# Artificial Intelligence in Water Treatment and Monitoring

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Contributor: Matthew Lowe , Ruwen Qin , Xinwei Mao

Artificial-intelligence methods and machine-learning models have demonstrated their ability to optimize, model, and automate critical water- and wastewater-treatment applications, natural-systems monitoring and management, and water-based agriculture such as hydroponics and aquaponics. In addition to providing computer-assisted aid to complex issues surrounding water chemistry and physical/biological processes, artificial intelligence and machine-learning (AI/ML) applications are anticipated to further optimize water-based applications and decrease capital expenses. Poor data management, low explainability, poor model reproducibility and standardization, as well as a lack of academic transparency are all important hurdles to overcome in order to successfully implement these intelligent applications. Recommendations to aid explainability, data management, reproducibility, and model causality are offered in order to overcome these hurdles and continue the successful implementation of these powerful tools.

artificial intelligence | water treatment | machine learning | hydroponics

## 1. Machine-Learning Models, Artificial-Intelligence Methods, and Smart Technology

ML models used in water applications are briefly summarized below. A brief mention of utilized AI methods is also included. A section on smart technologies as defined is included, which are considered the Internet of Things, smart sensors, and systems based on these technologies, and are often integrated with AI/ML models and methods. All of these techniques have been studied for uses in water- and wastewater-treatment processes including chlorination, adsorption and membrane filtration, water-quality management including dissolved oxygen and water level, as well as water-quality-index modeling and/or hydroponics and aquaponics farming.

### 1.1. Machine-Learning Models and Artificial-Intelligence Methods

AI and ML models and methods are briefly summarized. Their general usages, specific usages in water treatment and modeling applications, advantages, and disadvantages are highlighted to aid in the selection of appropriate models and methods for water treatment and monitoring applications. Further published textbook sources that supply the necessary foundational and in-depth explanations of these methods and models are also included in the final column. These water treatment and monitoring applications are not intended to be all-encompassing, but to represent the published journals that were selected based on the methodology explained above. Most of these included ML methods would fit the "black-box" archetype and would be considered a consistent "disadvantage" for many of the models (notably excluding GA/GPs).

### 1.2. Smart Technology—The Internet of Things (IoT) and Smart Sensing Technology

The Internet of Things is a descriptor for a network of physical objects that can connect to the internet (or other communication networks) and that are often endowed with some sort of analytical process (such as environmental sensing) using software, hardware or other technologies. In the context, the IoT in water applications often includes internet-enabled systems equipped with pressure sensors, flow sensors, and/or water-quality/characteristic sensors [1]. The intent is typically to exchange data with other connected devices or networks over the life and duration of the sensor or other technology [2], often for system optimization, transparency or ease of use [3]. The IoT creates a cooperative network of data collection that can be stored locally or offsite without a human ever physically needing to take the data themselves or operate the physical object. As such, the long-lasting function and life of the connected device must be maintained. Though not technically artificial intelligence, the IoT can be fused with AI to create what has been coined as the "Artificial Intelligence of Things", which would marry this data-collection process to feed AI with critical inputs for its learning process [4].

Smart sensing technology can be related to IoT, but often represents a broader breadth of systems that do not need to be defined by their collectiveness and can also include stand-alone or isolated systems/sensors. To achieve the designation of "smart" sensing technology, the sensors must have some function beyond their general sensing abilities [5], which is generally achieved through an actionable decision or automation. For example, a thermostat that both measures the temperature of a room and interfaces with a furnace in order to achieve a set temperature, thus not inherently requiring a connection with other smart devices in the home. The smart designation can be enhanced through the ability to wirelessly interact with other systems through Wi-Fi or Bluetooth capabilities.

## 2. Applications in Water and Wastewater Treatment

Artificial intelligence and machine-learning techniques have been studied in several water- and wastewater-treatment applications. This herein will serve as a cross-section of three common treatment processes employed at water- and wastewater-treatment plants. Much of the input data utilized by the journals were collected and disseminated by treatment-plant staff or other regulatory bodies, relying on traditional collection methods. Using smart-technology integration with the AI methods or ML models, the burden of data collection can be decreased. More data is also likely to increase the accuracy of selected ML models. Ultimately, this is not intended to represent the gamut of research into AI and ML application in the water-treatment industry but rather a representation of current research interest.

AI methods have been demonstrated to be effective in controlling chlorination, while ML models are effective in modeling DBP concentrations, as well as modeling important parameters for adsorption and membrane-filtration processes. The results are often evaluated using various statistical measures including the coefficient of correlation (R), the coefficient of determination ($R^2$), the mean average error (MAE), the mean square error (MSE), the root mean square error (RMSE), and relative error (RE).

## 2.1. Chlorination and Disinfection By-Product Management

Disinfection in a water- and wastewater-treatment plant is the process by which microorganisms and viruses are killed or inactivated, mainly with chlorine-based disinfectants [6]. While chlorination is effective as a disinfectant, it also poses human health hazards [7]. Beyond its ability to cause acute toxicity in humans, chlorine is also known to interact with bromide and organic matter naturally found in water systems to form what is known as disinfection by-products. Disinfection by-products (DBPs) are suspected human carcinogens and reproductive disruptors, and have received increased scrutiny from regulators all over the world [8]. DBPs mainly belong to two larger subcategories: trihalomethanes (THMs) and haloacetic acids (HAAs). THMs are regarded as the most common form of DBPs as their formation is associated with chlorine disinfectants [9]. Haloacetic acids are commonly tested for five or nine common haloacetic acids and are commonly referred to as HAA5 or HAA9. The entire mechanism behind the formation of DBPs in drinking water is not known, making their prediction and mitigation an ideal candidate for ML technologies. When learning has been achieved, mitigation through control using AI methods is possible.

Many researchers performed model testing on surface waters that undergo treatment at drinking-water plants utilizing chlorine as the primary disinfectant, though some studies did involve pre-chlorination peroxide/ozonation. Researchers also noted success in modeling DBP concentrations in the treated water-distribution networks, and directly at consumer homes and taps. Common model inputs include water temperature, pH, chlorine concentration, contact time, and TOC/DOC concentrations. Other successful models have implemented inputs using bromine concentration, $UV_{254}$, algae concentrations, chlorophyll-a concentrations, and DBP-precursor chemical markers.

The most tested ML model used for chlorination and DBP prediction is the ANN, with other applications involving support vector machines, fuzzy inference systems, and genetic algorithms. In comparative studies, ANNs typically outperformed both GAs and SVMs, though there are some cases of SVMs providing a slight advantage when $R^2$ is used as a point of comparison [2][9]. Common DBPs that were modeled and/or predicted include total trihalomethanes (TTHM) and total haloacetic acids (THAA), with some studies focusing on specific DBP compounds including dichloroacetic acid (DCAA), trichloroacetic acid (TCAA), bromochloroacetic acid (BCAA), HAA5, HAA9, trichloromethane (TCM), bromodichloromethane (BDCM) and dibromochloromethane (DBCM). Predictions for TTHMs or THAAs versus their compounds did not differ widely in statistical model-validation numbers.

## 2.2. Adsorption Processes

Adsorption processes are generally regarded as both a physical and chemical treatment option for removing a wide range of contaminants and pollutants in both the water-treatment and wastewater-treatment industries. The process of adsorption involves an exothermic mass-transfer surface process that causes the transfer of some target molecule (or adsorbate) from a fluid to a solid surface (or adsorbent, but also often referred to as the sorptive media in the industry) [10]. Due to the complexity of the interactions that affect the efficacy of an adsorptive process [11], it is often difficult for plants to precisely calculate the important parameters and ultimate removals of the adsorption process. Reducing this complexity would enable a treatment plant to extend a sorptive media's life and increase a treatment plant's effectiveness and confidence that it is effectively treating the water according to any applicable rules and regulations. To further optimize the process, researchers have identified models using ML to make important predictions for the adsorption process. ML for adsorption processes have the potential to support operator decisions.

Studies have been published modeling adsorption processes with water streams contaminated with metals, industrial dyes, and organic compounds. Adsorbent media ranges widely and includes carbonaceous materials and metal-based nanocomposites, among others. Inputs commonly used during ML modeling of adsorption processes include pH, water temperature, adsorbent dose, contact time, and initial adsorbate concentration. Individual models have included inputs utilizing adsorbent particle size, system flow rate, agitation speed, bed height, and BET surface area, among others. Studies that included various organic pollutants operated with varying compound-specific parameters such as target-contaminant molar mass. The majority of the published studies that are included pertained to models with outputs of adsorbate percentage removal (also known as adsorption efficiency), though some models sought to predict adsorption capacity, non-dimensional effluent concentrations, and the relative importance of input water-quality parameters.

For studies including metal, organic, and industrial-dye contaminants, the ANN was the most used ML model. Other models that researchers studied with notable success include ANFIS, SVM, and RF. On average, ANN, SVM, and RF ML models performed adequately, generally achieving $R^2$ values greater than 0.9, and in some cases, greater than 0.99 [12][13]. In most cases, SVM models performed slightly better than ANN models, producing both $R^2$ and RMSE values of better statistical value. In one case, the optimized ANFIS model performed poorly in comparison to other success models for adsorption processes, achieving an $R = 0.813$, and was noted as the worst performing in a comparison between ANN, ANFIS, and SVM models [14], though in another it achieved the adequate performance with an $R^2 = 0.9333$ [15].

## 2.3. Membrane-Filtration Processes

Membrane processes in water and wastewater treatment refer to the separation of contaminants using a barrier or filter. The water is passed through the membrane usually due to high-pressure differentials between one side of the membrane and the other side [16]. The smaller the pore size, the more pressure is required to pass the water through the membrane. Membrane processes are typically used for contaminants that are difficult or costly to remove by chemical or physical means, but also for contaminants that require a high level of removal that simply cannot be achieved by other chemical or physical means [17]. The most used membrane processes are microfiltration, ultrafiltration, nanofiltration, and reverse osmosis.

Researchers have created models that function with microfiltration, ultrafiltration, nanofiltration, and reverse osmosis. A study involving a submerged membrane bioreactor has also been included. Water sources tested using these models include a wide array of pollutants and natural compounds, including petroleum/oil, natural organic matter, various industrial and pharmaceutical wastes, and simple salt/ocean water. Similar to previous sections involving ML in water/wastewater-treatment applications, ANNs are the dominant model used. Other models that have been utilized for membrane-filtration-process modeling include ANFIS, SVM, and specific forms of ANNs including RNNs (some of which utilize LSTM).

ML techniques for modeling membrane-filtration processes seek to output several different variables, commonly including transmembrane pressure, permeate flux, and solute rejection. Inputs that exist in some of these published studies include pH, temperature, contact/filtration time, transmembrane pressure, and flux rate, among many, and more specific, options. Again, due to the range of models testing for different parameters, it is difficult to fully compare the statistical values that many of these studies obtained. Ultimately, ANN, RNN, and SVM models performed adequately well in terms of their respective $R^2$ values, consistently achieving values greater than 0.9, and in many cases, achieving values greater than 0.99 [18][19][20].

## 2.4. Artificial Intelligence in Water Treatment: A Brief Case Study of ANN, SVM, and RF Models for Adsorption-Efficiency Prediction

The published studies conducted by Bhaget et al. ([12]) focused on the prediction of copper-ion removal in an adsorption process relying on attapulgite clay as the primary adsorbent. Three models were developed and compared to determine the optimal form of prediction. These models included an artificial neural network, a support vector machine, and a grid-optimization-based random forest. This conducted by Bhaget et al. was selected due to their in-depth discussion of the construction of their model and their methods for input selection. This ultimately aids in furthering the development of these intelligent models and methods by allowing future researchers to better understand the processes and details of Bhaget et al.'s implementation.

The model inputs for all three intelligent options included initial copper concentration, adsorbent dosage, pH of the water, contact time, and the ionic strength of the solution (upon the addition of $NaNO_3$). Copper-ion concentration was held at a constant level of 50 mg/L to determine the effect the other input variables had on the adsorption efficiency. The adsorbent dosage varied from 2 to 15 g/L, pH varied from 2.0 to 12.0, $NaNO_3$ concentration varied from 0 to 0.5 mol/L, and contact time was evaluated varying from 5 to 120 min.

The models were all developed using open-source software for the programming language R, known for its usage in statistical computation. For training and testing, the dataset was divided into two with 80% used for training and the remaining 20% used for testing. The ANN model consisted of a four-layer model (one input layer, two hidden layers, and one output layer) where the first hidden layer contained five nodes, while the second hidden layer contained three nodes. Each neuron relied on a linear output function. The SVM model was developed using a linear kernel. Finally, the RF model utilized 76 samples to develop decision trees relying on the bootstrapping method (which divides data into several subsets through random replacement, allowing each decision tree in a forest to have its "own" random subset for training purposes [21]).

Tests were run on each model using a varying set of inputs. The input sets included: (1) initial copper concentration; (2) initial copper concentration and adsorbent dosage; (3) initial copper concentration, adsorbent dosage, and contact time; (4) initial copper concentration, adsorbent dosage, contact time, and pH; (5) initial copper concentration, adsorbent dosage, contact time, pH, and $NaNO_3$ concentration. The models were noted to perform best using all five inputs. Ultimately the RF and ANN models were determined to display the best performance in terms of accuracy, achieving correlation coefficients greater than 0.99, while SVM achieved a maximum correlation coefficient of 0.93.

## 3. Applications in Water-Quality Management

Artificial intelligence and machine-learning techniques have been studied in water-quality management. This here will serve as a cross-section of some water-quality-management models including dissolved oxygen, among other water-quality parameters and indices, and river-water-level monitoring.

ML models have been demonstrated to be useful for the prediction and modeling of water-quality-management parameters. The results were commonly evaluated using various statistical measures, potentially including the coefficient of determination ($R^2$), the mean square error (MSE), the root mean square error (RMSE), the normalized root mean square error (NRMSE), the mean absolute percentage error (MAPE), the Nash–Sutcliffe efficiency coefficient (NSE), the Pearson correlation coefficient (PCC) and/or accuracy (ACC).

### 3.1. Water-Quality Management

Water-quality management is an important task necessary for the health and good function of aquatic ecosystems. Often, human activity can hurt the water quality of rivers and other waterways, and tracking this effect is vital to maintaining these ecosystems. A commonly tracked parameter used to discern the health of a river or other waterway is the dissolved-oxygen concentration. Hypoxia (or the lack of dissolved oxygen in waterways) is becoming increasingly prevalent, generally because of increased nutrient loading and global warming [22].

Due to the interactions between dissolved-oxygen (DO) concentrations and human activity/pollution, it is increasingly important to measure DO as a means of predicting, and possibly preventing, hypoxic zones from dealing widespread damage to these aquatic ecosystems. Accurate and real-time results are often most favorable as moderate decreases in DO represent potentially fatal results in certain species [23]. In some cases, DO sensing can be obfuscated by environmental factors, demonstrating a present need for models and methods that can overcome the traditional sensing methods' shortcomings [24].

Common inputs for water-quality modeling using ML include pH, water temperature, and BOD levels. These inputs are also generally the same for water-quality-index (WQI) monitoring and BOD/COD modeling, with the inclusion of dissolved oxygen as an input in the case of the published studies for WQI included, while water-level monitoring relies exclusively on past water levels and robust training data.

While studies modeling aides for water-quality management using ML techniques mainly utilize ANNs, a wide array of other methods have also been studied including ANFIS, RNN, EML, RT, SVM, HW, and hybrid ML models utilizing some of them with RF models. Most studies' models demonstrated accurate predictions, but this is ultimately location dependent. On average, ANFIS models outperformed typical ANN and SVM models in almost all the published studies here and presented, and in some cases were outperformed by hybrid models. Water-level forecasts were accurately predicted using both ANN and ANFIS models, achieving $R^2$ values greater than 0.999 with both models.

## 3.2. Artificial Intelligence in Water-Quality Management: A Brief Case Study of ANFIS and ANN Models for WQI Prediction

ML-based models have been developed to predict the water-quality index for the river Ganga and its tributaries ([25]). Both models (ANN model and ANFIS model) relied on inputs of dissolved-oxygen concentration, pH, BOD, ammonium nitrate concentration, and water temperature. This case will highlight the methods used to achieve the AI models to better understand their construction and relative accuracy compared to one another. The research conducted by Gaya et al. was selected due to their inclusion of the ML models' structure, along with their decision to utilize similar ML models with varying structures to test the effect varying inputs and hidden layers had on model accuracy.

Both the ANN model and the ANFIS model were developed using programming packages within MATLAB R2017b. Both models utilized a dataset of which 70% was employed for training (referred to as calibration) and 30% was used for testing (referred to as validation). The ANN model was a simple three-layer neural network (one input layer, one hidden layer, and one output layer). Input data were normalized from 0 to 1 before being fed to the ANN model. As is commonly used with these models, the ANN model relied on backpropagation, meaning that input training data are fed through the model, passing through the output layer, where training error is propagated backward until the selected level of accuracy is achieved. The models were tested using five different structures that differed for the ANN and ANFIS model. For the ANN model, the structure was varied and included varying numbers of nodes. ANN model 1 (ANN-1) used one input node of dissolved oxygen, one hidden-layer node, and one output node. ANN-2 used two input nodes of dissolved oxygen and pH, two hidden-layer nodes, and one output node. ANN-3 used the previous plus BOD, three hidden-layer nodes, and one output node. ANN-4 used the previous plus ammonium nitrate concentration, four hidden-layer nodes, and one output node. ANN-5 used the previous water temperature, six hidden-layer nodes, and one output node. The best performing ANN model was noted as ANN-2.

The ANFIS models were tested using five different structures with variable input variables and two triangular membership function inputs with constant output. ANFIS model 1 (ANFIS-1) utilized all five input variables. ANFIS-2 utilized four input variables, ANFIS-3 utilized three input variables, ANFIS-4 utilized two input variables, and ANFIS-5 utilized two input variables. Interestingly, the best-performing model was noted as ANFIS-2, but variable combinations were not as readily available for ANFIS models as they were for ANN models. Both ANN and ANFIS models were noted for their relative success in predicting actual WQIs, achieving high determination coefficients greater than 0.99.

# 4. Applications in Water-Based Agriculture

Smart technology in conjunction with artificial intelligence and machine-learning methods has garnered interest in some sectors of the research community. This herein will serve as a cross-section of two water-based agricultural methods: hydroponics and aquaponics. Smart technology both coupled with and independent of AI methods and ML models (referred to below as “Smart Systems”) has been demonstrated to be effective in automating and monitoring the growth process and health of these water-based agricultural systems. The results are evaluated using various statistical methods including the system accuracy, the coefficient of determination ($R^2$), the mean average error (MAE), the false-positive rate (FPR), and the system error (Err).

## 4.1. Hydroponics and Aquaponics

Hydroponic farming and hydroponic systems are methods of plant cultivation that do not use soil. Plants are grown in (an often specifically tailored) nutrient solution that provides the plant with all its nutrient and water needs. While this is a far more technical form of cultivation compared to traditional farming, hydroponics has the distinct advantage of producing higher crop yields, with greater plant density in significantly less space and with lower average water usage [26]. Crops are grown suspended in a tailored nutrient solution that must also be kept at the proper pH for growing, and the growing rooms must be kept at the proper humidity and temperature [27]. Nutrient solutions are typically stored in separate tanks and are delivered to the crops utilizing a pump and pipe network.

Aquaponics is like hydroponics and is often considered a subset of hydroponic farming. Plants are still typically grown without the use of soils, but instead of relying on a tailored solution for nutrients, a more sustainable cycle is employed [28]. In aquaponic systems, plants receive their nutrients from the by-products of fish (typically fecal matter) stored in adjacent (or near-adjacent) tanks and connected through a pump and pipe network. In return, the crops often act as water purifiers for the fish through the removal of their by-products and fecal matter [29]. It is often a difficult process for cultivators to maintain and optimize hydroponic and aquaponic setups. Thus, researchers have been looking into artificial-intelligence models and have been more commonly using smart technology to help ease some of the burdens of controlling a hydro/aquaponics system.

For the purposes, AI methods, ML models, and smart applications used in the hydro and aquaponic studies are presented and referred to as “Intelligent Models, Methods and Technology”. In contrast to other sections presented, many of the applications involve control and monitoring using smart and/or internet-enabled devices, often using the IoT. Some of the included research do not rely on a proper IoT, and instead use smart sensors (that may have internet functionality) for control and automation. Like more traditional forms of AI and ML, these setups rely on the use of critical inputs for information monitoring and system action. Common aqua and hydroponic sensor data include pH, water temperature, air temperature, humidity, nutrient/plant height (often measured using an ultrasonic sensor), and electrical conductivity (which is meant to be analogous to nutrient loading). Other aquaponic-specific inputs include total dissolved solids and ammonia concentration.

In studies where IoT or smart sensing is utilized for monitoring system health and automation, outputs are commonly related to nutrient-pump feeding, humidity, temperature controls, pH control, and light control. To achieve these levels of automation, these IoT systems can be paired with AI methods and ML models, such as FIS or ANN. These systems are also paired with central control/processing units (though due to the scale of many of these studies, they are often technically considered microprocessors).

Arduino-based controllers are the most popular among the applicable published papers. Studies indicate that there has also been some success in implementing ML models for crop harvestability, crop height, fish weight, and nutrient solution constituent concentrations. These outcomes have been achieved using k-NN, SVM, and ANN. Studies integrating the models and smart technology have noted positive plant growth compared to traditional methods and have allowed operators to employ remote-monitoring techniques.

## 4.2. Smart Technology and Artificial Intelligence in Water-Based Agriculture: A Brief Case Study of IoT and FIS in Aquaponics

The published research conducted by Rozie et al. ([30]) implemented the IoT and an FIS using internet-connected sensors and data-connected rules and membership. The research conducted by Rozie et al. was included for its in-depth explanation and inclusion of the necessary sensors and tools to create an IoT network and a functioning automatic system using an AI method. Their clear explanation of the membership functions used to create their FIS is also an important reason why this case was selected. Ultimately, these inclusions and explanations will aid future researchers in reproducing the results presented below while also maintaining confidence in the knowledge that the system was sufficiently explained.

The IoT-based sensors captured data relating to pH, temperature, turbidity, dissolved oxygen, total dissolved solids, ammonia concentration, and water level while relying on them for a cloud-based storage system. Data were stored in various formats (CSV, excel, pdf, and images) with the intention of being used for creating a timeseries for the study and long-term observation of aquaponics processes and variables. Two of the aforementioned datasets, namely temperature and ammonia concentration, were additionally utilized for automation and control using the FIS.

Fuzzification of the data for the FIS was achieved using three membership functions: namely a temperature function with defined “cold”, “good”, “warm” and “hot” variables, an ammonia function with defined “safe”, “warning”, and “toxic” variables, and a motor-speed function with “slow”, “normal” and “quick” variables. The temperature and ammonia-concentration variables were defined using experience and knowledge derived from the Indonesian National Standards Agency. The motor-speed function was used to control the temperature and ammonia concentration by introducing clean and appropriate temperature water to the system. For example, when the membership function for temperature indicates “hot” and the membership function for ammonia concentration indicates “toxic”, the input for the motor-speed membership function would result in an output of “quick”, thereby quickly introducing freshwater to the system to cool water temperatures and dilute ammonia levels. All data were simultaneously recorded and uploaded to a web-application-based user interface and a TelegramBot live-chat feature to aid in remote control and monitoring of the system.

Utilizing the FIS, Rozie et al. were able to achieve acceptable temperature cooling in approximately 2 h versus the 3.5 h that a non-controlled system would naturally take to cool using fixed motor speeds. Ammonia control was also achieved and able to decrease ammonia levels from 0.19 ppm at its peak to approximately 0.04 ppm without direct human intervention. System updates directly to human monitors for other variable inputs recorded were sent to users within 3 s of appreciable changes.

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