Machine Learning (ML) Applications in Water Treatment: Possibilities and Advantages

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Abstract Artificial intelligence (AI), especially machine learning (ML) algorithms, has gained traction in water treatment processes (WTPs) for tasks such as process optimization, operational decision-making, and cost efficiency. Since 1997, at least 91 peer-reviewed studies have documented the use of AI in various WTP operations, including coagulation/flocculation (41 studies), membrane filtration (21), formation of disinfection byproducts (DBPs) (13), adsorption (16), and other aspects of plant management. This paper critically reviews these studies to evaluate how AI technologies have been applied in WTPs, highlighting both advancements and current limitations. AI has contributed significantly to improving the accuracy of predictions related to coagulant dosage, membrane performance (flux, fouling, and rejection), DBP formation, and contaminant removal. Notably, deep learning (DL) approaches have demonstrated strong feature extraction and data mining capabilities. These have enabled the development of image-based DL models capable of correlating floc morphology with coagulant dosages. Moreover, hybrid models—integrating AI with traditional regression or physical/kinetic approaches—have shown enhanced predictive capabilities. The review also identifies key future research directions aimed at further refining AI-based control systems for water treatment processes.

Keywords: Artificial intelligence; machine learning; water treatment process; coagulation & flocculation; disinfection byproducts

1. Introduction

Significant progress in sensor technology, data acquisition, storage, and processing capabilities has propelled the growth and integration of Artificial Intelligence (AI) across various domains. Among these, machine learning (ML)—a key branch of AI—has seen notable advancements in fields such as healthcare, finance, engineering, and economics. While numerous water treatment processes (WTPs) have been implemented in treatment facilities, rising concerns over increasingly complex water quality and tighter environmental regulations have created operational, financial, and efficiency-related challenges. Natural fluctuations in raw water quality further compound the complexity of maintaining consistent treatment performance (Chowdhury and Husain, 2020). Modeling and simulating the intricate processes within WTPs remains a difficult task. Many treatment plants rely on negative feedback control systems to make real-time adjustments based on continuous monitoring of water quality parameters (WQPs). These systems generate corrective signals when deviations from setpoints are detected, triggering metering pumps to adjust treatment inputs accordingly. For instance, Robenson et al. (2009) demonstrated the use of AI in optimizing coagulant dosing at the Segama WTP in Lahad Datu, Sabah, Malaysia, suggesting AI as a viable alternative to traditional jar testing methods. The use of AI in WTPs has largely focused on enhancing coagulation/flocculation, automation and control, cost-effectiveness, pollutant removal, effluent quality, and DBP regulation. This review provides a structured assessment of relevant literature addressing AI applications in WTPs, highlighting their benefits and existing limitations. The studies reviewed were categorized into four main areas: coagulation/flocculation, membrane-based filtration, DBP formation and mitigation, and contaminant removal through adsorption and other techniques. Opportunities for improving WTP operations and recommendations for future research are also discussed.

2. Methodology of article Collection

This review analyzed a minimum of 91 scholarly publications, dating back to 1997, that explored the application of artificial intelligence (AI) methods in water treatment processes (WTPs), including coagulation/flocculation (41 studies), membrane filtration (21), disinfection byproducts (DBPs) (13), and various other operational areas (16). The selection of these articles was guided by a scientometric approach—a quantitative technique used to evaluate research output, emerging themes, and patterns within academic literature. This study employs scientometric analysis to assess developments in AI applications for water treatment, with a focus extending as far back as 1990.

3. Results and Discussions

Unexpected fluctuations in the quality of incoming water create significant challenges for water treatment plant

(WTP) operators when determining appropriate coagulant dosages using traditional experimental or empirical methods. To enable real-time adjustment of coagulant levels, researchers have explored the application of artificial intelligence (AI) techniques in coagulation and flocculation (C/F) processes. These studies have aimed to forecast coagulant dosing requirements based on desired treatment outcomes—such as natural organic matter (NOM) reduction (Narges et al., 2021), turbidity control (Zangooei et al., 2016), process cost optimization (Malzer and Strugholtz, 2008), and prediction of treated water quality (Setshedi et al., 2021). AI models for coagulant dosage prediction typically utilize between three and twelve input variables, including turbidity (Turb), temperature (Temp), total dissolved solids (TDS), pH, color (Col), alkalinity (Alk), hardness (Hard), total organic carbon (TOC), dissolved organic carbon (DOC), dissolved oxygen (DO), electrical conductivity (EC), UV absorbance at 254 nm (UV254), chlorine (Cl_2), ozone (O_3), salinity (Sal), flow rate (Q), chlorine dioxide (ClO_2), and potassium permanganate ($KMnO_4$). Among these, Turb, Temp, Col, pH, and EC were the most frequently used parameters. Some models also incorporated coagulant dosage itself, along with other inputs like initial turbidity and mixing duration, to predict effluent turbidity.

Hybrid AI models have generally outperformed standalone approaches, displaying improved learning capability and more accurate predictions. General Regression Neural Networks (GRNN) yielded better outcomes with limited datasets, whereas Multi-Layer Perceptron (MLP) models proved more effective at full-scale WTP implementations. The speed at which machine learning (ML) models can be trained is particularly advantageous in dynamic treatment settings, facilitating quicker adjustments in coagulant dosing. In this context, Extreme Learning Machine (ELM) algorithms demonstrated faster training and better adaptability than Backpropagation Neural Networks (BPN). Most ML-based models have been developed using data gathered between 1997 and 2021 across a range of environmental conditions and operational uncertainties. With sufficient historical data, it is feasible to create comprehensive and resilient models for accurate coagulant dosing and effluent quality forecasting. Moving forward, research should focus on compiling and structuring such datasets to enhance C/F process modeling. Although deep learning (DL) techniques have been extensively applied in fields like autonomous driving, digital assistants, sentiment analysis, social networking, and healthcare, their adoption in WTPs remains limited. Nevertheless, DL offers exceptional capabilities in feature extraction and data interpretation, making it a promising tool for modeling C/F processes. For instance, DL-based image recognition frameworks could potentially be developed to correlate floc morphology with coagulant dosing or effluent water quality parameters. However, one of the key obstacles to implementing DL in WTPs is the scarcity of long-term, high-frequency datasets necessary for robust time-series modeling. Despite this, AI applications—particularly ML—have significantly enhanced the ability to predict coagulant requirements and effluent quality compared to traditional jar testing methods. These approaches have led to better process optimization and reduced operational costs (Malzer and Strugholtz, 2008). Moreover, the integration of AI into online control systems has improved the responsiveness and ease of managing C/F processes in WTPs.

Conclusions

This review examined literature published between 1997 and 2022 on the application of artificial intelligence (AI) methods in water treatment processes (WTPs), with many studies focusing on the coagulation/flocculation stage and the prediction of optimal coagulant dosages. AI models have demonstrated notable improvements in forecasting coagulant demand, membrane filtration behavior (including flux, fouling, and rejection), formation of disinfection byproducts (DBPs), heavy metal removal, and overall pollution control. Deep learning (DL) approaches, in particular, have shown strong capabilities in extracting relevant features and mining complex datasets. These strengths suggest the potential for DL-based image recognition systems that could map relationships between floc morphology and dosing levels. Hybrid modeling approaches—those that combine various AI methodologies—have generally achieved higher predictive accuracy. These systems are especially effective at modeling intricate, nonlinear interactions such as those seen in coagulant dosing, membrane performance, and adsorption mechanisms. AI tools offer significant advantages in handling complex data patterns that are not easily captured by traditional mathematical frameworks.

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