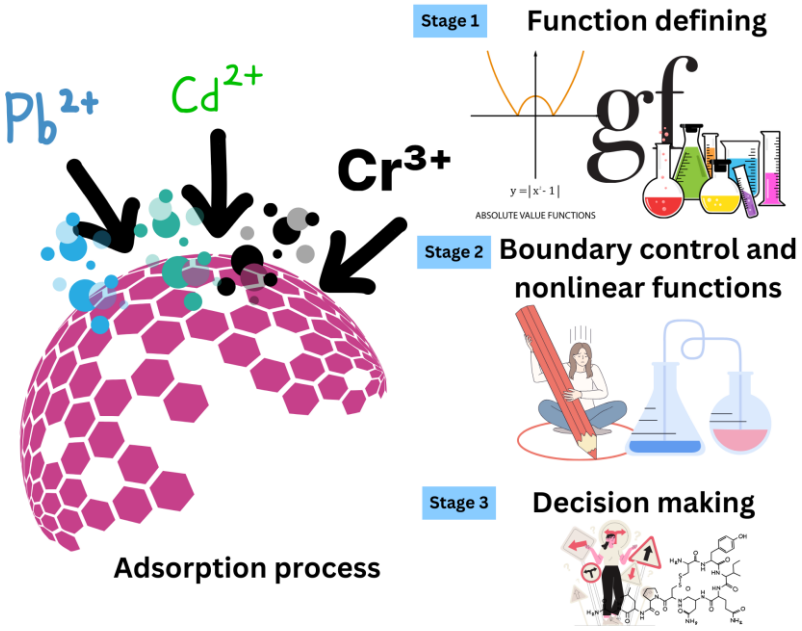


Figure 3. The specification of metaheuristics in WTPs by attention to adsorption process in this study.

State-of-the-art and the knowledge needs in the field

Adsorption processes are intricate and multifaceted, encompassing various aspects such as isotherm, kinetics, and thermodynamics. The Langmuir and Freundlich isotherms, described by Equations 7 and 8 respectively, delineate the relationship between adsorbate concentration (C_e) and adsorption capacity (qe). Meanwhile, the Lagergren pseudo-first order (Equation 9) and pseudo-second order (Equation 10) kinetic models explicate adsorption rates (k1, k2). Thermodynamically, the Gibbs free energy change (ΔG), enthalpy change (ΔH), and entropy change (ΔS) illustrated by equations Equations 11.12 and 13 are vital parameters reflecting the spontaneity, heat involvement, and randomness during adsorption. The intricate interplay of these factors complicates the prediction of adsorption behavior. Consequently, optimization of adsorption performance, central to efficient removal of pollutants, involves intricate mathematical modeling and experimental design. Maximizing adsorption capacity while minimizing costs is often addressed through response surface methodology (RSM) or artificial intelligence techniques. Equation 14 represents an illustrative optimization function, where Xi corresponds to various operating parameters. Achieving optimal conditions demands a nuanced understanding of the interdependent isothermal, kinetic, and thermodynamic factors, ultimately enhancing the efficacy of adsorption processes [28-31].

$$\text{Langmuir Isotherm: } qe=(Q_{max}\cdot K_L\cdot C_e)/(1+K_L\cdot Ce) \quad (7)$$

$$\text{Freundlich Isotherm: } qe=K_F.C_e^{1/n} \quad (8)$$

$$\text{Pseudo-First Order Kinetics: } \log((q_e - q_t)/ q_e) = -k_1 \cdot t \quad (9)$$

$$\text{Pseudo-Second Order Kinetics: } 1/q_t = 1/(k_2 \cdot t) + 1/q_e \quad (10)$$

$$\text{Gibbs Free Energy: } \Delta G = -RT \cdot \ln(K_c) \quad (11)$$

$$\text{Enthalpy Change: } 1/T = (\Delta H/R) + \ln(K_c)/R \quad (12)$$

$$\text{Optimization Function: Maximize } f(X1, X2, \ldots, Xn) \text{ subject to constraints} \quad (13)$$

Machine learning plays a crucial role in advancing the field of adsorption mechanism evaluation, offering a powerful tool for navigating the intricate relationships within isothermic, kinetic, and thermodynamic factors. The application of machine learning techniques in adsorption studies allows for the development of predictive models that can analyze and interpret complex data sets, making it easier to discern patterns and optimize adsorption performance. By leveraging algorithms, machine learning assists in the identification of key parameters influencing adsorption mechanisms, facilitating a more nuanced understanding of the intricate interplay between adsorbate concentration, adsorption capacity, and rates. This computational approach contributes significantly to the optimization of adsorption processes, providing a streamlined and efficient means of achieving optimal conditions for pollutant removal while minimizing costs. Through the utilization of machine learning, researchers can enhance the precision and efficacy of adsorption mechanism determination, ultimately advancing environmental remediation efforts [32-35].

In recent studies, the application of machine learning algorithms (MLAs) to model the adsorption efficiencies of various heavy metal–adsorbent pairs has been explored. Hafsa et al. (2020) investigated fourteen heavy metal–adsorbent pairs using support vector regression, random forest, stochastic gradient boosting, and bayesian additive regression tree models. Wet experiment-based measurements, along with synthetic data samples, were employed. Regression tree methods, BART, and RF demonstrated robust performance, achieving an impressive R2 of 0.96–0.99. This study provides a generalized methodology for applying ML in modeling not only specific adsorption processes but also comparable processes involving multiple HM-AD pairs [36]. Another study by Fanourgakis et al. (2020) proposed new descriptors for ML methods to predict gas adsorption capacities of nanoporous materials with electrostatic interactions. The study focused on CO2, H2, and H2S gases and employed probe atoms with electric dipoles as descriptors. The accuracy of the approach was validated against grand canonical Monte Carlo simulations, demonstrating the potential for ML to predict adsorption capacities in systems with electrostatic interactions [37]. Li et al. (2022) simulated the adsorption capacity of a nanocomposite material using ML techniques, addressing issues of generality in small datasets. AdaBoost and GA optimization models were employed, achieving high efficiency with low error rates, as indicated by RMSE criteria. Linear regression, Bayesian ridge regression, and Huber regression also demonstrated excellent performance [38]. In a

comprehensive review, Zhang et al. (2023) discussed the application of ML in pollutant adsorption, emphasizing the innovation ML brings to traditional adsorption models. The review covered various aspects, including adsorption efficiency, operating conditions, and adsorption mechanism. The authors provided general guidelines for applying ML in pollutant adsorption and identified existing challenges and future perspectives [39]. Fanourgakis et al. (2019) proposed descriptors for accurate predictions of gas uptake capacities in nanoporous materials using ML algorithms. The study showcased the improved accuracy of ML predictions, particularly at low pressures, compared to predictions based solely on structural features. The proposed algorithm demonstrated adaptability for diverse nanoporous materials [40]. Yin et al. (2022) implemented different models for predicting adsorption separation of a dye using porous materials. Tree models, including Multi-layer Perceptron, Passive-aggressive regression, and Decision Tree Regressor, were used, with the decision tree model showing the best performance. The study highlighted the potential of ML in correlating adsorption equilibrium data [41]. Taoufik et al. (2022) applied response surface methodology, support vector machine, and artificial neural network to study the sorption of caffeine on Cu–Al layered double hydroxide. The models showed high accuracy, with SVM achieving approximately 99.9% accuracy for test datasets. The proposed ML models provided reliable methods for monitoring and simulating the adsorption of pollutants [42]. In a study by Zhao et al. (2024), montmorillonite's adsorption behavior for pollutants was investigated using density functional theory (DFT) calculations and machine learning modeling. The gradient boosting decision tree (GBDT) model demonstrated a better fit for experimental data, and the study identified factors influencing adsorption, including pH levels and the molecular mass of pollutants [43]. These studies collectively underscore the diverse applications of machine learning in modeling adsorption processes, showcasing its potential for predicting adsorption efficiencies, gas uptake capacities, and separation of pollutants across various materials and conditions. The incorporation of synthetic data, novel descriptors, and optimization techniques highlights the evolving methodologies within the field. The studies contribute to advancing the understanding of adsorption processes and offer valuable insights for future research in this domain.

The present evaluation is centered around the design and implementation of a sophisticated online model aimed at monitoring and predicting the adsorption performance of heavy metals during the decontamination process. This intelligent system will leverage advanced features to enhance accuracy and efficiency in the assessment of adsorption capabilities. The primary objective of this review is to develop a smart online model that can dynamically analyze and adapt to changing conditions during the decontamination of heavy metals. By incorporating cutting-edge technologies and employing effective features, the proposed model seeks to provide real-time insights into the adsorption process. The inclusion of predictive capabilities will enable users to anticipate performance trends, optimize decontamination strategies, and respond proactively to emerging challenges. The underlying methodology involves the integration

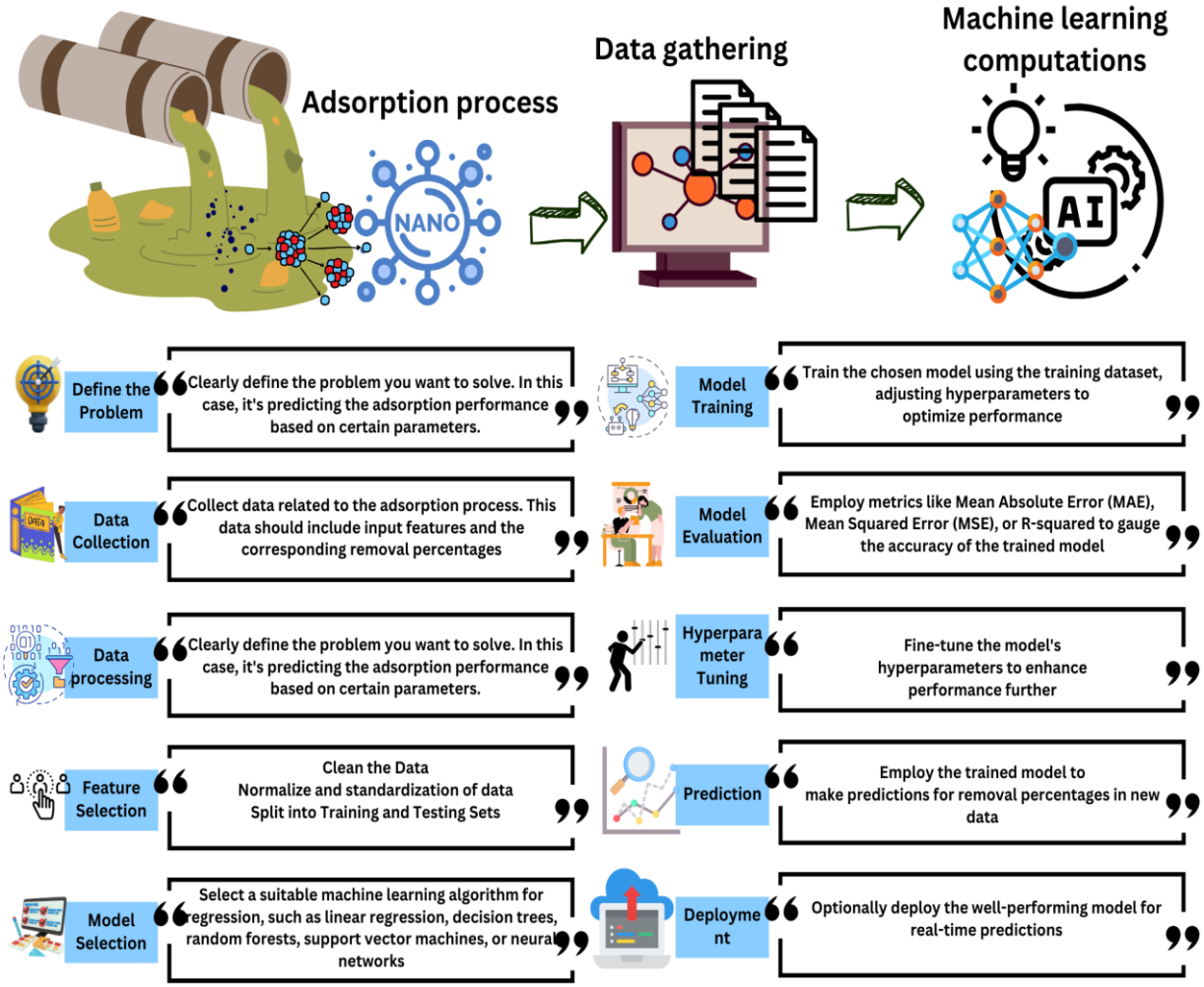
of data-driven algorithms that can learn and adapt based on historical and real-time data. This approach will facilitate the creation of a robust and versatile model capable of accurately predicting the adsorption efficiency for various heavy metals under diverse environmental conditions. The inclusion of effective features in the model ensures a comprehensive analysis, considering factors such as temperature, pH, concentration, and other relevant parameters that influence the adsorption process. Furthermore, the smart online model will provide a user-friendly interface, allowing stakeholders to easily access and interpret the predictions. The incorporation of visualization tools will enhance the understanding of the adsorption performance trends, enabling informed decision-making for process optimization and resource allocation.

This comprehensive review explores the application of metaheuristics in adsorption processes, showcasing diverse methods and tools for optimizing distinct adsorption scenarios. Nogueira et al. (2020) introduce a novel approach to optimize a pressure swing adsorption (PSA) unit for syngas purification using particle swarm optimization (PSO), emphasizing the generation of a substantial dataset for probabilistic confidence region construction around the optimal solution [44]. Ebrahimpoor et al. (2019) employ a bees-inspired algorithm coupled with artificial neural networks (ANN-BA) for optimizing the removal of acid red 27 dye using a polypyrrole/SrFe12O19/graphene oxide nanocomposite. The ANN-BA model outperforms D-optimal response surface methodology, demonstrating higher removal percentages and efficient utilization in wastewater treatment [45]. Silva et al. (2023) proposes a metaheuristic strategy, particle swarm optimization (PSO), for simultaneous optimization and material screening in adsorption heat pump design, showcasing its ability to evaluate broad temperature intervals and identify optimal adsorbents [46]. Lastly, Hossini Asl et al. (2024) investigate the use of mesoporous Fe-ZSM-5 nano-zeolite synthesized from coal fly ash for the removal of benzene, toluene, and m-xylene. Their study combines conventional and meta-heuristic neuro-fuzzy systems, revealing the potential of Fe-ZSM-5 as an effective adsorbent for hazardous hydrocarbons in aqueous media [47]. Together, these studies highlight the versatility and effectiveness of different metaheuristic approaches in optimizing adsorption processes, addressing various pollutants and adsorbent materials.

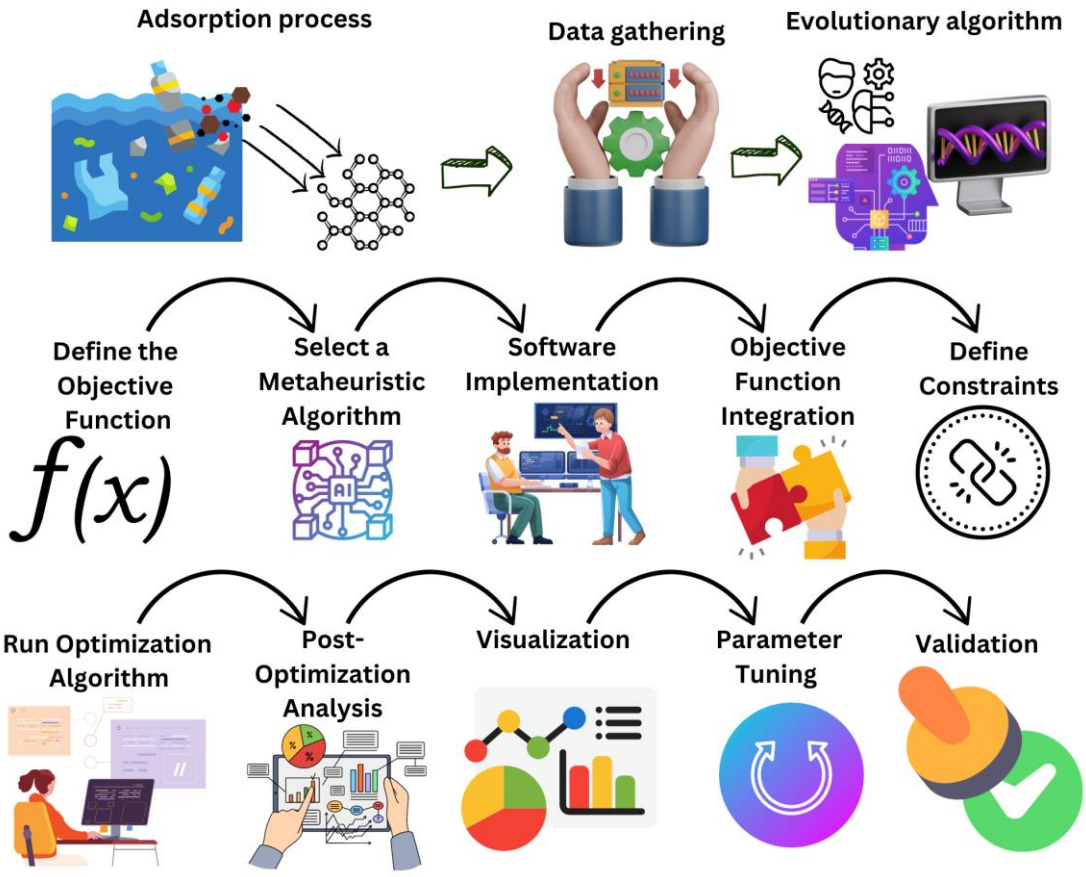
The current undertaking aims to develop an innovative and dynamic decision-making system designed to effectively control the adsorption process of heavy metals. This comprehensive system integrates key considerations related to isotherm, kinetic, and thermodynamic aspects, offering a multifaceted approach to optimize the removal of heavy metals from various environments. By focusing on isotherm aspects, the systematic review aims to understand the equilibrium adsorption behavior of heavy metals onto adsorbent surfaces. This involves studying the relationship between the amount of adsorbate and its concentration in the solution at constant temperature. Incorporating isotherm data into the decision-making system allows for a deeper understanding of the adsorption process and facilitates the selection of suitable adsorbents tailored to specific heavy metal removal requirements. The kinetic aspect of the decision-making system

involves analyzing the rate at which the adsorption process occurs. By incorporating kinetic parameters, the system can dynamically adjust and optimize conditions to enhance the efficiency of heavy metal removal. Understanding the adsorption kinetics is crucial for developing a responsive and adaptive system that can accommodate varying concentrations of heavy metals in real-time.

The execution framework of machine learning and metaheuristic algorithms in the adsorption process is exemplified in accordance with Figure 4. This scheme elucidates the systematic deployment and interaction of these algorithms, providing a comprehensive visual representation of their roles and relationships within the adsorption process.



(a)



(b)

Figure 4. The executive steps of (a) machine learning and (b) metaheuristic algorithms in adsorption process analysis.

Scientometric Analysis

As per 559 searched records in Scopus databank, the number of documents published annually on "Adsorption" and "Artificial Intelligence" has seen a significant rise over the years, as illustrated in Figure 5a. From 1986 until approximately 2017, there was a steady but low level of research activity in this area, with minor year-to-year variations. However, starting in 2018, the number of publications began to increase significantly, culminating in an exponential growth phase between 2020 and 2023. The peak, recorded in 2023 with more than 140 publications, highlights the growing importance of integrating AI with adsorption processes. This trend suggests that researchers increasingly recognize the potential of AI techniques to enhance the modeling, prediction, and optimization capabilities within adsorption applications, driven by a need for more effective and efficient solutions in environmental and industrial sectors.

Figure 5b provides insights into the distribution of publications across various academic journals. Notably, the Science of the Total Environment has seen a sharp increase in articles related to adsorption and AI in 2024, indicating a heightened interest in the environmental applications of these technologies. Similarly, the Journal of Molecular

Liquids and Chemical Engineering Journal have been consistently contributing to this research area since around 2020. Meanwhile, Desalination and Water Treatment also shows a notable, though more moderate, contribution. The increasing presence of relevant publications in prominent journals during 2023 and 2024 underscores the expanding interest across multiple scientific disciplines. It highlights the applicability of AI-enhanced adsorption processes in diverse fields, from molecular studies to broader environmental and engineering contexts.

The country-wise distribution of documents, depicted in Figure 5c, reveals that China leads the research output by a considerable margin, followed by India and the United States. This strong presence of China and India may be attributed to their focus on addressing water scarcity and environmental pollution, areas where adsorption and AI can play a vital role in providing efficient solutions. Iran, Saudi Arabia, and Egypt also contribute significantly to the research landscape, which may reflect the importance of adsorption technologies in addressing environmental challenges, particularly in water treatment, in these regions. Overall, Asian countries are at the forefront of applying artificial intelligence to adsorption, emphasizing the critical need for sustainable solutions to water and environmental issues across the continent.

The subject area analysis presented in Figure 5d demonstrates the multidisciplinary nature of adsorption research involving AI. Environmental Science (15.2%) and Chemistry (14.9%) are the leading subject areas, suggesting a significant focus on the environmental and chemical aspects of adsorption, including pollutant removal and process chemistry. Chemical Engineering (12.6%) and Engineering (11.3%) also feature prominently, highlighting the practical implementation of adsorption processes and their optimization using AI techniques. Fields such as Materials Science (9.1%), Energy (6.5%), and Physics and Astronomy (5.9%) indicate that adsorption, enhanced by AI, has found applications in developing novel materials, energy storage, and advanced physical processes. Other disciplines, including Biochemistry (4.8%) and Medicine (2.6%), indicate the role of adsorption in biological applications like drug delivery and biosorption. A notable portion falls under "Other" (11.8%), signifying that adsorption research transcends traditional disciplinary boundaries, reflecting its wide-ranging applications and growing relevance. Overall, the analysis of the figures highlights a rapidly growing interest in utilizing artificial intelligence to enhance adsorption processes. This interest spans multiple scientific disciplines and regions, with particular contributions from Asian countries and diverse academic fields. The recent surge in publications across leading journals since 2023 underscores the increasing recognition of the value that AI can bring to adsorption technology, particularly in solving critical challenges in environmental sustainability and industrial efficiency.

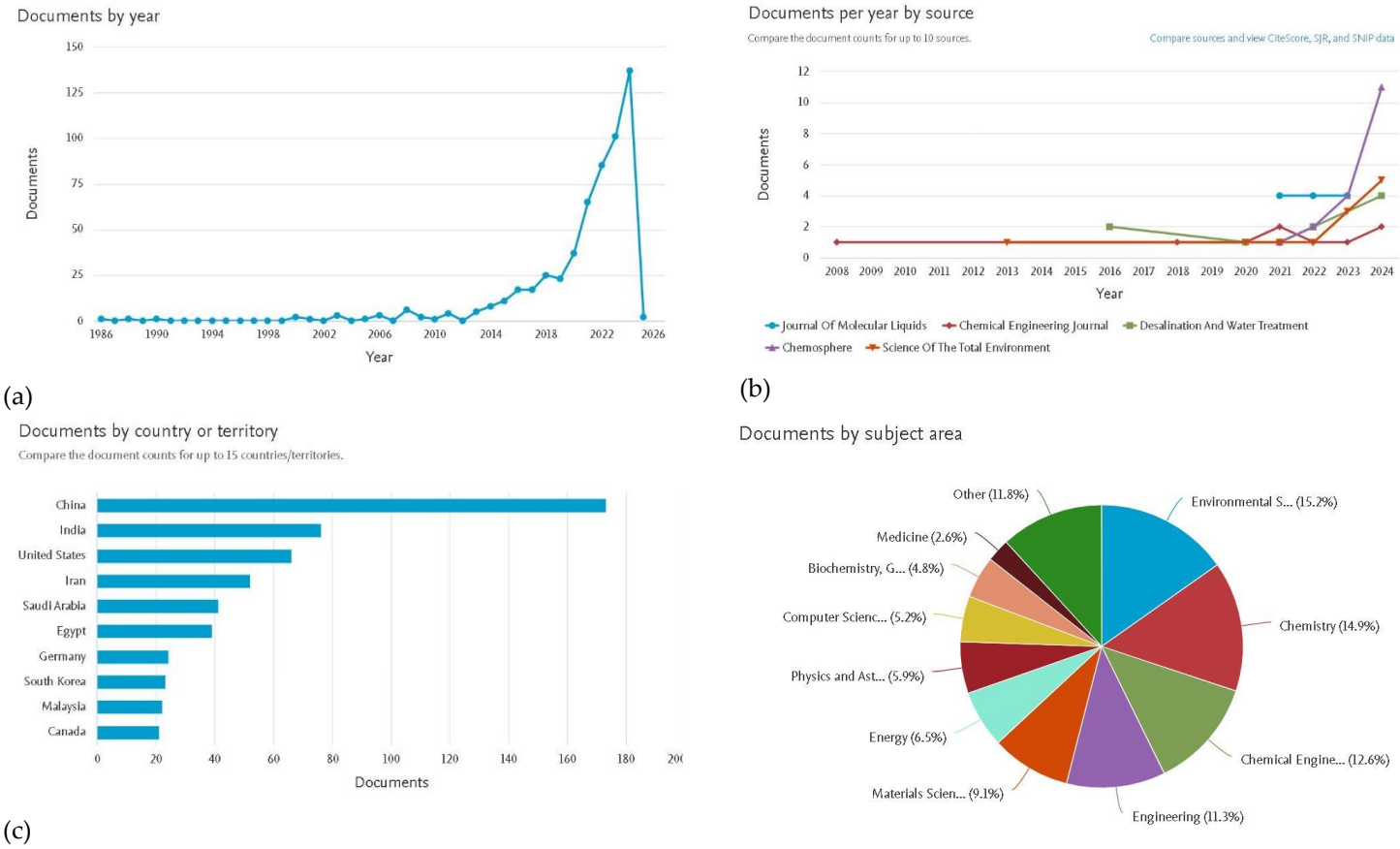


Figure 5. The outcomes of Scopus based analysis of AI-Adsorption topic as per (a) documents per year, (b) documents per year by source, (c) documents by country, and (d) documents by subject area.

Future studies

In future studies, the development of an advanced online predictive system for the application of Artificial Intelligence (AI) in controlling decontaminants in water and wastewater treatment systems should be prioritized. Such a system could incorporate machine learning models like Artificial Neural Networks (ANN), Adaptive Neuro-Fuzzy Inference Systems (ANFIS), and Random Forests (RF) to enhance real-time predictions and decision-making processes. By integrating these models into a comprehensive online dashboard, operators could monitor key water quality indicators, receive real-time contamination forecasts, and adjust treatment parameters dynamically to maintain regulatory compliance and optimize system performance. This approach would ensure effective and timely intervention, reducing the need for manual adjustments and enabling the automation of water treatment processes.

Another key aspect for future exploration is the development of an intuitive, user-friendly online dashboard that can seamlessly integrate predictive analytics and visualization tools. Such dashboards would empower plant operators to visualize data

trends and predictions through interactive charts and heatmaps, allowing for more efficient management of the water treatment system. Implementing AI models, such as Gradient Boosting Machines (GBM) or Support Vector Machines (SVM), for anomaly detection could also help identify unusual contamination events, making the system more robust and reliable. Leveraging cloud-based platforms could further enhance accessibility and scalability, enabling multiple treatment facilities to benefit from shared AI-based insights, thus contributing to smarter water resource management and better public health outcomes.

CONCLUSION

In conclusion, this systematic review highlights the transformative potential of Artificial Intelligence (AI) in optimizing the adsorption processes for heavy metal removal in water treatment plants (WTPs). AI, through machine learning (ML) and metaheuristic algorithms, has demonstrated its capability to enhance adsorption efficiency by providing data-driven insights, optimizing operational parameters, and improving the overall performance of the treatment processes. The integration of AI into WTPs allows for real-time analysis, predictive maintenance, and dynamic adjustments, significantly enhancing resource utilization and reducing environmental impact.

The adoption of ML techniques, including Support Vector Machines, Random Forests, and Artificial Neural Networks, enables accurate predictions of adsorption capacities by modeling complex relationships between parameters such as adsorbent mass, contact time, and pH. Moreover, the utilization of metaheuristics like Genetic Algorithms and Simulated Annealing optimizes the adsorption process by efficiently navigating the solution space and identifying optimal configurations. These techniques ensure that WTPs operate at peak efficiency, contributing to consistent delivery of high-quality water.

The review emphasizes the importance of a structured approach to AI implementation in WTPs, from data collection and pre-processing to model training, validation, and integration into control systems. This structured deployment ensures that AI models remain adaptable to changing conditions, thereby sustaining their effectiveness over time. Additionally, the combination of AI with conventional adsorption models, such as the Langmuir and Freundlich isotherms, allows for a more nuanced understanding of adsorption kinetics, thermodynamics, and equilibrium.

Ultimately, the incorporation of AI into adsorption processes not only enhances water quality control but also supports the development of intelligent, adaptive, and sustainable water treatment solutions. Future studies should focus on expanding the applicability of AI models to a wider range of pollutants and optimizing the integration of AI with other advanced treatment methods. By leveraging AI's predictive and optimization capabilities, WTPs can continue to advance towards achieving greater efficiency, reliability, and environmental sustainability.

CONFLICT OF INTERESTS

The authors confirm that there is no conflict of interest associated with this publication.

REFERENCES

1. Yaseen, Z.M., An insight into machine learning models era in simulating soil, water bodies and adsorption heavy metals: Review, challenges and solutions. Chemosphere, **2021**, 277, p.130126.

2. Zhu, X., Wan, Z., Tsang, D.C., He, M., Hou, D., Su, Z. and Shang, J., Machine learning for the selection of carbon-based materials for tetracycline and sulfamethoxazole adsorption. Chemical Engineering Journal, **2021**, 406, p.126782.

3. Yang, H., Huang, K., Zhang, K., Weng, Q., Zhang, H. and Wang, F., Predicting heavy metal adsorption on soil with machine learning and mapping global distribution of soil adsorption capacities. Environmental Science & Technology, **2021**, 55(20), pp.14316-14328.

4. Meng, M., Zhong, R. and Wei, Z., Prediction of methane adsorption in shale: Classical models and machine learning based models. Fuel, **2020**, 278, p.118358.

5. Nguyen, X.C., Ly, Q.V., Nguyen, T.T.H., Ngo, H.T.T., Hu, Y. and Zhang, Z., Potential application of machine learning for exploring adsorption mechanisms of pharmaceuticals onto biochars. Chemosphere, **2022**, 287, p.132203.

6. Kim, S.Y., Kim, S.I. and Bae, Y.S., Machine-learning-based prediction of methane adsorption isotherms at varied temperatures for experimental adsorbents. The Journal of Physical Chemistry C, **2020**, 124(36), pp.19538-19547.

7. Cao, L., Recent advances in the application of machine-learning algorithms to predict adsorption energies. Trends in Chemistry, **2022**.

8. Fanourgakis, G.S., Gkagkas, K., Tylianakis, E. and Froudakis, G.E., A universal machine learning algorithm for large-scale screening of materials. Journal of the American Chemical Society, **2020**, 142(8), pp.3814-3822.

9. Sarikas, A.P., Fanourgakis, G.S., Tylianakis, E., Gkagkas, K. and Froudakis, G.E., Comparison of Energy-Based Machine Learning Descriptors for Gas Adsorption. The Journal of Physical Chemistry C, **2023**, 127(43), pp.20995-21005.

10. Zhang, K., Zhong, S. and Zhang, H., Predicting aqueous adsorption of organic compounds onto biochars, carbon nanotubes, granular activated carbons, and resins with machine learning. Environmental Science & Technology, **2020**, 54(11), pp.7008-7018.

11. Hu, X., Alsaikhan, F., Majdi, H.S., Bokov, D.O., Mohamed, A. and Sadeghi, A., Predictive modeling and computational machine learning simulation of adsorption separation using advanced nanocomposite materials. Arabian Journal of Chemistry, **2022**, 15(9), p.104062.

12. Zhang, K., Zhong, S. and Zhang, H., Predicting aqueous adsorption of organic compounds onto biochars, carbon nanotubes, granular activated carbons, and resins with machine learning. Environmental Science & Technology, **2020**, 54(11), pp.7008-7018.

13. Moosavi, S., Manta, O., El-Badry, Y.A., Hussein, E.E., El-Bahy, Z.M., Mohd Fawzi, N.F.B., Urbonavičius, J. and Moosavi, S.M.H., A study on machine learning methods' application for dye adsorption prediction onto agricultural waste activated carbon. Nanomaterials, **2021**, 11(10), p.2734.

14. Kooh, M.R.R., Thotagamuge, R., Chau, Y.F.C., Mahadi, A.H. and Lim, C.M., Machine learning approaches to predict adsorption capacity of Azolla pinnata in the removal of methylene blue. Journal of the Taiwan Institute of Chemical Engineers, **2022**, 132, p.104134.

15. Abbasi, E., Moghaddam, M.R.A. and Kowsari, E., A systematic and critical review on development of machine learning based-ensemble models for prediction of adsorption process efficiency. Journal of Cleaner Production, **2022**, p.134588.

16. Nogueira, I.B., Martins, M.A., Regufe, M.J., Rodrigues, A.E., Loureiro, J.M. and Ribeiro, A.M., Big data-based optimization of a pressure swing adsorption unit for syngas purification: On mapping uncertainties from a metaheuristic technique. Industrial & Engineering Chemistry Research, **2020**, 59(31), pp.14037-14047.

17. Ebrahimpoor, S., Kiarostami, V., Khosravi, M., Davallo, M. and Ghaedi, A., Bees metaheuristic algorithm with the aid of artificial neural networks for optimization of acid red 27 dye adsorption onto novel polypyrrole/SrFe 12 O 19/graphene oxide nanocomposite. Polymer Bulletin, **2019**, 76, pp.6529-6553.

18. Silva, B.C., Rebello, C.M., Rodrigues, A.E., Ribeiro, A.M., Ferreira, A.F. and Nogueira, I.B., Metaheuristic Framework for Material Screening and Operating Optimization of Adsorption-Based Heat Pumps. ACS omega, **2023**.

19. Asl, S.M.H., Belviso, C., Masomi, M. and Tajbakhsh, M., Coal fly ash-derived Fe-ZSM-5 nano-zeolite for adsorption of mono-aromatics in aqueous media; hybrid meta-heuristic neuro-fuzzy modeling. Microporous and Mesoporous Materials, **2024**, 365, p.112831.

20. Azadikhah, K., Davallo, M., Kiarostami, V. and Mortazavinik, S., Modeling of malachite green adsorption onto novel polyurethane/SrFe12O19/clinoptilolite nanocomposite using response surface methodology and biogeography-based optimization-assisted multilayer neural network. Environmental Science and Pollution Research, **2022**, 29(24), pp.36040-36056.

21. Jaffari, Z.H., Jeong, H., Shin, J., Kwak, J., Son, C., Lee, Y.G., Kim, S., Chon, K. and Cho, K.H., Machine-learning-based prediction and optimization of emerging contaminants' adsorption capacity on biochar materials. Chemical Engineering Journal, **2023**, 466, p.143073.

22. Huang, M., Xu, H., Yu, H., Zhang, H., Micheal, M., Yuan, X. and Wu, H., Fast prediction of methane adsorption in shale nanopores using kinetic theory and machine learning algorithm. Chemical Engineering Journal, **2022**, 446, p.137221.

23. Zhang, X., Zheng, Q.R. and He, H.Z., Machine-learning-based prediction of hydrogen adsorption capacity at varied temperatures and pressures for MOFs adsorbents. Journal of the Taiwan Institute of Chemical Engineers, **2022**, 138, p.104479.

24. Da, T.X., Ren, H.K., He, W.K., Gong, S.Y. and Chen, T., Prediction of uranium adsorption capacity on biochar by machine learning methods. Journal of Environmental Chemical Engineering, **2022**, 10(5), p.108449.

25. Ebrahimpoor, S., Kiarostami, V., Khosravi, M., Davallo, M. and Ghaedi, A., Optimization of tartrazine adsorption onto polypyrrole/srfe 12 o 19/graphene oxide nanocomposite using central composite design and bat inspired algorithm with the aid of artificial neural networks. Fibers and Polymers, **2021**, 22, pp.159-170.

26. Zahmatkesh, S., Karimian, M., Chen, Z. and Ni, B.J., Combination of coagulation and adsorption technologies for advanced wastewater treatment for potable water reuse: By ANN, NSGA-II, and RSM. Journal of Environmental Management, **2024**, 349, p.119429.

27. Liu, W., Ji, Y., Huang, Y., Zhang, X.J., Wang, T., Fang, M.X. and Jiang, L., Adsorption-based post-combustion carbon capture assisted by synergetic heating and cooling. Renewable and Sustainable Energy Reviews, **2024**, 191, p.114141.

28. Birniwa, A.H., Ali, U., Jahun, B.M., Al-dhawi, B.N.S. and Jagaba, A.H., Cobalt oxide doped polyaniline composites for methyl orange adsorption: optimization through response surface methodology. Case Studies in Chemical and Environmental Engineering, **2024**, 9, p.100553.

29. Saba, B., Christy, A.D. and Shah, A., Hydrochar for pollution remediation: Effect of process parameters, adsorption modeling, life cycle assessment and techno-economic evaluation. Resources, Conservation and Recycling, **2024**, 202, p.107359.

30. Wang, G. and Chen, W., Molecular simulations of hydrogen adsorption on coal with different ranks: Implications for hydrogen geo-storage. International Journal of Hydrogen Energy, **2024**, 51, pp.10-20.

31. Li, X., Sun, X., Walters, C.C. and Zhang, T., H2, CH4 and CO2 adsorption on Cameo coal: Insights into the role of cushion gas in hydrogen geological storage. International Journal of Hydrogen Energy, **2024**, 50, pp.879-892.

32. Fan, X., Zhao, Z., Li, C., Li, X., He, Y. and Zhu, M., eep eutectic solvent intercalation graphene oxide with strong interfacial adsorption capacity towards efficient lubrication. Carbon, **2024**., 216, p.118508.

33. Pei, Y., Cheng, W., Liu, R., Di, H., Jiang, Y., Zheng, C. and Jiang, Z., Synergistic effect and mechanism of nZVI/LDH composites adsorption coupled reduction of nitrate in micro-polluted water. Journal of Hazardous Materials, **2024**, 464, p.133023.

34. Shao, M., Junejo, S.A., Zhang, B. and Huang, Q., Effects of explosion puffing on the native structural organization and oil adsorption properties of starch. Carbohydrate Polymers, **2024**, 324, p.121518.

35. Sellaoui, L., Gerhardt, R., Dhaoudi, F., Chebaane, S., Manai, L., Azhary, A., Saedoon, H., de Farias, B.S., Dotto, G.L., Cadaval Jr, T.R.S.A. and de Almeida Pinto, L.A., Novel films prepared from spirulina and chitosan for textile pollutant removal: Experiments and theoretical study of adsorption equilibrium via an advanced theoretical approach. Separation and Purification Technology, **2024**, 329, p.125158.

36. Hafsa, N., Rushd, S., Al-Yaari, M. and Rahman, M., A generalized method for modeling the adsorption of heavy metals with machine learning algorithms. Water, **2020**, 12(12), p.3490.

37. Fanourgakis, G.S., Gkagkas, K., Tylianakis, E. and Froudakis, G., A generic machine learning algorithm for the prediction of gas adsorption in nanoporous materials. The Journal of Physical Chemistry C, **2020**, 124(13), pp.7117-7126.

38. Weidong, L.I., Suhayb, M.K., Thangavelu, L., Marhoon, H.A., Pustokhina, I., Alqsair, U.F., El-Shafay, A.S. and Alashwal, M., Implementation of AdaBoost and genetic algorithm machine learning models in prediction of adsorption capacity of nanocomposite materials. Journal of Molecular Liquids, **2022**, 350, p.118527.

39. Zhang, W., Huang, W., Tan, J., Huang, D., Ma, J. and Wu, B., Modeling, optimization and understanding of adsorption process for pollutant removal via machine learning: Recent progress and future perspectives. Chemosphere, **2023**, 311, p.137044.

40. Fanourgakis, G.S., Gkagkas, K., Tylianakis, E., Klontzas, E. and Froudakis, G., A robust machine learning algorithm for the prediction of methane adsorption in nanoporous materials. The Journal of Physical Chemistry A, **2019**, 123(28), pp.6080-6087.

41. Yin, G., Alazzawi, F.J.I., Mironov, S., Reegu, F., El-Shafay, A.S., Rahman, M.L., Su, C.H., Lu, Y.Z. and Nguyen, H.C., Machine learning method for simulation of adsorption separation: comparisons of model's performance in predicting equilibrium concentrations. Arabian Journal of Chemistry, **2022**, 15(3), p.103612.

42. Taoufik, N., Boumya, W., Elmoubarki, R., Elhalil, A., Achak, M., Abdennouri, M. and Barka, N., Experimental design, machine learning approaches for the optimization and modeling of caffeine adsorption. Materials Today Chemistry, **2022**, 23, p.100732.

43. Zhao, C., Zhang, J., Zhang, W., Yang, Y., Guo, D., Zhang, H. and Liu, L., Reveal the main factors and adsorption behavior influencing the adsorption of pollutants on natural mineral adsorbents: Based on machine learning modeling and DFT calculation. Separation and Purification Technology, **2024**, 331, p.125706.

44. Costa, E.A., Rebello, C.M., Schnitman, L., Loureiro, J.M., Ribeiro, A.M. and Nogueira, I.B., Adaptive digital twin for pressure swing adsorption systems: Integrating a novel feedback tracking system, online learning and uncertainty assessment for enhanced performance. Engineering Applications of Artificial Intelligence, **2024**, 127, p.107364.

45. Ebrahimpoor, S., Kiarostami, V., Khosravi, M., Davallo, M. and Ghaedi, A., Bees metaheuristic algorithm with the aid of artificial neural networks for optimization of acid red 27 dye adsorption onto novel polypyrrole/SrFe 12 O 19/graphene oxide nanocomposite. Polymer Bulletin, **2019**, 76, pp.6529-6553.

46. Silva, B.C., Rebello, C.M., Rodrigues, A.E., Ribeiro, A.M., Ferreira, A.F. and Nogueira, I.B., Metaheuristic Framework for Material Screening and Operating Optimization of Adsorption-Based Heat Pumps. ACS omega, **2023**.

47. Asl, S.M.H., Belviso, C., Masomi, M. and Tajbakhsh, M., Coal fly ash-derived Fe-ZSM-5 nano-zeolite for adsorption of mono-aromatics in aqueous media; hybrid meta-heuristic neuro-fuzzy modeling. Microporous and Mesoporous Materials, **2024**, 365, p.112831.