Review article

A comprehensive review on modelling the adsorption process for heavy metal removal from waste water using artificial neural network technique

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ABSTRACT

Water is the most necessary and significant element for all life on earth. Unfortunately, the quality of the water resources is constantly declining as a result of population development, industry, and civilization progress. Due to their extreme toxicity, heavy metals removal from water has drawn researchers' attention. A lot of scientific applications use artificial neural networks (ANNs) because of their excellent ability to map nonlinear relationships. ANNs shown excellent modelling capabilities for the water treatment remediation. The adsorption process uses a variety of variables, making the interaction between them nonlinear. Selecting the best technique can produce excellent results; the adsorption approach for removing heavy metals is highly effective. Different studies show that the ANNs modelling approach can accurately forecast the adsorbed heavy metals and other contaminants in order to remove them.

1. Introduction

Researchers have been driven to investigate and create effective and clean water treatment methods by the ongoing flow of new inorganic pollutants into natural aquatic systems [1–3]. These wastewaters contain a variety of contaminants, each with unique characteristics and concentrations depending on where they came from. Before releasing treated wastewater into aquatic systems or soil, it is crucial to carefully choose and combine wastewater treatment procedures and methods [4,5]. Even at extremely low

concentrations, the majority of heavy metals are harmful to human health and the environment [5,6], even though they are normally present in minute amounts in natural waterways [7].

In all industries of electroplating process including conversion coating, milling, etching, cleaning, by anodization and electrolysis deposition, heavy metal ions may be produced, as shown in Fig. 1 [8]. Lead (Pb), zinc (Zn), copper (Cu), arsenic (As), cadmium (Cd), chromium (Cr), nickel (Ni), and mercury (Hg) are the heavy metals from diverse sectors that are most concerning [9–11].

Heavy metals have a negative impact on human health, including problems with nervous system function and growth and development. The maximum contamination level (MCL) limitations and toxicity caused by the emission of heavy metals were determined by the United States Environmental Protection Agency (USEPA), and are described in Table 1 [8,12]. In order to remove them from the environment, effective wastewater treatment is needed (Fig. 1).

Chemical precipitation [13], ion exchange [14], chemical oxidation [15], reverse osmosis [16], ultrafiltration [17], electrodialysis [18], electrocoagulation [19] and adsorption [20,21] are a few of the physical and chemical techniques used to remove heavy metals. Adsorption is the most effective strategy out of these because the others have built-in drawbacks including producing a lot of sludge, being inefficient, needing delicate working conditions, and being expensive to dispose of. Due to its reversibility, high-quality treated effluent, flexibility in design, and ability to regenerate the adsorbent, the adsorption approach is emerging as a potentially preferred alternative for the removal of heavy metals [22–24].

Alternatives to improve the simulation of adsorption processes for water treatment include artificial intelligence-based models. This sort of model's contribution to improving correlations and estimates of the adsorption of inorganic and organic adsorbates in single and multicomponent solutions has been acknowledged by a number of authors [25,26].

Over the past few decades, the use of artificial neural networks in adsorption modelling has grown dramatically. In the context of water purification, these artificial intelligence models have been used to correlate and forecast the kinetics, isotherms, and breakthrough curves of a broad range of adsorbents and adsorbates. Traditional adsorption models have significant shortcomings that artificial neural networks can address, especially when it comes to making better predictions under various operating situations. It is important to expand the use of these surrogate models for the prediction and modelling of adsorption systems with several adsorbates, or multicomponent adsorption, as they have mostly been applied to adsorption systems with only one pollutant [27].
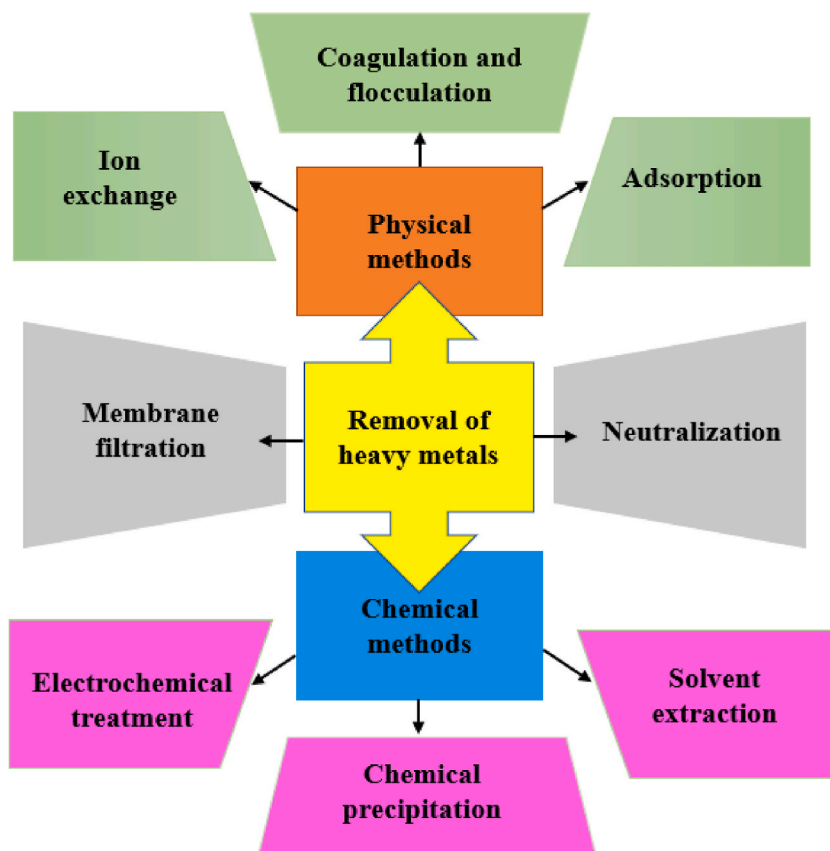

Fig. 1. Chemical and physical methods of heavy metal ions removal.

Table 1
Maximum contaminant level standers for the most hazardous heavy metals [8,12].

No.	Heavy metals	MCL standard (mg/l)	Toxicity effects
1	Arsenic (As)	0.05	Skin manifestations, vascular illness and visceral cancers
2	Chromium (Cr)	0.05	Nausea, Headache, diarrhea, vomiting and carcinogenic material
3	Cadmium (Cd)	0.01	Damage of Kidney, renal failure and human carcinogenic
4	Nickle (Ni)	0.2	Derma allergy, nausea, chronic asthma, cough, human Carcinogenic
5	Zinc (Zn)	0.8	Depression, lethargy, neurological signs and heavy thirst
6	Lead (Pb)	0.06	fetal brain damage, kidney diseases, circulatory and nervous systems
7	Copper (Cu)	0.25	Liver damage, Wilson illness and inability to sleep

2. Introduction of artificial neural networks

A system identification technique called an artificial neural network (ANN) can be used to explore phenomena that don't lend themselves to analytical modelling. In an effort to comprehend the human brain and mimic its functions, the creation of (ANNs) began in 1943 [28].

Lately, there has been great resurgence in the development of complex algorithms used as tool for computation. Numerous researches discussed the potential of (ANNs) as a tool for computing, representing, and acquiring a mapping from one input to another [29–31]. The ANN is regarded as an approximator in science, with the ability to find relationships in given data sets; it is likely that (ANNs) will be able to address challenging issues including nonlinear modelling, pattern recognition, association, and classification. McCulloch and Pitts (1943) proposed the (ANNs) concept, and Hopfield et al. (1982) [32] developed the (ANNs) development method. Since David et al. (1987) [33] rediscovered a rigorous mathematical framework like the back-propagation algorithm, there has been a significant increase in interest in computational machines. As a result, (ANNs) have been applied in a wide range of fields, including physics, finance, neurophysiology, robotics, image processing, and computer and electrical engineering [34]. Numerous chemical engineering applications have made use of ANN [35].

A variety of alloy and process design, materials specifications, and process control conditions utilized the (ANNs) technique [36]. The neural network's functionality and effectiveness are influenced by its structure, input and output normalization, data format, and appropriate activation function [37].

Neural network construction based on certain principles, for example the fact of processing information takes place at nodes, also referred to as neurons, and that every artificial neuron is a unitary computational processor with a summing junction operator and a transfer function. Fig. 2 shows the structure of an artificial neuron (node), and the parameters of the neural network weights and biases are used to connect inputs, neurons, and outputs [38].

Neural network characterization depends on its structural features, which show the node connections, activation function, and connection weighting scheme [39]. The conventional neural network topology consists of a large number of nodes arranged in a predetermined pattern. Additionally, the categorization of ANNs may be based on the direction of information flow during processing, as nodes in a feedforward network are oriented from the input layer to the output layer [40].
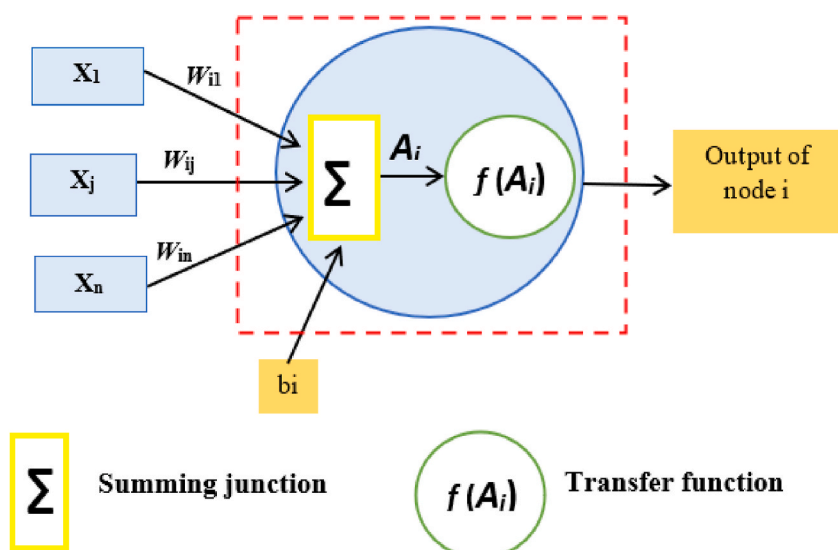

Fig. 2. The structure of an artificial neuron (node) [35].

The weights and bias are combined into a net input Ai, often referred to as an argument, via the summing junction operator of a single neuron *(i)*. W_{ij} is the connection weight, X_j is the input variable, *i* and *j* are the integer indices, *n* is No. of the input variables, and bi denotes to single artificial neuron bias. The net argument Ai is transformed into the scalar output by the transfer function of a single neuron (i).

In Table 2, the explicit connection for the summing junction operator and the types of transfer functions often used for multiple regression issues are given for a single artificial neuron. The three transfer functions that are most typically used to handle multiple regression issues are the linear transfer function (purelin), the log-sigmoid transfer function (logsig), and the hyperbolic tangent sigmoid transfer function (tansig) as shown in Fig. 3 [26,27,32].

The back-propagation network and the radial-basis-function network are the two network architectures that are most frequently employed for classification issues. There are a number of additional neural network types for classification networks, including probabilistic, fuzzy artmap, learning-vector-quantization (LVQ), and others [41]. The backpropagation network (BPN), a multilayer feed-forward neural network based on error reverse spread, is one of the most developed and commonly used ANN types. Back-propagation networks or its variant forms are used in up to 80% of neural network models, which is statistically significant [41]. Computing the partial derivatives of the function with respect to any bias or weight in the network is the aim of backpropagation.

A BPN has no connections to neurons in the same layer and at least three layers: an input layer, a hidden layer (implicit layer), and an output layer. The input layer distributes and collects inputs. The nonlinear relationship between the inputs and outputs is captured by the hidden layer. The calculated results are produced by the output layer. The back-propagation method suggested in Ref. [9]serves as the foundation for the development of the BPN. The objective of the network training process is to modify weights. Network training is an unconstrained nonlinear minimization problem [42]. Theoretically, every function with a finite number of discontinuities can be approximated by networks with biases, a sigmoid layer, and a linear output layer [13]. Fig. 4 [41] shows a hierarchical feed forward BPN frame.

In order to implement the back-propagation (BP) process, the input data must first be provided to the network with estimated errors, then the sensitivity being propagate from the output to the input layer, and both biases and masses values were adjusted [43]. This approach has considered to be effective in modelling applications, where the necessary estimated properties provided as inputs to a wide range of algorithms [44]. The MSE is used to optimize the training phase's epochs and neuron counts in order to enhance network performance. The network weights are chosen at random; choosing the right ones during training is crucial for reducing the error that have been estimated. There is typically no single technique for providing an exhaustive initial estimate of training set examples without beforehand knowing the convergence and outcomes of the setting training process; as a result, a variety of training methods using a variety of data should be used at first for the algorithm validation. The information that characterizes the behavior throughout the array of inputs and outputs must be included in the training set. The trained neural networks need to simplification the involved response in the training set. Afterward, making comparison between the trained and untrained verification data in the full range with the trained and untrained network's output.

There are two training approaches: supervised and unsupervised, and they apply to both classification and regression. By adjusting the weight values between the connections to predict an output's value, the network is trained using the supervised approach (s). While there are no target outputs from the taught inputs in the unsupervised training approach [45].

3. ANN applications

The use of neural network techniques in numerous scientific fields is well known. The basis radial function of (RBFNN), NARX-NN, ANFIS, and GRNN are only a few examples of the several ANN versions that have been employed in the solar research community, according to Yadev and Zhang's comprehensive analysis of solar radiation modelling [5,46,47].

Removal based on Humic acid optimization (HA) from municipal solid waste biochar was studied by Genuino et al. (2017) using the ANN, along with the effects of precipitant volume, extractant dose, KOH solution concentration, and contact time [8]. In the case of membrane processes [48], oxidation processes (AOPs) [49], ANN approaches were successfully used for optimization and prediction. The refined palm oil process was improved and forecasted by Tehlah et al. (2016) using two ANN forms. Inputs parameters for the first model were pressure (P), column temperature (T), and flow rate of feed (F), whereas for the second one, only pressure (P) and column temperature (T) were needed (T) [13]. For twin-screw extruder modelling, Shirazian et al. (2017) used ANNs. Various configurations of ANN have been used with a various hidden layer counts, types of activation function, and node counts to find the ideal conditions for an effective prediction model [50]. In order to determine the electricity consumption for the intelligent building that requires constant monitoring, Pombeiro et al. (2017) used ANN techniques. Several parameters were taken into account in the system modelling including the occupancy that calculated using WiFi traffic, weather, and time of day [51]. Using the ANNs technique, it was possible to

Table 2
Transfer functions of artificial neurons used for solving multiple regression problems.

Descriptions	Notation	Transfer function equations
linear transfer function	*purelin*	$f(A_i) = A_i$
Log-sigmoid transfer function	*logsig*	$f(A_i) = \dfrac{1}{1 + e^{-Ai}}$
Hyperbolic tangent sigmoid transfer function	*tansig*	$f(A_i) = \dfrac{1 - e^{-Ai}}{1 + e^{-Ai}}$

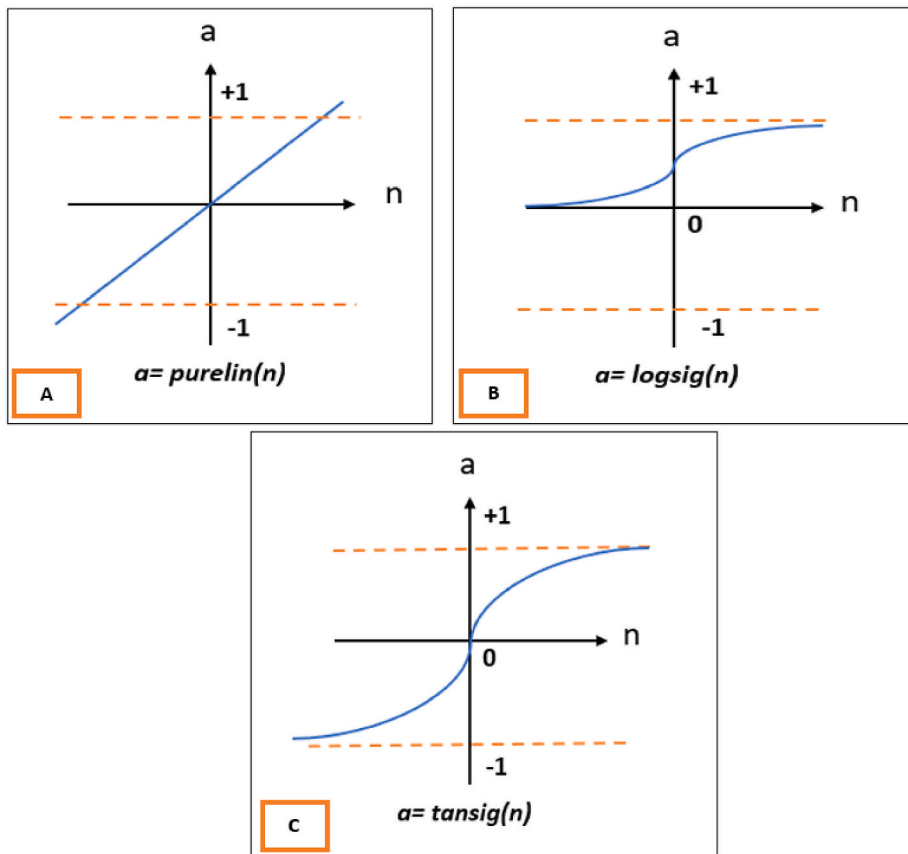**Fig. 3.** The most used transfer functions to solve multiple regression problems, A: *purelin*, B: *logsig* and C: *tansig*.

X : input variables   *Y : Output variables*   (*w*): Weights

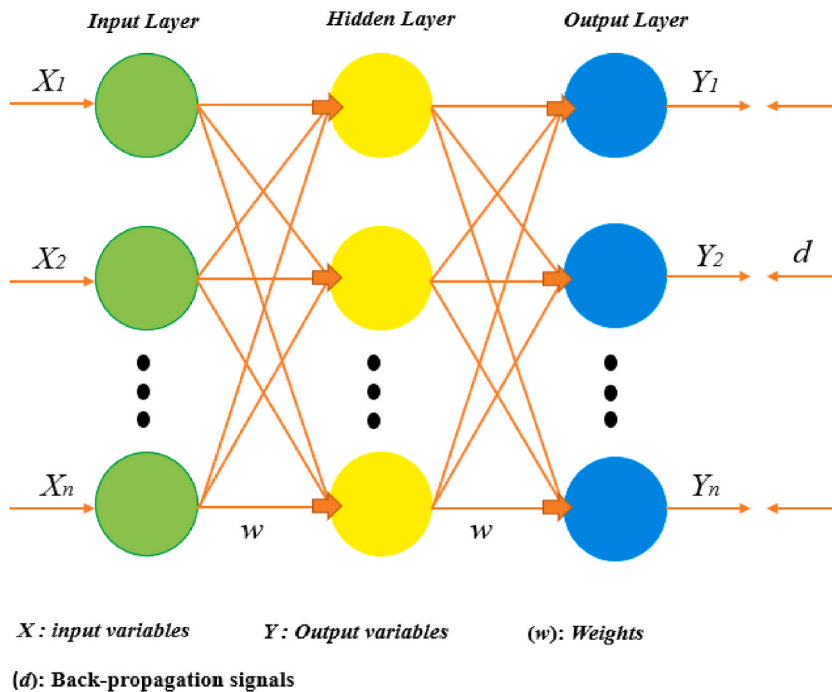(*d*): **Back-propagation signals**

Fig. 4. General structure of Back-propagation network (BPN).

forecast the wellhead choke liquid critical-flow rates as a function of the gas-liquid ratio, choke size, and wellhead pressure. Other parameters included in the modelling system were temperature, specific gravity of oil and gas [52].

Concrete characteristics were also predicted using conventional aggregate and ANN modelling techniques [22,53–56]. However, some research has been done using recycled aggregate and the ANNs technique to simulate the compressive strength of concrete [57]. In order to train, validate, and analyze the ANNs model, cone penetration test (CPT) data were used. This model was then used to characterize the behaviour of pile settling [58]. In this study by Hamad et al., 16 feed-forward back-propagation of ANN models were created and used in the modelling of 240 data sets (2017). Roadway temperature, speed in average, categorization, volume of traffic, and levelling the noise were the variables included in the model [59].

The pure refrigerants surface tension [60], pore structure of carbon aerogels [61], the heat reflux extraction [62], the TiO_2 reinforced composites and Nano TiB_2 [63], the ultrasound-assisted bleaching of olive oil [64], the solar system [65], the MgO/oil nano-lubricants [66], and the characterization of wave resource [67] are some other fields in which researchers have used artificial neural networks for modelling. Additionally, Table 3 presents the artificial neural network used in numerous scientific fields.

4. ANNs and remediation of waste water treatment

The development of the empirical model is approximated mathematically using artificial neural networks (ANNs). Kim et al. (2015) created a model employing ANN techniques studying total nitrogen (TN), total phosphorus (TP) concentrations, dissolved oxygen (DO), and pH to assess the quality of water bodies to have a reasonable accurate results [73]. The mean value prediction of four variables related to water quality using the ANN algorithm to show that the ANN technique surely cannot give the best outcome without choosing the proper methodology. Additionally, the results showed that the best single ANN model has a lesser capacity for generalization than the ensemble ANN model [74]. The multilayer perceptron (MLP) ANN technique was used by Vakili et al. (2016) to estimate the thermal conductivity of graphene nanofluids. The prediction results demonstrate the great precision and certainty of the ANN model [75]. Shetty et al. (2003) described how to estimate membrane fouling for drinking water nanofiltration using the ANN approach. The ANN inputs included physical and independent factors like flow rate and water quality parameters including total soluble solids (TDS), UV_{254}, and pH [76,77].

Furthermore, ANN was used to predict the wastewater separation percentage (SP) from the wastewater using membrane distillation (MD), with voltage, flow rate, and temperature being the key process variables [78–80]. For prediction of SP and ED cell current efficiency (CE), the number of nodes and hidden layers that work best is (4:6:2:1) [81]. Additionally, the electrodialysis (ED) cell was utilized as an adsorbent to demonstrate the removal of lead ions from water utilizing the voltage, flow rate, temperature, and lead ions concentration as the input variables for the ANN [82]. In the assessment of the Fenton process performance in landfill leachate treatment, three objectives were utilized to cover a variety of post-treatment product parameters, including mass removal efficiency (MRE), sludge and supernatant, and mass content ratio (MCR).The average error (AE), correlation coefficient (R2), and root mean square error (RMSE) were provided for the model evaluation, and the ANN model demonstrated a satisfactory result [83]. The most common mechanism for all reactions was found to be coagulation. The process parameters in a study by Won et al. (2016) that employed the ANN to evaluate the water quality at the Cheongpyeong dam downstream included chlorophyll-a, turbidity, TP, TN, electric conductivity, pH, DO, and temperature.

ANNs aims to lessen stochastic component, periodicity, and trend effects. The stratified sampling method was utilized to improve the performance of ANN models [84,85]. A water bloom model was created using the ANN system in order to prevent erupting water blooms, adopt emergency response measures, and provide a technical foundation for bettering the lake and river environmental systems [80]. The Danube River's dissolved oxygen (DO) was predicted using ANN applications. Water quality parameters were monitored in 1912, and the data were split into two sets: an extreme set with monitoring records of outlier levels and a regular set with minimal variability and normally distributed data. It is well recognized that the phosphorus dosage, pH biological oxygen demand (BOD), and temperature have a major impact on the dissolved oxygen level [86,87].

Hong et al. (2018) developed a reliable model for estimating the accumulation of heavy metals in urban roads using the ANN model technique. The distribution of heavy metal loading and the hazard of an extensive ecological map have been created as a result of the findings. The resulting maps can serve as a foundation for prioritizing the locations where safe storm water can be reused, and they can also be utilized as a tool for urban land use planning in storm context [88]. The next section reviews a few of these studies. The

Table 3
The application involved ANNs.

Application	Algorithm	Remarks	Ref.
Wireless sensor networks (WSN)	Adaptive neural fuzzy inference system	The model outperforms measurement accuracy in different environments conditions.	[68]
Enhancer regions	Recurrent neural network (RNN)	The produced model detailed information on the histone profiles contribute to putative enhancers presence.	[69]
Fetal state from the cardiotocogram	ANFIS	The ANFIS topology multi-layer with large input features was tested by hardware and software restrictions.	[70]
Phosphate concentrate grade	Feed forward neural network (FFNN)	The BP model achieve a prediction results with an error of less than 5%.	[71]
Elbow joint motion	Feed forward neural network	The set up dynamic model is appropriate for concentrating on the elbow joint movement qualities under electrical incitement.	[72]

adsorption techniques of heavy metals considered one of the many applications of the ANN modelling system. Different water treatment procedures are modelled using ANNs; a number of these procedures are included in Table 4.

5. ANN technique and adsorption process

The technique of ANN considered an appropriate for predicting the experimental data of patterns in water pollution treatment, such as the adsorption technique's removal of dyes from water solutions [94]. Utilizing Penicillium YW 101 biomass as an adsorbent, dye compounds were removed. The significance of process variables such as initial concentration, contact time, temperature, and pH was examined [95]. Adsorbent parameters such as primary dye concentration, solution pH, adsorption period, and adsorbent dosage were evaluated for the amido Black 10B removal from aqueous solution using the adsorption approach, and the ANN technique was employed for optimization [96]. Pistachio (Pistacia Vera L.) shells from Antep have been used as an adsorbent to remove Pb^{+2} from aqueous solutions using a determined approach of adsorption. Yetilmezsoy et al. (2008) constructed an ANN model to determine best conditions for Pb^{+2} ion removal, the impacts of operational parameters such as contact duration, temperature, beginning pH, Pb^{+2} initial concentration, and adsorbent dosage were examined [97,98]. Furthermore, black cumin was used as an adsorbent of lead ions, and the ANN technique has been used to model and evaluate the biosorption of heavy metals. Temperature, biosorbent mass, and pH were among the process variables whose effects were examined [99]. Yasin et al. (2014) created an eco-friendly environment for pb^{+2} removal from solutions in order to optimize and simulate the lead ions. As a lead absorber, tartrate-Mg-Al layered double hydroxides were applied. Levenberg-Marquardt (LM) algorithm was used to train the ANN model, utilizing lead ion concentration, adsorbent dosage, solution pH, and contact time as model inputs [100].

The application of the ANN approach to model the removal of zinc ions (Zn^{+2}) from leachate showed excellent accuracy. Hazelnut shell was used as the adsorbent by Turan et al. (2011) in the development of an ANN model for the removal of (Zn^{+2}) ions. It was important to investigate the impacts of operation factors such as temperature, operation time, adsorbent loading, and pH in order to reach the highest condition for (Zn^{+2}) ions adsorption. The ANN model is capable of properly forecasting the zinc elimination, as shown by the coefficient of correlation ($R^2 = 0.99$) when the experimental and ANN model data were compared [101]. A second study was presented on the removal of Cu^{+2} from water, and the impacts of important variables like contact time, adsorbent dosage, pH, and temperature were examined. The amount of Cu^{+2} extracted from water was calculated using the ANN technique. The first model included a three-layer structure with 8 neurons in the second layer and 4 neurons in each of the first and third layers. Additionally, the accuracy of the radial basis function (RBF) was evaluated in comparison to other network types. The ANN model had a high level of accuracy, as evidenced by its coefficient of correlation (R2 = 0.999) [102]. The ANN was also used by other researchers to create a model that predicts the removal of copper ions using discarded flax meal as an adsorbent [103]. Esfahani et al. (2015) conducted a batch experiment and employed the ANN modelling method to accurately predict the experimental data for chromium with an R2 value of 0.9803 [104]. Naked ZVIN and S-ZVIN were to simulate the exclusion of chromium from water and evaluate their efficiency. A second study was carried out to obtain the best variable values for the most effective disposal of heavy metal ions Pb^{+2} and Cu^{+2} by rice straw powder. The root mean squared error (RMSE) was employed as a gauge to determine the model topology [105].

The input variables employed in Khajeh et al. (2017) research for cobalt and manganese ions removal by using tea waste were the eluent flow rates, eluent concentration, eluent volume, concentration of PAN (complexing agent), the concentration of tea waste quantity, and pH [106]. Hamid et al. (2016) used surface-oxidized cellulose nanowhiskers (CNWs) as a Cu+2 absorber and studied the effects of sorbent dosage, Cu+2 ion concentration, and temperature on the removal of Cu+2 from water. The redesigned CNWs have higher surface area per unit mass than the original CNWs, according to this study. the construction and improvement of a prediction model for the ANN system-based evaluation of Cu+2 performance. Among the measures utilized to assess the ANN model were the absolute average deviation (AAD), the determination coefficient (R2), and the root mean squared error (RMSE) [107].

The impacts of various operating parameters, such as contact time, adsorbent dosages, Pb^{+2} ion concentration, and pH of solution, were investigated when using six different bio-sorbents to remove Pb^{+2} ions from water. To demonstrate the viability of ANN, three training methods—Scaled Conjugate Gradient, Levenberg-Marquardt, and Backpropagation—each had a different transmission role in the hidden layer and a linear transfer function at the output layer [108]. An effective tool for analyzing and simulating systems whose interest response varies on a wide range of variables and where the link between dependent and independent system components is unknown is the artificial neural network (ANN). In recent years, the ANN has been successfully used for metals biosorption [109–111]. Recent studies have used several neural network methods to predict the adsorption process for removing pollutants using various adsorbents. Some of these studies are shown in Table 5.

6. Conclusion

The use of artificial neural networks (ANNs) is considered as a valuable modelling tool for addressing and mapping the environmental concerns, particularly in the field of water treatment. The increased ability of processes modelling to remove of hazardous contaminants, especially heavy metals that has a significant effect on human health. This study has concentrated on: (a) the background and capabilities of artificial neural networks; (b) the application of ANNs to science; (c) ANNs and water treatment remediation; and (d) ANN and adsorption. In comparison to the commonly used traditional modelling techniques, ANNs modelling method demonstrated its high capacity to represent the adsorption system using different adsorbents with a significant deal of efficiency. This study revealed that ANNs were highly effective at simulating the adsorption system for heavy metal removal from water using different adsorbents.

Table 4

The methods modelled using ANNs technique for water treatment.

Prediction	Algorithm	Remarks	Ref.
Water allocation trade prices	Artificial Neural Network-Bayesian	The model accuracy (RBASIC = 0.93, RFULL = 0.99 and RINTER. = 0.96).	[89]
Bathing water quality	Feedforward neural network	The computational forecasting costs are decreased by the neural networks comparing to the process-based model.	[90]
Oil–water two-phase flow	Feedforward neural network	modelling of the experimental results used the deep neural network algorithm.	[91]
Chemical and physical parameters	Feedforward neural network	Presented equations and models are reliable tools for water quality parameters investigation.	[92]
Oxidant demand	Feedforward neural network	The designated architecture consisted of a feed-forward perceptron with four inputs and one hidden layer are applied.	[93]

Table 5

The artificial neural network use for modelling the adsorption system.

Adsorbent	Algorithm	Pollutant	Remarks	Ref.
Biochar	Forward Back Propagation	(Cd^{2+}), nickel (Ni^{2+}), zinc (Zn^{2+}) and copper (Cu^{2+}) ions	The ANN model presented the lowest errors for the adsorption breakthrough curves.	[112]
Poly-luminium	Feed forward back Propagation	Dye	This study presented that the optimizing and predicting of the colour removal.	[113]
polyaniline nano-adsorbent	Feed forward back propagation neural network	Methyl orange	The optimum architecture of ANN model is 5-12-1 presented an R^2 of 0.9475.	[114]
activated carbon	adaptive neuro-fuzzy interference system (ANFIS)	nickel	The developed ANFIS and ANN models are able to predict the experimental outcomes with R^2 of 0.9943and 0.9926, respectively.	[115]
Functionalized carbon nanotubes	Feed-forward back propagation and Layer recurrent and ANFIS	Lead	The ANN model presented a MSE of 1.66 10^{-4} and R^2 of 0.9956	[116, 117]
Functionalized carbon nanotubes	NARX neural network and Feed-forward back propagation	Arsenic	The NARX model results revel that the NARX model is capable to estimate the arsenic ions elimination from water using the functionalized CNTs as adsorbent.	[118, 119]
Functionalized carbon nanotubes	NARX neural network	Mercury	The maximum RE was 3.49%, R^2 of 0.9998 and MSE of 4.28 × 10^{-6}.	[120]

Author contribution statement

All authors listed have significantly contributed to the development and the writing of this article.

Data availability statement

Data will be made available on request.

Acknowledgment

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