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Review

Development of artificial intelligence for modeling wastewater heavy metal removal: State of the art, application assessment and possible future research

Suraj Kumar Bhagat**, Tran Minh Tung, Zaher Mundher Yaseen*

Faculty of Civil Engineering, Ton Duc Thang University, Ho Chi Minh City, Viet Nam

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A B S T R A C T

The presence of various forms of heavy metals (HMs) (e.g., Cu, Cd, Pb, Zn, Cr, Ni, As, Co, Hg, Fe, Mn, Sb, and Ce) in water bodies and sediment has been increasing due to industrial and agricultural runoff. HM removal in nature is highly stochastic, nonlinear, nonstationary, and redundant. Over the last two decades, the implementation of artificial intelligence (AI) models for HM removal has been massively conducted. The divergence in the selection of predictors, target variables, the optimization, normalization of the algorithm, function, and architecture of AI models are time-consuming processes, which limit the optimal use of such models for HM removal simulation. The selection of sustainable, cost-efficient, and user-friendly treatment techniques that have minimal reverse impact on the ecosystem is immensely challenging. The focus of the established researches is to find an optimal AI models for specific removal techniques. Predictors and target variables can be sorted using several techniques, and the selection of algorithm, function, and architecture based on individual treatment techniques have been coherently ordered and argued. In this review, each element of the predictive models and their corresponding treatment processes, including its pros and cons, are discussed thoroughly. The performance matrices are also discussed in accordance with the behavior of each model. Moreover, multiple perspectives that can enlighten interested multi-domain scientists and scholars, such as AI model developers, data scientists, wastewater treatment researchers, and environmental policymakers, on the actual status of the models' progression are summarized. A comprehensive gap and assessments are also conducted to provide an insightful vision on this topic. Finally, several research directions, which could bridge the gap in the same domain are proposed and recommended on the basis of the identified research limitations.

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* Corresponding author.
** Corresponding author.
E-mail addresses: 186204003@student.tdtu.edu.vn (S.K. Bhagat), yaseen@tdtu.edu.vn (Z.M. Yaseen).

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1. Introduction

As reported by the World Health Organization (WHO), the entire ecosystem and human health are threatened by serious exposure to heavy metals (HMs) (Enochs et al., 1994; Jaishankar et al., 2014; Järup, 2003). The serious point is that the majority of the popular HMs reported with increasing trends in water bodies except Pb and Zn within 1970–2017 periods (Li et al., 2019). Recently, most HMs, such as Cr, Mn, Co, Ni, As, and Cd, in water bodies have been reported to have exceeded the permissible limits set by the WHO and United States Environmental Protection Agency (USEPA); the statistics of popular HM concentration in surface water bodies are listed in Table 1 (Kumar et al., 2019). These data reveal the point of attraction by esteemed researchers who contribute to research on HM removal techniques. Environmental science and engineering researchers work tirelessly to minimize the load of popular HMs that are released in the ecosystem by various industries, such as agriculture, textile, mining, pharmaceutics, and food processing (Hymavathi and Prabhakar, 2017; Kumar et al., 2019; Sharma, 2014; Viessman et al., 1998). In the last two decades, various treatment techniques have been developed to remove HMs from water and wastewater; these techniques are categorized in Fig. 1. HM removal is expensive and laborious. In addition, the procedure requires skilled supervision and is time consuming. Various studies on the optimization and simulation of HM prediction and removal have been increasingly conducted over the last two decades to overcome these issues (Fig. 2).

Various artificial intelligence models, such as neural network, logic, regression, and hybrid models have been developed to understand the uncertain nonlinear pattern of HM removal using different treatment techniques. Moreover, these models have been compared with various conventional models, such as mathematical, isotherm, statistical, empirical, and physical models. These classical tools must determine a target for all groups of input variables to model and optimize contamination removal techniques; therefore, the target may vary, but remaining variables must remain constant at a time (Singh et al., 2010). These mentioned works increase the cost, time, and tedious laboratory work while implementing the HM removal process (Tak et al., 2015). Hence, it opens the door of soft computing (SC) aid. Fig. 3 illustrates that artificial neural network (ANN) has been the predominant model in maximum time owing to the fact that it is a new soft computing intervention that aids HM removal techniques. AI models are not limited to HM removal prediction; these models can also be used for thermal and process engineering (Shanmugaprakash et al., 2018). The main challenges in building such models are the number of datasets and optimizing process prior to model building, weight minimization, and bias in the selection of an appropriate optimization algorithm, which has a massive effect on the performance of predictive models (Guyon and Elisseeff, 2003; Wu et al., 2008). Model construction requires expertise to understand the stochastic behavior of data and the nature of the experimental process of HM removal and achieve reliable performance. Furthermore, the selection of training, validation, and testing tools for AI models are complicated (Tan, 2018).

Predictive models can potentially reduce the burden on environmental science and engineering in terms of cost, workforce, space requirement, and time consumption. AI models do not have a precise formula to understand architecture and algorithm; such a formula could facilitate the selection of variables (samples) (Jang et al., 1997). Hence, those can be solved in several ways, such as trial and error, which starts with a simple network to a complex one until the prediction value does not correspond to or near that of the experimental data. A solution can be achieved by observing the problem behavior and selecting an appropriate AI model architecture (Anupam et al., 2014).

Various HMs are released into water bodies by different industries (Barman et al., 2000; Sharma and Agarwal, 2009). Some

Table 1
The concentration of different HMs (μg/L) existed in the surface water bodies (statistical analysis), (Kumar et al., 2019).

	Cr	Mn	Fe	Co	Ni	Cu	Zn	As	Cd	Hg
Minimum	0.001	0.15	0.001	0.06	0.001	0.00067	0.01	0.22	0.003	0.007
Maximum	21800	77000	63500	42970	38100	27400	54000	86100	13700	8
Mean	413.27	2562.15	1654.05	3994.82	945.86	537.87	723.11	3981.78	180.88	1.01
Standard Deviation	128.24	747.74	541.75	135.24	191.84	138.71	213.10	145.96	62.80	0.54
Coefficient of variation	478.71	432.87	322.94	292.32	669.54	500.72	579.3	440.66	614.25	168.34

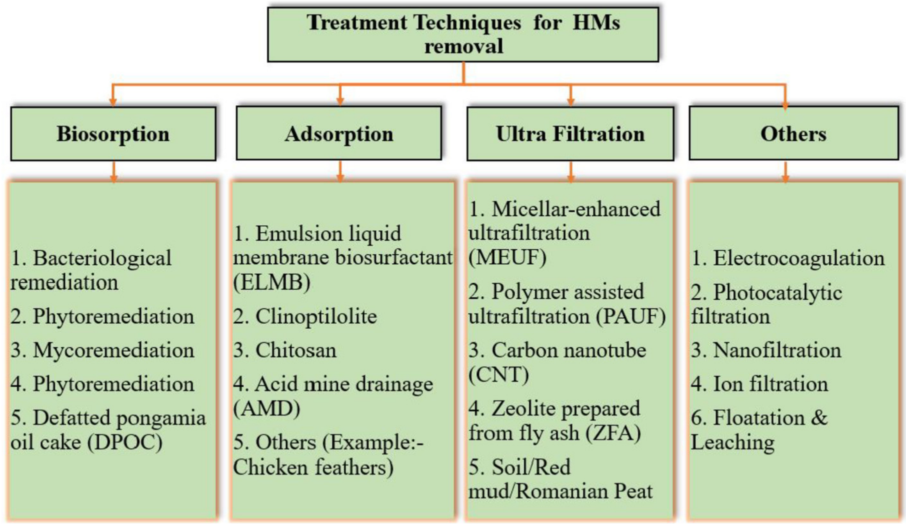

Fig. 1. Classification tree of Treatment Techniques of Heavy Metal removal.

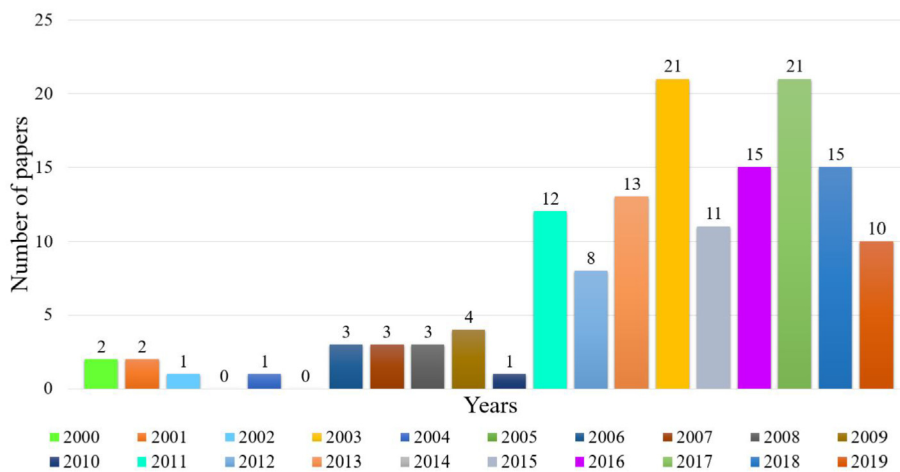

Fig. 2. Year versus number of papers on HMs removal and prediction by AI models.

are highly toxic to the ecosystem and human health; how HMs cause human body intoxication is discussed in Engwa et al. (2019). Common HMs, such as Cr, Ni, As, and Cd, have been reported to possess a high risk for cancer (Kumar et al., 2019), thus attracting considerable attention from researchers led the priority of HMs selection by these valued works indicated in Fig. 4. Nonlinearity is observed in the development of various AI models, their optimization approaches, the selection of different algorithms and types of functions to build the appropriate AI models, for which several researchers conducted the works on the complex behavior of HMs removal process by different treatment techniques (Fig. 5). Selecting appropriate optimization and simulation algorithms according to the experimental design leads to the optimal performance of the model and has the highest agreement with actual experimental data.

Research on HM simulation using AI models has progressed remarkably. However, to the best knowledge of the authors, this study is the first to review novelty works, such as the critical analysis and exploratory data analysis (EDA) of different variables; the normalization, optimization, algorithms, functions, and architecture of different AI models for simulation; and prediction of various HM removal techniques. Some reviewed research works are based on either HM removal techniques without the incorporation of AI modeling intervention (Fu and Wang, 2011; Ngah and Hanafiah, 2008) or water treatment techniques with a limited number of HMs, along with nutrients and persistent organic pollutant removal with a few number of AI models, such as ANN (e.g., backpropagation (BP), multilayer perceptron (MLP), radial basis function (RBF), particle swarm optimization (PSO), genetic algorithm (GA)), boosted regression tree (BRT), response surface methodology (RSM), and self-organizing map (SOM) (Fan et al., 2018). However, Fu and Wang (2011) reported various HM removal techniques without introducing AI models; these techniques required expensive instruments and skilled supervision and was time consuming. Furthermore, Fan et al. (2018) reviewed only 11 published works based on HM removal; thus, other major toxic HMs, such as Cu, Zn, Ni, and Hg were not covered. However, they reviewed the fundamental of heavy metal removal process and advantages of AI tools. The lack of review papers on the evaluation of AI models for HM removal prediction has led to the collective preparation of the current review. Total number of 152 esteemed manuscripts are explored, based on types of toxic HMs removal, considerable range of explanation for AI models for each target in terms of accuracy, critical assessment reported in scientifically

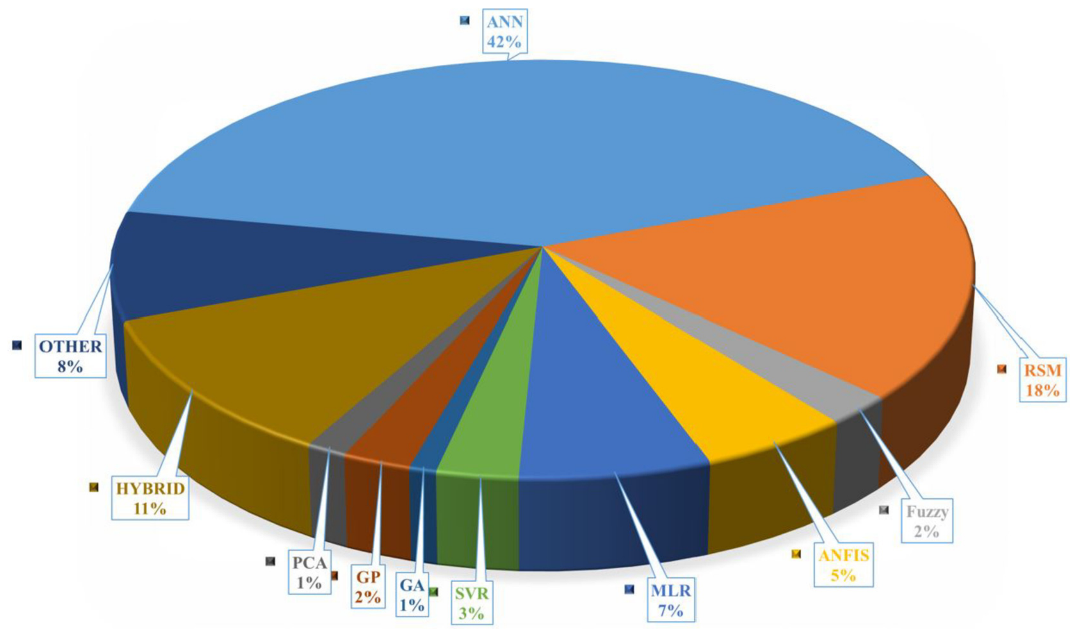

Fig. 3. Percentage of each model used to predict the HMs removal in past 20 years.

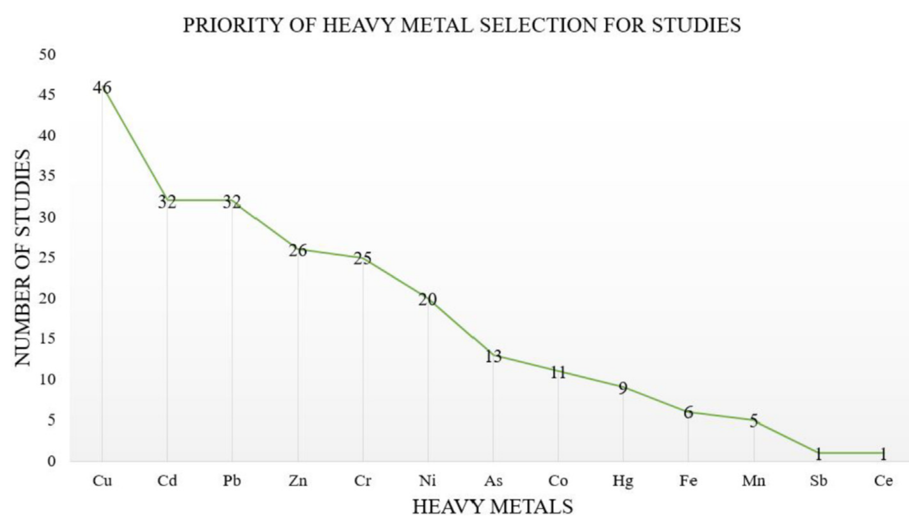

Fig. 4. Heavy metal selection for studies among researches.

coherently. All papers included in this review are those indexed in ISI and Scopus only; conference proceedings are excluded.

The advances in HM removal modeling and simulation achieved through numerous AI models have largely outperformed conventional models with respect to performance and increased the number of associated research, resulting in remarkable investigations since the early 2000 (Fig. 2). Reviews on AI modeling for HM removal are insufficient; hence, researchers are always interested in studies on reliable architectures, suitable algorithms, and various EDA process and functions for training the appropriate model for specific data/variables of HM treatment techniques.

To achieve the best performance of the model, all factors or the synergistic effect of HM remediation process for its modeling design must be friendly resemble according to the optimization of the input data for maximizing the target (output) and prediction value accurately. Various factors, such as different EDA processes, data optimization and normalization, number of hidden layers, number of neurons in the hidden layers, type of training algorithm, type of transfer functions, initial weights, and number of iterations of the training process (epoch), must be understood to achieve maximum accuracy. Different algorithms, including the Levenberg–Marquardt (LM), BP, MLP, and evolutionary algorithm (EA), are available; however, the best algorithm as per the characteristics of the dataset and the architecture of the AI model must be selected to produce a model that best fits the target.

This review research aims to provide a comprehensive survey on exhaustively categorized AI models and enumerate their advantages and advanced application in HM removal techniques. In turn, this assessment will inspire ideas for prospective research. This comprehensive evaluation focuses on the black box, fuzzy logic, kernel, evolutionary, and hybrid models of AI for the optimization and prediction of HM removal through various treatment techniques. Fig. 3 displays the implementations of different AI model versions. Given the abundance of papers that introduce the main

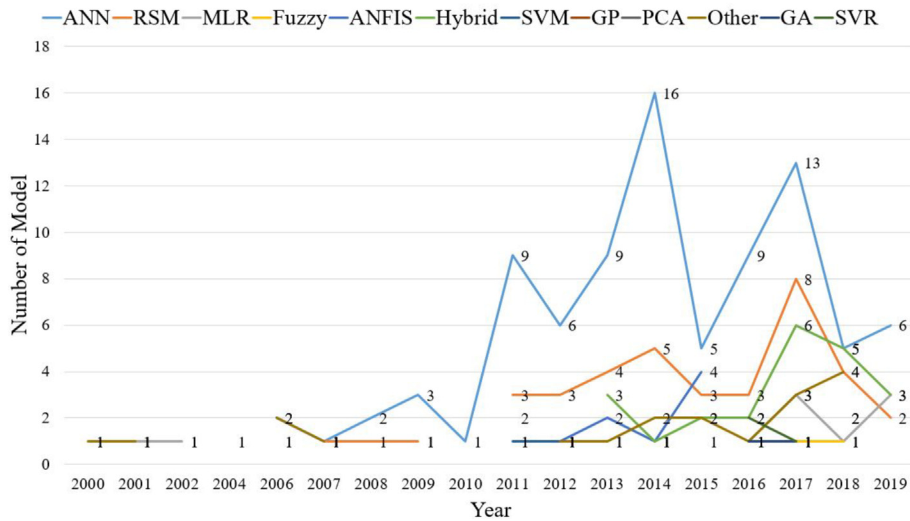

Fig. 5. Number of each model year wise.

concept of AI models, this review does not discuss the theoretical and mathematical approaches of AI models but rather presents the main ideas and cites several references for the readers to follow. Details, including authors, years of publication, treatment techniques, source of samples (HMs) for experiments, proposed predictive models, input–output variables, performance metrics (PM) evaluation, and research findings, of the selected papers are tabulated in Tables 2–6 according to the applied models. The process of building AI models for HM removal including the proposed models, algorithms, functions, merits, demerits and established arguments based on similar target, similar experimental design, and similar algorithm used to build the AI models are presented in Section 2. The evaluation and assessment of various treatment techniques are reported in Section 3 in which all HM removal treatment techniques in line with sustainable adsorbents are summarized, along with their affinity toward specific HM, user-friendliness, economy, reverse impact on the ecosystem, simulation, the prediction produced during the elimination process, and their suitability for the proposed model. The reviewed research assessments, evaluations, and prospective research possibilities are presented in Section 4. The trend of productive HM removal models, its development in the past two decades, its pros and cons with the critical gap between the research, as well as the prospective possible work are listed. Section 4 also describes the development of the treatment techniques and the possible research direction that could contribute important results. Section 5 contains the summary of the manuscript and presents opportunities for prospective researchers who want to contribute to the same field.

2. Applied soft computing models for HM simulation

2.1. Black box models (ANN, RSM, and MLR)

The black box model is not new to the engineering field but has not been extensively explored for optimum use, especially in environmental engineering. Black box explains independent and dependent variables but not the processing between these variables. In the last two decades, black box models have been mostly used as ANN, RSM, and multiple linear regression (MLR or MnLR or MNLR). Here, 90 of the finest works are reviewed and reported. Table 2 compares the types of treatment techniques for various HMs, and the grouping and prediction of HMs with ANN, RSM, ANN-RSM, and ANN-MLR models are reported in the next section.

The neural network was first proposed by McCulloh and Pitts in 1943 (McCulloh and Pitts, 1943). ANN is a mathematical and statistical model that attempts to mimic the human brain's mechanism. The process of learning and then memorizing the actual relationship of the mechanism between the input/output and their nonlinearity has attracted many researchers. ANN consists of three layers, namely, the input, hidden, and output layers. These layers comprise neurons, connectors, nodes, and learning algorithms that must be trained to achieve maximum accuracy. Neurons and nodes are the processing units where weights connecting the neurons of different layers and organize the ANN model. The backpropagation neural network (BPNN), feedforward back propagation neural network (FFBP), Levenberg-Marquardt (LM), MLP, MLR, Multi-layer perceptron (MLP), multivariable nonlinear regression (MNLR), multiple nonlinear regression (MnLR), and the RBF training algorithm have been used widely in HM removal modeling. In addition, different training functions, such as *Trainscg*, *Trainlm*, *Traingdm*, *Traincgp*, and *Trainrp*, and transfer functions, such as tangent sigmoid (*tansig*), *logsig*, and *purelin* have been utilized. Transfer functions are used to synthesize the neurons/model between the input and hidden layers and the hidden and output layers. One or more hidden layers can exist. The theoretical and mathematical concepts of ANN are discussed in another paper (Demuth et al., 2014). Approximately 57 papers on ANN for predicting several HMs and their combinations using different treatment techniques are reviewed in the following subsection.

2.1.1. ANN model for single HMs

A comparison of two results for Cu removal reveals that the ANN model is effectively trained by either the LM (using the *tansig* and *purelin* functions on the 11 neurons of the hidden layer and on the output layer, respectively) or the RBF feedforward algorithm, as reported by (Kabuba et al., 2014; Messikh et al., 2014), respectively. Furthermore, Messikh et al. (2014) highlighted the profits of ANN by establishing membrane stability through the optimization of the best variable to obtain maximum accuracy.

Two studies on the simulation of sulphur removal capacity have been reviewed. These studies applied the MLP and LM algorithms to train the ANN model, depicting potential predictability with a high determination of coefficient (R^2), a low average absolute deviation (AAD) and root mean square error (RMSE) (Acharya et al., 2006; Vasseghian et al., 2014). Furthermore, Oguz and Ersoy (2014) and Oguz (2014) investigated Co(II) and Fe(III) removal, respectively. The first study used minimax algorithm normalization techniques with seven variables in the BP and LM algorithms of the ANN model. In the second study, the scale and shift factor normalization techniques for input data, which were used to train the hyperbolic *tangent* and the linear function of the LM algorithm of the ANN model, were investigated. The LM algorithm exhibited higher accuracy compared with the BP algorithm. However, Yildiz (2017) proposed a BP algorithm for its simplicity and high training capacity with a low mean square error (MSE) value, which illustrated the potentiality of the AI model.

Esfandian et al. (2016) reported an inclusive comparative study between a data-driven model (i.e., ANN) and traditional adsorption isotherm models (i.e., Morris–Weber, Lagergren, and pseudo-second order) for Hg(II) metal removal. Some of the variables were fetched from theoretical models, such as the Langmuir, Freundlich, Dubinin–Radushkevich, and Temkin models. ANN exhibited a better predication capability compared with traditional models, but the authors reported that this model requires further advancement to elucidate the broad view of adsorption mechanism with comprehensive analysis.

In 2011, two comprehensive studies were reported (Rahmanian et al., 2011b; Turan et al., 2011a) to highlight the competence of the different functions of ANN in removing Zn(II). Both studies used a different approach to design the ANN model as per their treatment techniques and input data, and both reported that the LM-BP algorithm is superior to resilient BP, gradient descent, gradient descent with momentum BP, gradient descent with adaptive layer recurrent (LR), BP, and adaptive LR-BP. However, they differ in choosing the optimization and network design functions. The full factorial design (FFD) and cubic spline curve fitting (CSCF) functions were utilized by Turan et al. (2011a) to estimate the optimal values for the variables reported, whereas FFD was utilized by (Rahmanian et al., 2011) for optimization, and the *logsig* processing with the hyperbolic *tangent* function was used to train the LM algorithm.

Five studies are presented for the same output, that is, the removal of Cd(II) ion (Ahmad et al., 2014; Ahmad and Haydar, 2016; Nasr et al., 2015; Siva Kiran et al., 2017; Yurtsever et al., 2014). The LM with the hyperbolic *tansig* function was reported to be the most suitable (Ahmad et al., 2014). Meanwhile, Ahmad and Haydar (2016) used different outputs, such as the breakthrough curves of the column process and the coefficient of the Thomas and Yan models, to achieve the best fittings of the proposed model. Multiple regression was used to optimize the input data for the FANN_TRAIN_RPROP function for training, the FANN_ELLIOT for the hidden layer, and the FANN_SIGMOID_SYMMETRIC to build the ANN model, to achieve high performance (Yurtsever et al., 2014). Nasr et al. (2015) used an adaptive neural fuzzy interference (ANFIS) model to evaluate the influence of input variables on output variables and then proposed an ANN model with a hyperbolic *tangent* transfer function in the hidden layer to identify the pattern understanding and the linear transfer function at the output to match with the actual data of the batch process. In 2017, Siva Kiran et al., used the Box–Behnken (BB) experimental design grouping with ANN and the DIRECT algorithm to train the model for optimal performance.

For As(III) removal, four studies reported that the BPNN trained by the LM algorithm for the ANN model is popular as it adjusts the weight and bias of the network with a high correlation coefficient (R) and a low MSE (Altowayti et al., 2019; Giri et al., 2011; Gnanasangeetha and SaralaThambavani, 2014; Mandal et al., 2014b). These studies used 60%–75% range of data for training purposes. In the 60% case, normalization techniques were proposed to minimize the effect of scaling along with *sigmoid* transfer function from input and hidden layers, whereas all others used *tansig* for the same, and *purelin* was used at output layer neurons by all four studies.

Five studies on Cu(II) ion removal are reviewed (Abdollahi et al., 2019; Geyikçi et al., 2013; Oguz and Ersoy, 2010; Prakash et al., 2008; Turan et al., 2011b). Prakash et al. (2008) used the BP recurrent network (Elman) with three hidden layers of the ANN model, whereas the LM-BP network with the hyperbolic *tangent* function was reported as a potential model for predicting the same output mentioned by (Oguz and Ersoy, 2010). A newly proposed network (i.e., RBF) was compared against the LM-trained feedforward network in which the competency of RBF was high as reflected by the low MSE and high R^2. Geyikçi et al. (2013) applied the LM algorithm to a feedforward MLP network using the *tansig* and *logsig* functions at the hidden and output layers, respectively, resulting in improved performance. Abdollahi et al. (2019) suggested that GA could be used to optimize the grouping of input variables to maximize the target. GA is a reliable data optimizer that can enhance the accuracy of the feedforward BP network trained by the LM algorithm for the same target.

Six thorough studies confirm the Pb(II) ion removal prediction efficiency of different algorithms of the ANN model (Fiyadh et al., 2017; Gomez-Gonzalez et al., 2016; Kardam et al., 2012; Singha et al., 2015; Shojaeimehr et al., 2016; Yetilmezsoy and Demirel, 2008). Principal component analysis (PCA) was used to validate the input data for the LM training algorithm of the BP network, showing the lowest MSE value among the 11 different topologies (i.e., FRCGBP, PCGBP, PCGBP, LMBP, SCGBP, BFGS, QNBP, OSSBP, BGD, VLRBP, and BGDM), followed by the Broyden–-Fletcher–Goldfarb–Shanno (BFGS) algorithm (Yetilmezsoy and Demirel, 2008). Kardam et al. (2012) also reported the potential of the same algorithm, as validated by sensitive analysis. Singha et al. (2015) worked on three algorithms (i.e., BP, LM, and scale conjugate gradient (SCG)) with different transfer functions at the hidden layer to train the ANN model; they tested the BP algorithm with a transfer function between 1 and 25 raised up to the highest value of R and the lowest value of chi-square (χ^2) to reveal the best prediction model. Recently, Gomez-Gonzalez et al. (2016) conducted an intensive research on optimization techniques (i.e., GA, pattern search (PS), simulated annealing (SA), and the gradient-based method) and predictive models (i.e., isotherm models, such as Langmuir and Freundlich, and a data-driven model such as ANN). They found that the PS method, which used the LM algorithm to train the ANN model, is the best by ignoring the local minima and accelerating the convergence for the feasible optimizing power. In 2016, another study also delivered LM-trained BP network, which had optimal efficiency to produce the lowest MSE and mean relative error (MRE) values and the highest R^2 values (Shojaeimehr et al., 2016). In 2017, an exhaustive comparative study was conducted between two neural networks, namely, FFBP with three hidden layers and LR with five hidden layers along with different transfer functions, such as *Trainbfg*, *Trainbr*, *Traincgb*, *Traincgp*, *Traincgf*, and *Trainlm*. The study was conducted to develop a design for the best performance. The best evaluated values of PM were found by utilizing the *Trainbr* function in the three-layered FFBP neural network architecture (Fiyadh et al., 2017).

Seven exclusive work findings of Cr(VI) HM removal are presented in this section. Aber et al. (2009) and Asl et al. (2013) used a multilayered FFNN trained by BP algorithm to achieve high accuracy. In the same year, Singha et al. (2013) established an ANN model with BP and LM algorithms as the best model for the same experimental design. Anupam et al. (2014) compared the resilient and BFGS quasi-Newton backpropagation algorithm among six possible algorithms, which adjusted their weight and bias easily using the *trainrp* and *poslin* functions to design the best performance of the ANN model. Ramazanpour Esfahani et al. (2014) applied *trainscg* and the training-and-test-approach to design a common neural network of an ANN model. In another study, 1–30 neurons at a hidden layer of a feedforward BP network, which was trained using LM-BP algorithm, was used by (Debnath et al., 2016). They found that eight neurons were the best with the *tansig* and *purelin* functions, which were adjusted to calculate the best prediction performance. This year, Tümer and Edebali (2019) established five neurons at the hidden layer of the FF-BP neural network model, which was trained by the *trainlm* and *purelin* functions to achieve the highest accuracy of the model.

2.1.2. ANN model for the alliances of HMs

Laberge et al. (2000) used the MLP algorithm to train the ANN model for the prediction of a mixture of Cu, Zn, and Cd from municipal sludge. Fagundes-Klen et al. (2007) investigated individual and binary mixtures of Cd and Zn ion biosorption. They conducted a comparative study between traditional isotherm and data-driven models, i.e., ANN, which showed improved performance.

Kamiński et al. (2009) proposed the MLP network for the adsorption of a single or mixture of three HMs (Cu(II), Zn(II), and Cr(VI)). The proposed model showed potential predictability of one ion, two ion groupings, and three ion mixtures at a time. After a couple of years, Tomczak (2011) used EA to identify the adsorption dynamics model, whereas MLP topology was used to describe a sorption isotherm for the same arrangement of ions and experimental design, as reported by (Kamiński et al., 2009).

In 2012, Drăgoi et al., studied the competence of a clonal selection neural network for the experimental data of a series of simulations with high measurement errors to understand the sorption process of Cd, Co, Ni, Hg, and Cu. In another study, Tomczak and Kaminski (2012) used the LM training algorithm to design an MLP-based ANN model for HM prediction (Cu(II), Zn(II), Ni(II)). Researchers addressed seven different types of HM input combinations and achieved an output with a high R^2 value and low MSE (δm). The adsorption capacity of Cu(II), Zn(II), and Ni(II) ions was exhibited chronologically (high to low).

Two intensive studies were conducted on same adsorbent, i.e., Romanian peat to adsorb Cd, Co, Ni, Hg, and Cu in one experiment; and Pb instead of Cu in another (Gabriel D. Suditu et al., 2013; Gabriel Dan Suditu et al., 2013). In the first experiment, they used GA to optimize the variables during the sorption process and in another treatment process. Modular neural networks were proposed for data optimization. Both studies used the MLP algorithm to train two hidden layers of the ANN network. The inverse modeling concept was also suggested to achieve improved efficiency of the ANN model.

Wilson et al. (2013) utilized the Bayesian regularization algorithm to train a single-layer chemometric tool (ANN) to determine the effect of various binary and tertiary combinations of HMs, and the best removal sequence was $Pb^{2+v} > Cu^{2+} > Zn^{2+} \geq Cd^{2+}$ HMs removal percentage with the best performance by the model.

Mendoza-Castillo et al. (2014) highlighted the advantages of the ANN model by establishing the importance and consequence of both sorbent and HM characteristics in addition to metal sorption kinetics and isotherms. ANN was built with the BP algorithm to evaluate the most relevant parameters of HM removal. The treatment was administered using lignocellulosic sorbents (i.e., biomass lignin content), concentration of acidic groups, metal molecular weight, and hydration energy, which were distinguished among other reviewed studies.

Reynel-Avila et al. (2014) proposed the Taguchi's experimental design and an ANN model to analyze the variables of HM (i.e., Cd, Ni, and Pb) removal prediction. The BP algorithm trained the MLP network of the ANN model, and the weight and bias were adjusted using the trial-and-error method. The ANN model exhibited a more promising prediction ability compared with conventional isotherm models, such as the Langmuir and non-modified Sips models.

Esmaeili and Aghababai Beni (2015) studied the potential topology of an ANN with two hidden layers, which were trained by the MLP algorithm for Ni and Co HM biosorption capacity. In another study, Podder and Majumder (2016) evaluated the LM-BP algorithm to optimize the neural network structure to be the best fit for the variables of the As(III) and As(V) metal sorption prediction.

Khandanlou et al. (2016) reported the highest efficiency of incremental BP among quick propagation (QP), batch BP, GA, and LM algorithms for ANN model training to minimize the RMSE value for Pb and Cu ion removal prediction.

The biosorption prediction of Cd(II), Pb(II), and Ni(II) was elucidated with high accuracy using an LM-BP-trained algorithm of ANN model (Varshney et al., 2016).

Early this year, changes in the selection of variables were observed. Rossi et al. (2019) revealed in an intensive research on Cd and Ce ions, which were used as plant physiological parameters, and the ratio of v/m as an independent variable that these HMs accumulate in different parts of a plant as dependent variables (Table 2). The MLP algorithm was used to train the ANN model for predicting the accumulation of Ce and Cd ions in different parts of the plant; the model performed well.

In 2018 and 2019, two comprehensive studies in which output parameters included a breakthrough curve, equilibrium concentrations, and the adsorption capacity of bone char, have been reported; the adsorbent technique in these studies was used for the binary, tertiary, and quaternary groupings of HMs (i.e., Cu–Zn and Cd–Ni–Cu–Zn) (Hernández-Hernández et al., 2017; Mendoza-Castillo et al., 2018). The forgoing studies applied the BP and multilayer feedforward algorithms to train the ANN model; however, the later research utilized the BFGS optimization method to lessen the objective functions (Mendoza-Castillo et al., 2018). These output variables limit the efficiency and robustness of the ANN, resulting in incorrect prediction due to high modeling error.

2.1.3. RSM model for single HMs and HM alliances

The RSM model, which comprises mathematical and statistical approaches, was introduced by (Box and Wilson, 1951) and developed suitably toward HM experimental design by (Gifi, 1990; Ross and Ross, 1988). In HM removal treatment techniques, RSM is performed in three steps: 1) designing the experiment, 2) building the model, and 3) estimating the effect of variables and response within the range (Jain et al., 2011; Myers et al., 2016). The theoretical and mathematical concepts of RSM are presented in the work of (Myers et al., 2016). RSM in HM removal techniques demonstrate competency in terms of economy by optimizing the experiments, thus achieving maximum response (Ashan et al., 2017; Jain et al., 2011). In addition, RSM is utilized by researchers for HM removal to determine the linearity, interaction, and quadratic effects between the variables and the accuracy of the model (Jain et al., 2011; Sabonian and Behnajady, 2014). The center composite design (CCD), BB design (BBD), and fractional factorial design of FFD algorithms have been used to construct the RSM model.

The authors of this study have reviewed approximately 10 exclusive works based on the RSM model alone. The RSM model has been used to optimize input variables to achieve the target. Four works on Cu(II) ion removal are reported (Cojocaru and Zakrzewska-Trznadel, 2007; Kavosi Rakati et al., 2019; Özer et al., 2009; Xiarchos et al., 2008), whereas the others focused on Cr, Ni, Cd, Pb, and Co (Cobas et al., 2014; Dil et al., 2017c; Esmaeili and

Khoshnevisan, 2016; Gusain et al., 2016; Hymavathi and Prabhakar, 2017; Jain et al., 2011). In most of these works, the authors reported that pH, initial concentration of HM, initial concentration of adsorbent, molar ratio, weight ratio, and contact time against a target of HM removal (in percentage) were found relevant to the response. The RSM was designed using CCD, FFD, BBD, and MLR as per their experimental design requirement. CCD was found to have a good fitting with a quadratic surface model and could establish a second-order response surface model and experimental process optimization. This design was also ideal for sequential experimentation along with reasonable input data to achieve the target (Dil et al., 2017c; Hymavathi and Prabhakar, 2017; Kovalova et al., 2012; Özer et al., 2009). FFD was used for the ratio of the molar-to- weight variable in place of the CCD to optimize the experimental design process, whereas MLR was used to reduce the value of the sum of the squares of the residual (Cojocaru and Zakrzewska-Trznadel, 2007; Xiarchos et al., 2008). By contrast, three factorial BB models were found suitable for the rotatable quadratic design and could be executed freely (Gusain et al., 2016; Jain et al., 2011). The BBD was used to predict Cr(VI) ion removal and optimized the $CaCl_2$ pretreatment process to enhance the performance of the model (Cobas et al., 2014). Analysis of variance (ANOVA) was performed to validate the competence of the quadratic or factorial design model, as revealed by different indicators, such as the f-value, p-value, R, and R^2. Indeed, the experimental designs can be positively modeled as an advancement of the AI models to simulate HM removal efficiency.

2.1.4. ANN and RSM model for the same treatment technique or target

Nineteen papers are reviewed, and the ANN and RSM models are compared in this section. In accordance with the reviewed papers, this section is subcategorized as per the target, where ANN shows superiority over the RSM model as per the following reviewed exercises for each target variable.

i. Case of Cu(II)

Bhatti et al. (2011) reported that the ANN-GA model demonstrated a better prediction capability for Cu(II) removal compared with the quadratic model designed by the CCD of the RSM model. Reportedly, ANN could more competently arrest the nonlinear experimental data to evaluate the combined regression coefficient for removal efficiency and energy consumption. Another work showed that the CCD of RSM could potentially establish the single and combined effect of various treatment techniques on Cu(II) removal efficiency. Optimized variables were obtained from the CCD-trained RSM model and fed to the BP algorithm of the ANN, which was constructed by the *poslin* function of the input-to-hidden-layer modeling and the *purelin* function of the hidden-to-output-layer modeling to achieve high accuracy (Ghosh et al., 2013). In another study, the LM BP algorithm of the ANN model trained with functions *transig* and *purelin* at the input-to-hidden and hidden-to-output layers exhibited superiority over the RSM model in terms of the fitting of variables for the maximum prediction value. Here, RSM was utilized to display the linear effect of variables and their interaction on the target effectively (Shojaeimehr et al., 2014). A research reported that the CCD algorithm of the RSM model outperforms the BBD- and FFD-designed model with respect to the linear and interactive session between the variables. The RSM also removed less effect variables and fed them to the LM to design the ANN, which produced a prediction value near the actual result (Podstawczyk et al., 2015). Meanwhile (Blagojev et al., 2019; Uddin et al., 2018), applied the BBD algorithm to train the RSM model for optimizing the variables to maximize the response; they used the LM and GA algorithms to train the ANN model to achieve the best prediction performance.

ii. Case of Cr(VI)

Krishna and Sree (2013) conducted a comparative study between ANN and RSM for Cr(VI) removal. BBD was used to design RSM for variable optimization, and GA was used for the ANN model. ANN demonstrated better competency in predicting the Cr(VI) removal efficiency compared with the RSM model (Krishna and Sree, 2013). In the same year, Cr(VI) ion prediction was studied using the RSM and ANN models. The multilayer feedforward network's BP algorithm was used to build the ANN model, which exhibited a better predictive model compared with the CCD-trained RSM model, as indicated by the PM matrices (Shanmugaprakash and Sivakumar, 2013). After one year, another modified adsorbent (Table 2) was used to predict the same HM using an ANN model that was trained by additional data obtained from a proposed mathematical equation, which was linked with the percentage removal and optimized input parameters of the RSM model; the predicted value of the ANN model with the additional data from the mathematical equation was better than those of the RSM and normal ANN models (Sabonian and Behnajady, 2014). In the following year, the quadratic equation from multiple regressions was used to strengthen the CCD for less experimental data. This study used the CCD of the RSM model for the input variables to obtain the best yield. Moreover, a modified version of CCD, that is, a face-centered central composite design, was used to develop a link between the variables and the target. Along with the traditional trend of a transfer function (*tansig* and *purelin*), the gradient descent transfer function was used with momentum BP (*traingdm*) to construct the ANN topology to obtain updated weight and bias values according to the momentum. ANN displayed superiority over RSM in terms of predictive capability, as indicated by the PM matrices (Mandal et al., 2015a). After two years, Ashan et al. established the Cr(VI) ion prediction and removal percentage by applying the ANN and RSM models; the performance evaluation indicates that the simulation by the ANN model (in the case of RSM-optimized data) was better than that of RSM and ANN optimization and simulation (Ashan et al., 2017).

iii. Case of Pb(II)

In 2012, the CCD and LM/MLP algorithms were used for the RSM and ANN model for Pb removal prediction; the LM training module of the ANN was better than the MLP training module, as indicated by the improved predictive fitting with real data. This training used the *tansig* function at the hidden layer and the nonlinear function, *logsig*, at the output layer. The ANN model performed better than RSM in terms of prediction (Bingöl et al., 2012). In another study, the BBD algorithm was applied for the same target using the RSM and ANN models; here, the ANN model used the MLP training module and exhibited improved performance (Geyikçi et al., 2012). Another study that combined the Pb(II) and malachite green dye removal processes exhibited the use of CCD to prepare the RSM model for highlighting the best independent variables; the *transig* and *purelin* transfer functions at the hidden and output layers of the ANN model outperformed RSM's prediction ability (Dil et al., 2017b).

iv. Case of As(II and V)

Research on As(III) and As(V) sorbent on rice polish adsorbent used CCD algorithm for the RSM model to evaluate the single and combined effects of independent variables on responses. In the same experiment, the MLP network was used for the learning techniques of the LM BP of the ANN model for prediction, which exhibited a better performance compared with RSM (Ranjan et al., 2011). Another study was performed to optimize the variables using the BBD of the RSM model for As(V) removal (phytoremediation technique); here, multilayer feedforward neural networks (MLP) and a BFGS algorithm were successfully used to develop an ANN model, which produced a better prediction result compared with the RSM (Titah et al., 2018).

v. Case of Ni(II)

Oladipo and Gazi (2014) proposed a hyperbolic *tangent* function to construct a three-layered feedforward network of an ANN model to optimize the weight and bias of the topology. The ANN was evaluated in terms of the effect of various variables of the Ni(II) metal removal process on the modified adsorbent, and then a sequence of variables were reported as per their effect. In addition, CCD was used to strengthen the RSM model for input parameter optimization and maximize the breakthrough time and uptake capacity of batch adsorption. The ANN and CCD matrices presented a linear pattern with marginal irregularities from the actual line.

vi. Case of Cd—Co and azo dyes

A removal study based on a combination of HMs (i.e. Cd^{2+} and Co^{2+} ions) and azo dyes (i.e., methylene blue (MB) and crystal violet (CV)) established that the CCD of RSM produces optimized data with an improved understanding of the synergistic effect of variables against the output (Dil et al., 2017a). The LM algorithm of the FFBP topology of ANN was used with the *tansig* and *purelin* transfer functions to match the variables for the predictability of the removal percentage. The ANN displayed a slightly better performance compared with the RSM model (Dil et al., 2017a).

vii. Case of Zn(II)

Shanmugaprakash et al. (2018) recommended the LMBP learning technique to train the MLP topology of an ANN and utilized numerous optimized variables, which were gathered by the CCD of RSM, to produce the best predictive value of the Zn(II) removal efficiency dataset.

2.1.5. ANN and MLR for the same treatment technique

Multivariate and linear regression analyses have been used frequently in HM removal techniques since the study of (Yu et al., 2001). MLR revealed the correlation between two or more nonlinear variables (Ashrafi et al., 2019). In detail, the theoretical and mathematical concepts of MLR can be drawn from previous studies (Dunn and Clark, 1987; Myers and Myers, 1990) In this section, various works are reported and reviewed to compare the performance of the ANN and MLR models. Shandi et al. (2019) reported that the LM algorithm was better than the BP algorithm in designing an ANN model due to its powerful nonlinear mapping capacity of Cu(II) removal efficiency. By contrast, the twin logarithm of the MnLR model was designed to assess the previous experimental process. Both models show promising PMs (Table 2); an ANN model was also used to conduct sensitivity analysis to identify the variables' relationship with the target, revealing that all input variables have their own effect, whereas the initial concentration of Cu(II) has a maximum effect on the biosorption process (Shandi et al., 2019).

In the adsorption of Pb(II) onto carboxylate-functionalized walnut shells (CFWS) adsorbent was applied the three-layer feedforward ANN model, which was trained using the LM algorithm and the *transig* function; here, ANN outperformed MLR. However, MLR is well known for simplicity, transparency, and easy interpretability in terms of determining the cause—effect relationship between dependent and independent variables (Ashrafi et al., 2019). Both models were used to optimize the variables for improved fitting and produce a low prediction error. ANN has a marginally higher prediction value and a better statistical quality compared with MLR.

The biosorption prediction of Ni(II) and Co(II) was studied using two different models, namely, ANN and MNLR (Allahkarami et al., 2017). The BP learning methods of ANN evaluated the weight starting at the output layer and moving back through the hidden layer of the network, whereas the trial-and-error method was used to find the optimum number of hidden layers and neurons in each layer. The model evaluators showed that the performance of ANN was better than that of MNLR. The Ni(II) removal prediction by both models was better than their Co(II) removal prediction.

Three other works on the prediction of HM concentration in soil due to mining and agricultural activities are reviewed. In 2002, Kepler and Sommer reported from Spain field spectral measurement and geochemical variables to build up the chemometric experimental model using the ANN and MLR models. The feedforward network of ANN performed slightly better than the MLR model in terms of all metal determination at once, unrestrictedly. Soil remediation was achieved by removing the topsoil using heavy machinery for the detection of nine HMs. Out of the nine HMs, six (i.e., As, Fe, Hg, Pb, S, and Sb) were detected accurately by the MLR and ANN models (Kemper and Sommer, 2002). In 2009, ANN and MLR models were built using 13 properties of agricultural soil from Germany and the solution phase as input and the sorption phase as output. This experiment was conducted for nine HMs (i.e., Cd, Cr, Cu, Mo, Ni, Pb, Sb, Tl, and Zn). The authors used the intelligent problem solver (IPS) and two-fold cross-validation methods to determine the lowest error of the network and avoid the overfitting problem of ANN. However, no considerable difference was found between these two models, except in the cases of Cr and Cu. ANN and MLR are potential tools for sorption modeling; these models increased detection efficiency when the topsoil data were divided into subsoil data (Anagu et al., 2009). After two years, researchers from Iran introduced the BPNN and general regression neural network (GRNN) algorithms to the ANN and MLR models to predict four HMs (i.e., Cu, Fe, Mn, and Zn) from acid mine drainage (AMD). Surprisingly, GRNN, which is supervised, learns fast without categorization, and evaluates each output freely, showed better fitting with three input data (i.e., pH, SO_4, and Mg^{2+}), predicting the concentration of four HMs more accurately than another model (Rooki et al., 2011).

2.2. Fuzzy logic (TS, Mamdani, genetically generated fuzzy knowledge bases (GGFKB), and fuzzy-based decision support system (FDSS))

Since 1965, fuzzy logic (if—then rule) has been introduced to various fields of science and engineering to solve multidimensional problems (Zadeh, 1965). In environmental science, introducing a fuzzy model to solve water HM problems is time consuming. The main advantage of fuzzy logic over neural network is it avoids the pattern between the investigational data and the feedback by using a linguistic expression to present uncertainties (Mandal et al., 2015b; Rebouh et al., 2015). Furthermore, fuzzy logic, with the optimized input variable obtained by ANN, forms a new robust model called ANFIS. ANFIS reduces time and facilitates detection by simplifying the mathematical model for a system (Sonmez et al., 2018). The theoretical and mathematical concepts of fuzzy logic from basic to advance have been discussed in previous studies (Brown, Martin and Harris, 1994; Jang et al., 1997; Nauck et al.,

Table 2
The summarized details (calibration approach, predictive models, input/output variables, performance metrics and research remark) of the reviewed researches on heavy metal variables using the feasibility of ANN, RSM and MLR models over the period (2000–2020).

Sl. No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
1	Laberge et al. (2000)	Bioleaching by *Thiobacillus ferrooxidans*/Municipal sludge	Neural networks (NN)	several hydraulic retention times(HRT), FeSO4_7H2O concentrations, pH, oxydo-reduction potential and initial metal concentrations/metal (Cu, Zn and Cd) solubilization percentages	MAD	NN architect successfully with the best output of solubilization of these metals with mean absolute deviations. HRT found sensitive to predict the solubilization of these three metals.
2	Kemper and Sommer (2002)	Removal of topsoil by heavy machinery/Mining accident in Spain	ANN, MLR	Depth of soil for a different range, Reflectance spectra of a soil/ Concentrations for As, Cd, Cu, Fe, Hg, Pb, S, Sb, and Zn	R, R^2, SEP	Out of nine heavy metals, six were perfectly suitable to both ANN and MLR with a high-performance matrix. The remaining three heavy metal (Cd, Cu, Zn) did not show potential attraction for these models.
3	Acharya et al. (2006)	Bio sorption by (*Acidithiobacillus ferrooxidans*)/Three types of coal (Assam, coal, Polish coal and Rajasthan lignite)	ANN	Type of coal, initial pH, pulp density, particle size, residence time, media composition and initial sulphur content of coal/sulphur removal percentage	MAD	Very first-time Multi-layer perceptron (MLP) of ANN reported predicting Bio-sorption (*A. ferrooxidans*) techniques for sulphur removal
4	Cojocaru and Zakrzewska-Trznadel (2007)	Filtration by dead-end and cross-flow polymer assisted ultrafiltration (PAUF)/Aqueous Solution	RSM	feed concentration of polyacrylic acid, a ratio of polymer to copper and pH of feed solution/removal of Cu(II) ions	R^2, adj R^2	FFD of RSM used to optimize the variables and predict the response with a high value of determination of coefficient adjusted by MLR. ANOVA also performed to raise the quality of the model and produce the R^2 value for its prediction.
5	Fagundes-Klen et al. (2007)	Bio sorption (*Sargassum filipendula*)/ synthetic solution	ANN	The equilibrium concentrations of the fluid phase/equilibrium concentrations of the bio sorbent for Cd and Zn	AAD, objective function	Adsorption (Langmuir –Freundlich) isotherm was suited better for equilibrium data of the binary system. ANN was better efficient then adsorption isotherms model to estimate the equilibrium concentration.
6	Prakash et al. (2008)	Bio sorption by sawdust of mango tree (*Mangifera indica*)/Aqueous Solution	ANN	the initial ion concentration, pH, temperature and particle size/% adsorption efficiency for the removal of Cu (II)	MSE	The researcher found the momentum-training algorithm of back-propagation recurrent of ANN as an operative method in modeling, estimation and prediction of the biosorption process to remove the Cu (II) ion from aqueous solution.
7	Yetilmezsoy and Demirel (2008)	Adsorption by Antep Pistachio (*Pistacia Vera* L.) shells/Aqueous solution	ANN	adsorbent dosage, initial concentration of Pb(II) ions, initial pH, operating temperature, and contact time/ Adsorption efficiency of Pb (II) ions removal	MSE, R	Authors revealed that desorption studies may be needed further. This adsorbent is cheaper than membrane filtration inline to renewal sources of Antep Pistachio shells. ANN-Levenberg-Marquardt algorithm (LMA) performed well with predicting the value of adsorption efficiency.
8	Xiarchos et al. (2008)	Filtration treatment by micellar-enhanced ultrafiltration (MEUF)/ Aqueous solutions	RSM	Surfactant (SDS) concentration, pH and surfactant/metal (S/M) ratio/Rejection coefficient(%) of Cu removal	Fisher test (F-test), R^2	CCD and FFD of RSM utilized to alleviate the process variables to achieve maximum response and confirmed with F-test, whereas, the value of R^2 revealed the degree of agreement between predicted rejection coefficient (%) and experimental one.
9	Aber et al. (2009)	Electrocoagulation/synthetic and real wastewater from an electroplating factory	ANN	Current density (j), time of electrolysis (tEC), initial concentration of Cr(VI) and the concentration of electrolyte/ residual Cr(VI) concentration	R^2, MSE	The iron anode was better than aluminium one to removal chromium ion due to Fe^{2+} produced from the iron anode and reduced to chromate ion electrochemically. The authors found the best R^2 value using ANN prediction and Experimental data.
10	Anagu et al. (2009)	sorption models/133 agricultural sites across Germany	ANN, MLR	13 soil properties and solution phase concentrations/sorbed phase concentrations	RMSE, ME, EF	ANN and MLR used to develop sorption model as a function of 13 basic soil properties. ANN worked effectively when topsoil data divided into subsoil data. Moreover, ANN showed a better result than MLR in terms of EF.
11	Kamiński et al. (2009)	Sorption on chitosan foamed structure/aqueous solution	ANN	Initial concentration Ci/amount of adsorbed metal Cu^{+2}, Zn^{+2} and Cr^{+6} ions.	R^2, MRE	All three metal ions assessed at individual concentration level and as well as in the combination of each other for Langmuir-Freundlich

Table 2 (*continued*)

Sl. No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
						equation not necessary for ANN. MLP of ANN was best fitted between input and output for the best result of predication of removal of heavy metals.
12	Özer et al. (2009)	Adsorption by green seaweed (*Enteromorpha prolifera)*/Aqueous solution	RSM	Initial pH, temperature, initial Cu(II) ion concentration and biosorbent concentration/Cu(II) ion removal percentage	R^2	CCD used to design the experimental process to make better fitting for the RSM model to predict the Cu(II) removal efficiency. RSM evaluated by R^2 and scored high value.
13	Oguz and Ersoy (2010)	Adsorption(Shells of Sunflower)/ aqueous solution	ANN	the treatment time (t), the concentration of initial Cu_o^{2+}, adsorbent dosage, pH, flow rate, bed depth and particle size./Cu_o^{2+} concentration as a function of reaction time	RMSE	The authors found the best variables of the system behaviors for the adsorption process and simulated with LM-BP algorithm of ANN model to predict near actual values.
14	Bhatti et al. (2011)	Electrocoagulation system [Al(III) ions generated from sacrificial cathode]/ Synthetic wastewater	ANN, RSM	Cu concentration, pH, voltage and treatment time/Cu removal efficiency and energy consumption	Combined regression coefficient, R^2, MSE	CCD of RSM and ANN-GA showed advantage at their own stage such as RSM assessed voltage and treatment time as a positive correlation with removal efficiency but the negative effect on energy utilization. ANN was more capable to arrest the nonlinear data of experimental results with combined regression coefficient for removal efficiency and energy consumption.
15	Jain et al. (2011)	Biosorption by *Helianthus annuus* flowers (SHC)/Aqueous solution	RSM	the pH of the solution, initial Cr(VI) concentration and adsorbent dose/ Cr(VI) adsorption	R	BBD of RSM used to optimize the quadratic equation data and called timesaving technique by reducing the number of experiments to optimizing the variable input effectively.
16	Ranjan et al. (2011)	Bioadsorption by rice polish/aqueous solution	ANN, RSM	pH, initial arsenic concentration, temperature, and biomass dose(for batch mode) and bed height, flow rate, and initial arsenic concentration (for column mode)/uptake capacity of the sorbent for As(III) and As(V)	R^2	ANN and RSM models have used to assess the predictability. ANN found better than RSM model in the line to a limited number of experiments with accuracy, whereas, RSM reported useful for interactions between different components.
17	Giri et al. (2011)	Biosorption by *Bacillus cereus*/Aqueous solution	ANN	The initial concentration of arsenic (III), biosorbent dosage, temperature and contact time/As (III) sorption %	ARPE, R^2	Although, with the high value of the degree of correlation estimated for ANN predictive tool of biosorption efficiency. The authors recommended that fast convergence proficiency together with ANN might be tested with experimental data and more number of variables to exploit the fundamental principle of biosorption.
18	Rahmanian et al. (2011b)	Filtration treatment by micellar-enhanced ultrafiltration (MEUF)/ Aqueous solutions	ANN	TMP, pH, Feed SDS concentration, S/M ratio, L/M ratio, Electrolyte concentration, (Brij35/SDS) modal ratio/permeate flux and rejection rate of metal (Zn) ion from wastewater	AARE	ANN and FFD have designed for the prediction of permeate flux and rejection of metal ion removal. These models showed dependable and truthfulness with AARE value.
19	Rooki et al. (2011)	NA/amount of acid mine drainage (AMD)	ANN, MLR	pH, SO_4 and Mg^2/heavy metals concentrations (Cu, Fe, Mn and Zn)	R	Best ANN (BPNN and GRNN) and MLR architecture have been set best on correlation coefficients to predict the heavy metals from AMD. GRNN found a better model than others to predict with more agreement to experimental data.
20	Turan et al. (2011b)	Adsorption by Pumice of Soylu Mining Industry/WW from Elektrosan Elektrocopper Industry & Trade Co. Ltd. in Samsun, Turkey.	ANN	initial pH, adsorbent dosage, temperature, and contact time/ maximum removal of Cu(II) ions	R^2	Radial basis function (RBF) established as a feasible better than traditional network type for the prediction of % adsorption efficiency for the removal of Cu (II) ions from industrial leachate by pumice.
21	Turan et al. (2011a)	hazelnut shells (Corylus pontica) as a biosorbent/Industrial waste of Elektrosan Electrocopper Industry in Samsun, Turkey	ANN	Initial pH, adsorbent dosage, contact time, and temperature/Zn (II) removable capacity (Rem%).	R^2, RMSE	The authors found LM-BP of ANN is the significant tool to predict the removal capacity of hazelnut shells with cost-effective and less computational time.
22	Tomczak (2011)	sorption on chitosan foamed structure/aqueous solution	ANN	Equilibrium concentration, C_{ei}, of a given component (for one component,	R^2, MRE	ANN used with MLP and EA algorithm to the proposed model for suitability of

(*continued on next page*)

Table 2 (*continued*)

Sl. No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
				binary and ternary systems)/amount of metal (Cu(II), Zn(II) and Cr(II)) ions adsorbed		Chitosan for sorption process in order of highest concentration for zinc ions, higher for nickel ions and lowest concentration for copper ions, respectively. EA showed better performance of prediction.
23	Bingöl et al. (2012)	Biosorption by black cumin (*Nigella sativa*)/Aqueous solution	ANN, RSM	pH, biosorbent mass and temperature/sorbed amount of lead	R^2, RMSE	Predictability of ANN revealed better than RSM based on the validation data set. The study presented a high level of non-linear relation ANN model with experimental results.
24	Dră;goi et al. (2012)	Biosorption by peat bed (lignin, cellulose and humic substance)	ANN	the metal type described by its electronegativity of Cd, Co, Ni, Hg and Cu), sorbent concentration, the pH of the initial solution, initial concentration of the solution containing metal ions, solution temperature, and contact time/sorption process	R^2, MSE	Clonal Selection Neural Networks (CS-NN) has been used to develop an optimum neural network model, which estimates the efficiency of the sorption process depending on working conditions.
25	Geyikçi et al. (2012)	red mud of Seydiş ehir Aluminium Plant, Konya, Turkey/industrial sludge leachate of an accumulators production plant, Turkey	ANN, RSM	Dosage, time and pH/Removal of Lead	MSE, RMSE, R^2, ADD	Box–Behnken design (BBD) used for both ANN and RSM model to optimize the input for better yield of the target. RMSE, R_2 and ADD were used to compare ANN and RSM. Better statistical parameters made by ANN than RSM.
26	Kardam et al. (2012)	Biosorption by Nanocellulose Fibers (rice straw)/synthetic solution	ANN	Biomass doses, Metal concentration, volume, contact time and pH/Pb % sorption efficiency	MSE	Complex sorption process has been assessed and optimized by ANN which used Levenberg–Marquardt algorithm (LMA) of BP algorithms to train the model with a minimum mean squared error (MSE).
27	Tomczak and Kaminski (2012)	Adsorption by Clinoptilolite/Aqueous solution	ANN	7 different combination of input in terms of heavy metals/adsorption capacity of Cu(II), Zn(II), Ni(II)	R^2, *m*	MLP of ANN model addressed to predict the heavy metal of either single or in-group.
28	Asl et al. (2013)	Adsorption by zeolite (ZFA) of raw fly ash (RFA)/Aqueous solution	ANN	initial pH, adsorbent dosage, contact time and temperature/percentage adsorption the efficiency of Cr(VI) ions	R^2, MSE	Sensitivity analysis showed that MSE values are inversely proportional with a number of variables used in the ANN model. Therefore, the researchers open a new area of research to understand the dynamic behavior of the process with other phenomenal in detail with advance ANN model.
29	Gabriel Dan Suditu et al. (2013)	Biosorbent by Romanian peat (from Poiana Stampei)/Aqueous solution	ANN	Metal electronegativity, a dose of peat, pH, temperature, initial concentration of the pollutant in solution and contact time/efficiency of heavy metal(Cd, Co, Ni, Hg, Cu) ions removal	MSE, r	ANN-GA proved the reliability and efficiency based on performance and presented in general form. GA of ANN used to avoid the overfitting of the model.
30	Gabriel D. Suditu et al. (2013)	Biosorbent by Romanian peat (from Poiana Stampei)/Aqueous solution	ANN	Metal nature (electronegativity), sorbent dose, pH, temperature, initial concentration of metal ion, contact time/amount of retained metal(Cd, Co, Hg, Ni, Pb) ion per unit mass of sorbent	MSE, E_r, r	For each metal, the best among entire database has been achieved by MNN, used for training and testing of ANN, and found a better performance of the model with MLP algorithm with simple structure and faster training. Inverse modeling also used to determine the leader parameters to pre-established values of adsorbed metal ion per unit mass of peat.
31	Geyikçi et al. (2013)	Adsorption by single-wall carbon nanotubes (SWCNTs)/Aqueous solution	ANN	initial concentration, PH, time and adsorbent dosage/percentage of Cu ions removal	R^2	Authors found LM learning algorithm to train the feedforward MLP network model superior overall previous adsorption isotherm model to design the experiment well and to predict the metal removal percentage with high determination coefficient.
32	Ghosh et al. (2013)	Biosorption by orange peel/aqueous solution	ANN, RSM	pH, copper concentration and contact time/removal (%) of copper	R	ANN and RSM reported unique in their respective place. CCD of RSM optimized the best process variables, whereas, error backpropagation of ANN imitated the best model to predict with better correlation value.
33	Krishna and Sree (2013)	Adsorption by ragi husk powder/synthetic wastewater	ANN, RSM		MSE, R^2	Using GA to design ANN produced a better result for the prediction of metal

Table 2 (*continued*)

Sl. No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
				pH, adsorbent dosage and initial chromium(VI) concentration/ percentage of metal removal		than BBD for RSM. Nevertheless, BBD model optimizes the experimental data better.
34	Shanmugaprakash and Sivakumar (2013)	Defatted *Pongamia* oil cake (DPOC)/ synthetic aqueous solution	ANN, RSM	pH, initial Cr(VI) ion concentration, temperature and dosage in the case of the batch mode and bed height, flow rate and initial Cr(VI) concentration in the case of continuous mode/ biosorption of Cr(VI) in case of both mode	R^2, RMSE, AAD	The first time, Inline to the non-linear behavior of adsorption operating parameters of Cu (VI) removal of both batch and continuous process, have been studied with ANN model and found precisely efficient to predict Cu(VI) removal over RSM model.
35	Singha et al. (2013)	Biosorption by eight adsorbent(sawdust of teakwood, neem bark, rice straw, rice bran, rice husk, hyacinth toots, neem leaves, and coconut shell)/Aqueous solution	ANN	Initial pH, initial Cr(VI) ion concentration, adsorbent dosages, and contact time/percentage removal of Cr(VI)	MSE, R, AARE	BP and LM both algorithms were suited to producing the best ANN model for Cr (VI) removal percentage predictability with a high value of R and low value of AARE.
36	Wilson et al. (2013)	simultaneous and automated Biosorption by potentiometric sensor array [vegetable wastes based on flow-injection potentiometry (FIP) and electronic tongue detection (ET)]/ Aqueous solution	ANN	Furrier and breakthrough coefficient/ removal of Cu2+, Cd2+, Zn2+, Pb2+ and Ca2+	RMSE, R2, Intercept and slop	Binary and tertiary combination of metal as an input selected. The best removal sequence of $Pb^{2+}>Cu^{2+}>Zn^{2+}\geq Cd^{2+}$ reported by this new integrated biosorption approach with the more reliable predictable model of ANN.
37	Ahmad et al. (2014)	Biosorption by immobilized *Bacillus subtilis* bead (IBSB)/Aqueous solution	ANN	pH, biosorbent dosage, contact time, initial cadmium ions concentration and temperature/biosorption capacity for cadmium ions	R^2	With the highest value of determination coefficient, ANN found best simulation model for batch biosorption process of IBSB.
38	Anupam et al. (2014)	Physisorption by powdered activated carbon/simulated wastewater	ANN	Adsorbent dose, wastewater pH, initial pollutant concentration and contact time/adsorption efficiency and adsorption capacity for adsorptive removal of Cr(VI)	R^2, MSE	Resilient and BFGS quasi-Newton backpropagation algorithm of ANN used to predict adsorption capacity and trainrp and poslin of ANN used to predict adsorption efficiency and showed the best result as per their evaluation matrix.
39	Cobas et al. (2014)	Biosorption by *F. vesiculosus*/Aqueous solution	RSM	pH, biomass dosage and $CaCl_2$/Cr(VI) removal percentage	R^2	Three factorial Box-Behnken based design of RSM revealed a high degree of predictability and robustness. Authors also investigated Freundlich isotherm suited well.
40	Gnanasangeetha and SaralaThambavani (2014)	Adsorption by zinc oxide nanoparticle entrenched on activated silica (ZnO-NPs-AS) which extracted of *Azadirachta indica*/Aqueous solution	ANN	the initial concentration of As^{3+}, adsorbent dosage, contact time, pH and agitation/As sorption capacity	RMSE, R^2	LM of ANN found greater than BP along with performance matrix result.
41	Kabuba et al. (2014)	Adsorption by Clinoptilolite/Aqueous solution	Neural network	pH, temperature, initial concentration/ Cu(II) ion removal	MSE, R^2	BP of a neural network trained the model to an obtained high degree of prediction ability of the model.
42	Mandal et al. (2014b)	Adsorption by hybrid material of cerium hydroxylamine hydrochloride (Ce-HAHCl)/Aqueous solution	ANN	adsorbent dose, pH, contact time, agitation speed, initial concentration and temperature/removal % efficiency of As(III)	R^2, ARPE, MSE	Backpropagation algorithm of ANN was trustworthy to predict the adsorption efficiency of As ions with difference variables input.
43	Mendoza-Castillo et al. (2014)	Biosorption by lignocellulosic wastes, namely jacaranda fruit, plum kernels and nutshell/Aqueous solution	ANN	Sorbent characteristics, Metal ion properties, Sorbent characteristics, Metal ion properties/removal of Pb(II), Cd(II), Ni(II) and Zn(II)	R, MSE, MRE	The nonlinear relationship between the sorbent features and the sorbate characteristics established and predicted the sorption of HMs by ANN, successfully.
44	Messikh et al. (2014)	Adsorption by emulsion liquid membrane process/Aqueous solution	ANN	emulsification time, ultrasonic power, stirring speed, sulfuric acid concentration, extractant concentration, surfactant concentration, internal phase/organic phase volume ratio, emulsion/external phase volume ratio, copper concentration, contact time, extractant concentration, stirring speed/stability of membrane and Cu removal efficiency	R^2, RMSE	ANN build-up by RBF feed-forward algorithm to set the stability of membrane and extraction of copper.
45	Oguz and Ersoy (2014)	Biosorption by sunflower biomass/ Aqueous solution	ANN	The treatment time, initial Co(II) concentration, biosorbent dosage, pH, bed depth and particle size, flow rate/ Co(II) concentration as a function of reaction time	R^2, SDR, MAR, RMSE	All performance indicators illustrated well to predict the Co (II) removal by sunflower as an adsorbent by proposed LM of the ANN model. Minimax-algorithm normalized the input and output variables.
46			ANN, RSM		R^2	

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Table 2 (*continued*)

Sl. No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
	Oladipo and Gazi (2014)	Adsorption by Alginate-based composite bead (ABCB)/aqueous solution		Dosage, contact time, initial concentration and pH/uptake capacity and removal percent of (Ni)		CCD of RSM depicted to optimize the input parameters on breakthrough time and removal % of nickel. ANN and CCD are reliable in matching with the result of batch experimental values.
47	Ramazanpour Esfahani et al. (2014)	Sorption by sepiolite-stabilized zero-valent iron nanoparticles (S-ZVIN)/ Aqueous solution	ANN	pH of aqueous solution, S-ZVIN concentration, Initial Cr(VI) concentration and Chloride ion concertation/removal efficiency(%) of Cr(VI)	R^2, MSE	This study approved the quantitative role of each input variables of the removal efficiency of Cr(VI) with almost a unit determination coefficient of ANN.
48	Reynel-Avila et al. (2014)	Adsorption onto chicken feathers using Taguchi's experimental design// Aqueous solution	ANN	The initial concentration of Pb(II), Cd(II), Ni(II), pH/removal of HMs	R^2, MSE	Pb(II) illustrated better adsorption among ternary aqueous solution by using Taguchi's experimental design and ANN model for modeling the sorption of HMs.
49	Sabonian and Behnajady (2014)	Photocatalytic remediation by nanoparticles of TiO_2−P25/Aqueous solution	ANN, RSM	The initial concentration of Cr(VI), the dosage of TiO2 catalyst, light irradiation time, and pH/percentage of Cr(VI) reduction	R^2, MSE	Optimized data set and a result of the proposed mathematical equation obtained from RSM used to train the ANN model to predict the percentage error reduction of Cr (VI) adsorption and exhibited low MSE and high R^2 value.
50	Shojaeimehr et al. (2014)	Adsorbent by light expanded clay aggregate (LECA)/Aqueous solution	ANN, RSM	initial pH, temperature, initial Cu^{2+} concentration, and sorbent dosage/ removal efficiency of Cu^{2+}	R	ANN raised up with better correlation coefficient and a tool for Cu2+ removal efficiency by using BP and CCF algorithm than RSM.
51	Vasseghian et al. (2014)	Flotation and leaching methods/ bitumen of mines (Kermanshah/Iran)	ANN	the floor, the collector, shaking, pH, solid weight percent and particle size/ percentages of ash and sulphur removal	R^2, RMSE	LM found the accurate model to predict the sulphur removal through flotation and leaching methods.
52	Yurtsever et al. (2014)	Biosorption by valonia tannin resin(VTR)/Aqueous solution	FANN	Operating temperature, initial pH, initial Cd(II) ion concertation, particle size, agitation rate and contact time/ Cd(II) ions adsorption uptake at equilibrium conditions	R^2, MSE	ELLIOT and SIGMOID SYMMETRIC function at the hidden and output layer of ANN used, respectively. Input variables data set have been optimized with multiple regression analysis for four-layer (2-hidden) of ANN model prediction
53	Esfandian et al. (2016)	Biosorption by brown algae (*Sargassum bevanom*)/Aqueous solution	ANN	Initial concentration of mercury, pH, contact time, sorbent dose/Hg(II) removal efficiency	R^2, MSE	ANN model agreed more with experimental data as it is exhibited by MSE and R^2 value. ANN also compared with adsorption isotherm models (Morris−Weber, Lagergren, and pseudo-second-order. To estimate sorption capacity, the sorption data were imported in the Langmuir, Freundlich, Dubinin−Radushkevich (D −R) and Temkin models) and showed superior to them.
54	Esmaeili and Aghababai Beni (2015)	Biosorption (Sargassum glaucescens (brown algae)/effluent of zinc ingot plant in Shahrekord	ANN	Bias, pH, Dosage, Time/Biosorption efficiency of Ni and Co	R^2	The efficiency of *S. glaucescens* ANP (alginate nanoparticles) was set more for nickel ions removal than cobalt and established the best variables to raise efficiency by ANN.
55	Mandal et al. (2015a)	Adsorption by cerium oxide polyaniline (CeO_2/PANI) composite/ synthetic solution	RSM, ANN	Adsorbent dose, contact time, pH, temperature and initial concentration/ removal percentage of Cr(vI)	R^2, MSE, RMSE, MAPE, AARE, Relative error (%)	RSM used to optimize the response by adjusting the different variables, where, ANN showed better predictability of removal efficiency of metal ions with a low score of MSE and AARE and high value of R^2.
56	Nasr et al. (2015)	Biosorption by rice straw/Stock solution	ANN, ANFIS	Biosorbent dose, pH and initial Cd(II) concentration at two-level (low and high)/Cd(II) removal	R	ANFIS evaluated the influence of the variables on output, whereas, ANN predicts the Cd(II) ion removal efficiency with a high value of R.
57	Podstawczyk et al. (2015)	Biosorption by flax meal (oil extraction with supercritical CO_2.)/Aqueous solution	ANN, RSM	metal ions concentration, biosorbent dosage and solution pH/Biosorption efficiency of Cu (II) ion	R^2, MSE, F-value, p-value	Central composite design (CCD) projected the best utility for modeling and optimization among Box −Behnken design (BBD) and full factorial design (FFD). ANN showed more accuracy in line to dependent variables than RSM in the prediction of Cu^{2+} removal
58	Singha et al. (2015)		ANN		MSE, R, AARE, σ, $\chi2$	Authors reported statistical analysis that ANN model with BP algorithm (1

Table 2 (*continued*)

Sl. No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
		Biosorption by rice wastes, hyacinth roots, neem leaves and coconut shells/ aqueous solution		initial pH, initial Pb(II) ion concentration, adsorbent dosages, and contact time/removal of Pb(II) ions		and 25 transfer function in a single hidden layer) produced top predictableness of the percentage removal.
59	Yildiz (2017)	Adsorption by peanut shell/Aqueous solution	ANN	Sorbent amount, initial concentration and initial pH/Zn(II) adsorption capacity	R^2, MSE	ANN was suitable for the prediction as low MSE exhibited, where, Freundlich showed better fitting than the Temkin isotherm model.
60	Ahmad and Haydar (2016)	Biosorption by immobilized *Bacillus subtilis* bead (IBSB)/stock solution	ANN	The influent concentration of metal ions, bed depth of column, flow rate, column internal diameter and the mass of the biosorbent filled inside the column/Thomas model constants i.e. k_{TH} and q_o, or Yan model constants i.e. a and q_o for Cd ion	R^2, RMSE	The best breakthrough curves and parameters of the empirical model of the biosorption process were caught by the ANN model, which modeled with LM algorithm.
61	Debnath et al. (2016)	Adsorption by $CaFe_2O_4$ magnetic nanoparticles (CaF-MNPs)/aqueous solutions	ANN	pH, adsorbent dosage, initial Cr(VI) ion concentration and contact time/ percentage removal of Cr(VI)	R^2, MSE	ANN model predicted the target and be quite agreeable with experimental data as shown by a low value of MSE and high value of R^2.
62	Esmaeili and Khoshnevisan (2016)	Alginate-coated chitosan nanoparticles (Alg—CS—NPs)/aqueous solutions	RSM	The contact time, pH, biomass dose, and initial Ni ion concentration/ Removal efficiency of Ni	R^2	RSM model used to optimize the process for achieving the best removal efficiency of Ni ion, and ANOVA used to determine the adequacy and significance of the model with R^2.
63	Gomez-Gonzalez et al. (2016)	Biosorption by coffee grounds(CG)/ aqueous solutions	ANN	Different pH values/adsorption capacity of lead ions	R	Despite being less capable in the physical interpretation of the isotherm models, ANN stands up the best predictive model among Langmuir and Freundlich isotherm model. The pH was 5 for best removal %.
64	Gusain et al. (2016)	Adsorption by nanocrystalline zirconia/Aqueous solution	RSM	Initial concentration, pH, Adsorbent dose/% removal of Cd ions	R, R^2	Adsorption process optimized by BBD of RSM model. Best-input variables reported achieving the maximum output as removal (%) Cd ion. Predictive model acted with a high value of correlation coefficient.
65	Khandanlou et al. (2016)	Sorption by nanocomposites of rice straw and Fe_3O_4 nanoparticles/ Aqueous solution	ANN	Initial ion concentration, adsorbent dosage, removal time/removal efficiency of Pb(II) and Cu(II) ions	RMSE, R^2	Five algorithm named as quick propagation (QP), Batch Back Propagation (BBP), Incremental Back Propagation (IBP), genetic algorithm (GA) and Levenberg-Marquardt (LM) algorithms have been used to topologies the ANN and IBP of ANN stood up to be the best predictive model for removal efficiency of Pb and Cu ions with the highest R^2 and lowest RMSE indicators.
66	Podder and Majumder (2016)	Biosorption (Phycoremediation of *Botryococcus braunii*)/synthetic wastewater	ANN	Initial pH, Inoculum size (%v/v), contact time, initial concentration/% removal of both As (III) and As(V) ions	R^2, MSE, AE, SD	LM of ANN found suitable to predict the % removal of ions by the phycoremediation process; though, the authors reported, it needs more data to comprise the analysis of the principle of removal of ions by the same technique.
67	Shojaeimehr et al. (2016)	Biosorption by *Gundelia tournefortii*/ Synthetic wastewater	ANN	Temperature, initial Pb ion concentration, initial pH, biosorbent dosage, and contact time/Pb(II) adsorption capacity	R^2, MSE, MRE	ANN model designed with LM-BP algorithm and found the best suited predictive model for Pb ion prediction along with a high value of R^2, and low value of MSE and MRE.
68	Varshney et al. (2016)	Biosorption by itaconic acid grafted poly (vinyl) alcohol encapsulated wok pulp (IA-g-PVA-en-WP)/stack solution	ANN	Different metal concentration, varied biosorbent dose, varied contact time/ Sorption efficiency of Cd(II), Pb(II), Ni(II)	R^2, MSE	LM-BP algorithm used to train the ANN model for best prediction ability with high R^2 value. Sensitivity analysis reduced the time of modeling run by removing low sensitivity values of input channels.
69	Allahkarami et al. (2017)	Biosorption (by carboxymethyl chitosan bounded Fe3O4 nanoparticles)/Aqueous solution	ANN, MNLR	pH, contact time, initial concentration of metal ions and adsorbent mass/ amount adsorbed of Ni(II) and Co(II)	R^2, MSE	Both ANN and MNLR predictive model showed perfectly with their performance matrix, though ANN performed with more in terms of accuracy.
70	Ashan et al. (2017)	Adsorption by NiO nanoparticles/ Aqueous solution	ANN, RSM		R^2, MSE	Optimized data has been used to evaluate the performance of ANN

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Table 2 (*continued*)

Sl. No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
				Initial Cr(VI) concertation, amount of adsorbent, contact time and pH/Cr(VI) adsorption %		predictability and found the performance indicator near one.
71	Dil et al. (2017a)	Adsorption by nano-rods (ZnO-NRs-AC)/stock solution	ANN, RSM	Initial heavy metal (Cd^{2+}, Co^{2+}) and azo dyes concentrations [Methylene Blue (MB) and Crystal violet (CV)], adsorbent dosage and ultrasonic time/adsorption efficiency of heavy metals (Cd2+, Co2+ ions) and azo dyes (MB and CV)	R^2, RMSE	RSM used to optimize the best parameters of the adsorption process to evaluate the maximum adsorption efficiency whereas, ANN trained with LM algorithm picked up a better predictive model to use these input variables to estimate future absorption capacity.
72	Dil et al. (2017b)	Absorption by Copper oxide nanoparticle-loaded activated carbon (CuO-NP-AC)/aqueous solutions	ANN, RSM	Pb2+ ions and MG concentration, pH, amount of adsorbent and ultrasound, irradiation time/removal of Pb^{2+} and Malachite Green (MG)	R^2, MSE	ANN and RSM have been used to determine the optimum input variable to achieve the best output dependent variable and ANN found slightly better with R2 value than RSM.
73	Dil et al. (2017c)	Adsorption by modified genetic megnatic nanomaterials/Aqueous solution	RSM	Initial Pb^{2+} ion concentration, pH, adsorbent mass and ultrasound time/percentage removal of Pb^{2+}	R	CCD of RSM used to optimize the data and CCD evaluated by ANOVA and calculated the value of R to calculate the prediction value of lead removal efficiency and experimental value by this adsorbent.
74	Fiyadh et al. (2017)	Adsorption by deep eutectic solvents functionalized CNT/Aqueous solution	ANN	pH, adsorbent dosage, contact time and Pb^{2+} initial concentration/removal percentage of Pb(II)	R^2, MSE, RMSE, RRMSE, MAPE	The FFBP and layer recurrent used to train the ANN. FFBP used further to set the design as R^2 and MSE showed better than layer recurrent result.
75	Hernández-Hernández et al. (2017)	Adsorption by reverse stratified bone char/Aqueous solution	ANN	Metal properties (molecular weight, electronegativity and ionic radius), feed concentration, feed flow, stratified bed length and the operating time of the adsorption column/ratio (*Ct,i*/*C0,i*) of the breakthrough curve of copper and zinc	Modeling error %	ANN model is challenging for binary adsorption process with maximum modeling error in the breakthrough zone of C_t/C_0 patterns.
76	Hymavathi and Prabhakar (2017)	Biosorption by *Cocos nucifera* L. leaf powder/Stock solution	RSM	The initial concentration of Co(II), pH, adsorbent dosage, and temperature/percentage adsorption of Co	R^2	CCD of RSM utilized to predict the response and evaluated an R^2 by ANOVA. Value of R^2 was near one, which showed excellent performance of the model.
77	Oguz (2014)	Sorption by ignimbrite/aqueous solution	ANN	pH, the sorption time, the concentration of initial Fe3+, bed depth, flow rate and particle size and/Fe_o^{3+} concentration as a function of reaction time for Removal of Fe^{3+} ion	R^2, RMSE	Sensitive analysis performed to assess the vital input variables of ANN on removal efficiency. In addition, ANN used to predict removal efficiency.
78	Siva Kiran et al. (2017)	Bio sorption by three species of *Spirulina (Arthrospira) maxima*, *Spirulina (Arthospira) indica* and *Spirulina (Arthospira) Platensis*/Aqueous solution	ANN, BB	Initial concentration Cd, biosorbent dosage, agitation speed and pH/% adsorption of Cd	R	BB modeled for optimization of input variables for best output. Coupled BB_ANN model found a predictive model with high correlation coefficient for low concentration of Cd ion removal process.
79	Mendoza-Castillo et al. (2018)	Adsorption by bone-char/Aqueous solution	ANN	the initial metal concentrations of four metals (Cd2+, Ni2+, Cu2+ and Zn2+ ions)/equilibrium concentrations and adsorption capacity ($q_{e,i}$)	R^2, Modelling error (*ei*, %)	This study revealed that the output variable of a binary, tertiary and quaternary mixture of heavy metals play a key role to design the best predictive model. Equilibrium concentration used as output variable may cause incorrect prediction, whereas, designed adsorption capacity ($q_{e,i}$) − based ANN model is capable and flexible to predict precisely even in multi-component composition behavior of bone char.
80	Shanmugaprakash et al. (2018)	Biosorption by Pongamia (*Pongamia Pinnata)* oil cake/	ANN, RSM	For Batch mode: pH, temperature, the dosage of biosorbent and For Continuous mode: flowrate, initial concentration of Zn(II) ion, bed height/Zn(II) ion uptake rate	R, AAD, MPE, RMSE, SEP, R	Uptake capacity of Zn (II) ion found better in batch mode than a continuous mode of biosorption process. ANN predictability stands up better than RSM for Zn (II) ion uptake rate along with higher performance indicators.
81	Titah et al. (2018)	Phytoremediation by Ludwigi octovalvis/solution of As(V) salt	ANN, RSM	As concentration in the soil, sampling day, and aeration rate/total As removal from soil (%) efficiency	R^2, AAD, RMSE, adjusted R^2	Multilayer feedforward neural networks and a BFGS algorithm used to construct ANN biases and weight with the highest R^2 and lowest AAD and RMSE value than RSM model.

Table 2 (*continued*)

Sl. No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
						However, both models are good for optimization of the variables.
82	Uddin et al. (2018)	batch adsorption experiments of pottery sludge/synthetic solution	ANN, RSM	pH, initial Cu2+ concentration, contact time, temperature/removal percentage of Cu2+	MSE	BBD of RSM was implemented to optimize the mathematical model of isotherm and LM of ANN sought well to deep prediction values.
83	Abdulhussein and Alwared (2019)	Sodium Dodecyl Sulfate (SDS) as a surface-active agent and sunflower seed husk/Synthetic solution	ANN	contact time, surfactant concentration, flow rate, initial copper concentration and sunflower seed husk dosage/removal efficiency of Cu (II) in %	RMSE	LM used to architect the ANN model for predicting the Cu ions and evidenced its capacity for this aim. The scholars confirmed the significant correlation of the pH and time-dosage variables on the flotation process and sorptive floatation process, respectively by sensitive analysis.
84	Altowayti et al. (2019)	Removal by indigenous *Bacillus thuringiensis* strain (WS3) from arsenic-laden tailing dam/aqueous solution	ANN	contact time, temperature, pH, As (III) concentrations and adsorbent dosages/ As (III) adsorption	R^2, MSE	The Langmuir equation revealed better fitting than the Freundlich model for ANN and revealed by a good degree of correlation (R^2) between the actual and predicted removal of As (III).
85	Ashrafi et al. (2019)	Adsorption by carboxylate-functionalized walnut shell (CFWS)/ Aqueous solution	ANN, MLR	pH, initial concentration, adsorbent dosage and contact time/removal percentage of Pb^{2+}	MSE, MAE, R^2	ANN produced better statistical quality and lower prediction error than MLR. Moreover, the initial concentration of Pb ion picked up with the highest significance for the removal percentage of Pb ion by both models.
86	Blagojev et al. (2019)	sugar beet shreds/aqueous solution	ANN, RSM	initial concentrations of Cu(II) ions, the adsorbent dose and pH of the inlet solution/critical time (best capacity of adsorbent showed until this time)	R^2, SSer	Authors found the best predictive critical time from ANN-GA while pH was a significant parameter as a result of a BBD of RSM model. They proposed a parallel sigmoidal model (PS) based on the asymmetric shape of the breakthrough curves.
87	Kavosi Rakati et al. (2019)	Polyaniline modified chitosan embedded with (ZnO/Fe3O4) nanocomposites/Aqueous solution	RSM	pH, contact time, initial concentration of copper, temperature, and adsorbent dosage/ removal of Cu (II)	R^2	CCD of RSM used to evaluate the best range of input variables to maximize the adsorption capacity. Quadratic models used to describe the relationship between response and variables precisely.
88	Rossi et al. (2019)	Phytofiltration by *Brassica Napas*/ Aqueous solution of Engineered nanoparticles (CeO_2) and HM (Cd)	ANN	Leaf fresh weight, root fresh weight, leaf dry weight, root dry weight, net photosynthesis rate at day 60, stomatal conductance at day 60, and F_v/F_m at day 60/percentage of Cd and Ce in root and leaf of *Brassica Napas*	MSE, R	Physiological parameters of the plant have been used as input variables to training the ANN model prediction for Ce and Cd accumulation in root and leaf of a plant. ANN model displayed slightly better prediction for Cd than Ce by performance indicators such as higher R and lower MSE value, respectively.
89	Shandi et al. (2018)	Removal achieved by raw *Gundelia tournefortii* (GT)/Aqueous solution	ANN, MnLR	pH, contact time, adsorbent dosage, initial concentration and temperature/ Biosorption capacity of Cu (II)	R^2, MSE	The authors used the MnLR and ANN to optimization and prediction, Both models showed potential to do it, Sensitive analysis conducted with ANN and established the initial Cu (II) concentration; which was the most effective parameters against others on biosorption capacity.
90	Tümer and Edebali (2019)	Sorption by commercial resins (Amberjet 1200H and Diaion CR11)/ Aqueous solution	ANN	contact time, adsorbent dosage, pH, and initial concentration/removal efficiency of Cr (III)	R^2, MSE	The feasibility of the ANN models was examined for the resin removal of trivalent Cr and demonstrated a reliable intelligent predictive model.

1997). In general, BP or the combination of BP and least squares assessment is applied to HM parameter prediction. Several fuzzy models, such as Takagi–Sugeno (TS), Mamdani, and GGFKB, have been applied to HM removal studies as listed in Table 3 (a and b).

Elektorowicz and Qasaimeh (2004) demonstrated a hybrid model (i.e., GGFKB), that is more reliable and user-friendly than the FDSS in terms of predicting mercury metal adsorption.

Fuzzy set theory has been investigated for HM removal techniques in terms of optimization and prediction. Singh et al. (2006) compared the potentials of the ANFIS and ANN models for Cd removal prediction. A total of 20 neurons were designed at the hidden layer of the FFBP network of the ANN model. Fuzzy interference used the optimized membership function, fuzzy logic operators, and if–then rules to input variables and improve target yielding. The ANFIS model outperformed the ANN model in terms of accuracy by holding the irregularities and uncertainties of variables against target.

The findings of three comprehensive research works based on

Table 3a
The summarized details (calibration approach, predictive models, input/output variables, performance metrics and research remark) of the reviewed researches on heavy metal variables using the feasibility of fuzzy logic models over the period (2000–2020).

Sl. No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
1	Elektorowicz and Qasaimeh (2004)	Biosorption by wetland plant (floating and rooted)/	Fuzzy logic model	pH, temperature, initial mercury concentration and chloride concentration/mercury uptake efficiency	NA	GA used to optimize the data to train the fuzzy-based decision support system (FDSS) to catch up with the highest degree of predictability; moreover, they did not use any performance indicator.
2	Singh et al. (2006)	Adsorption by hematite ore/ Aqueous Solution	ANN, Hybrid Neuro-Fuzzy Model, ANFIS	Initial Cd (II) concentration, agitation rate, temperature, pH/Adsorption	R^2, % error	Hybrid Neuro-Fuzzy model reported the best model to predict the adsorption process of Cd(II) ion with the lowest value of error than ANFIS and single-layered feed-forwarded of ANN, respectively.
3	(Rahmanian et al., 2011a)	Filtration treatment by micellar-enhanced ultrafiltration (MEUF)/ Aqueous solutions	Fuzzy logic model	SDS feed concentration (C_{SDS}), surfactant to a metal molar ratio (S/M ratio), pH/ permeate flux and rejection factor for Pb removal	ARE, AARE, SD	BBD used to attain the maximizing Pb removal by MEUF process and then after the Fuzzy logic model designed to predict the permeate flux and rejection factor for Pb removal and illustrated maximum agreed of correlation with experimental data.
4	(Rahmanian et al., 2011)	Filtration treatment by micellar-enhanced ultrafiltration (MEUF)/ Aqueous solutions	Fuzzy logic model	SDS concentration, pH and surfactant/ metal ratio/permeate flux and rejection for Z(II)	R^2, AARE, SD, CE	FFD optimized variables applied to the ANFIS model to predict the permeate flux and rejection for Zn (II). This model showed a high degree of acceptance with actual data.
5	Rahmanian et al. (2012)	Filtration treatment by Micellar-enhanced ultrafiltration (MEUF)/ Synthetic wastewater	ANN, RSM, Adaptive neuro-fuzzy inference system (ANFIS)	Initial surfactant concentration, Surfactant to Metal ratio and Feed solution pH/permeate flux and the rejection rate of Pb^{2+} removal efficiency.	R^2, MSE	Authors proposed RSM to assess the process but ANN and ANFIS model found reliable to predict the MEUF method performance. Moreover, ANFIS showed better correlations than ANN.
6	Bingöl et al. (2013)	Adsorption by Date palm (*Phoenix dactylifera* L.) seeds/ Aqueous solution	MLR, ANFIS	pH, biosorbent mass and temperature/ Cu(II) removal	R^2, RMSE	Polynomial regression method i.e. ANFIS found better to predict Cu(II) ion removal onto Date palm than MLR by using high R^2 and low RMSE value.
7	Turan and Ozgonenel (2013)	Adsorption by leachate(Clinoptilolite)/ effluent of ETI Copper Works in Samsun, Turkey	ANFIS, 2^3 full factorial design	Initial pH, adsorbent dosage, and contact time/Cu(II) ion removal	R^2	ANFIS express a high degree of predictability for Cu (II) removal than a traditional mathematical model.
8	Jafari and Jafari (2014)	Biosorption by *Vibrio parahaemolyticus* (PG02)/ Aqueous solution	ANN, ANFIS, RSM	pH, temperature, and initial mercury(Hg^{2+}) concentration/ mercury removal percentage	R^2, SD, SSE, MSE, RMSE	CCD of RSM used to assess the impact of operational parameters and found better than ANN and ANFIS. Where LM of ANN showed up than Gaussian MF of ANFIS as revealed by R^2 value. Though, Authors suggested all three models have well fitted the experimental data and can be applied for prediction of the mercury metal.
9	Mandal et al. (2015b)	Adsorption by zirconium oxide ethylenediamine adipate (ZEDA)/Stock solution	ANFIS	Operational parameters (Dose, pH, time, temperature, initial concentration) and experimental design parameters (bed height and flow rate)/efficiency of As(III) and Cr(VI) removal	R, AARE, MSE	ANFIS optimized the variables for a maximum response as well as predict the output with a significant score of R and AARE.
10	Rebouh et al. (2015)	Biosorption by wheat straw/ Aqueous solution	ANFIS, Langmuir, Freundlich and Redlich-Peterson	Initial metal ion concentration, Initial pH, temperature, contact time, straw particle size(granulometry), and biosorbent chemical treatment/percentage removal of Cu(II) and Cr(VI)	R^2, RMSE	ANFIS exhibited better result over conventional method such as Langmuir, freundlich, redlich-peterson inline to interpolated, extrapolated data, fast result and accuracy obtained by indicators.
11	Ronda et al. (2015)	Biosorption by untreated and chemically treated olive stone(OS) obtained from oil extraction plant, Jaén Spain/ Stock solution	ANFIS, full factorial design method	The concentration of the chemical agent, pH and initial lead concentration/ Biosorption capacity of Pb(II)	R^2	ANFIS outperformed FFD method to predict the metal adsorption. Treated OS showed better adsorption capacity than the untreated one.
12	Javadian et al. (2017)	Adsorption by activated carbon nanocomposite(NiO/ Rosa Canina-L seeds)/aqueous solution	Fuzzy-logic-based model	pH, contact time (min), dosage (g) and initial concentration of Pb (II)/adsorption of Pb (II)	R^2	Proposed Madami type of fuzzy logic model by means of 26 if-then rules found a suitable realistic prediction for removal performance of sorbent.
13	Jana et al. (2018)	Filtration treatment by micellar-enhanced ultrafiltration (MEUF)/ aqueous solutions	RSM_BBD (Box-Behnken design) and an interval type-2 fuzzy logic controller (IT2FLC)	SDS feed concentration, surfactant to the metal molar ratio (S/M ratio) and solution pH/lead removal	R	This study produced all systematic integrated approach for modeling process condition and their prediction so that MEUF process can be enhanced. Although, after all, rigorous study, authors suggested to have quantitative and its financial effects with more

Table 3a (*continued*)

Sl. No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
13	Lashkenari et al. (2018)	Adsorption by γ-Fe_2O_3/ Polyrhodanine nanocomposite	ANFIS, two empirical models (Thomas and Yoon methods)	Treatment time, initial concentration of Zn ion, column height, flow rate/effluent-to-influent concentration of Zn (C_t/C_o)	R, RMSE, MAE, N–S	accurate tools such as interpretative structural modeling method, Simulink, fuzzy artificial neural network, to evaluate the scale of efficiency. Prediction of effluent-to-influent concentration of Zn (C_t/C_o) reported with ANFIS, Thomas, Yoon model and ANFIS stood up than other two with a high value of R and less value of RMSE and MAE.

Table 3b
The summarized details (predictive models, river or region, input/output variables, performance metrics and research remark) of the reviewed researches on heavy metal variables using the feasibility of fuzzy logic models over the period (2000–2020).

Sl.No.	Reference	Predictive models	River or region	Input/Output	Performance Matrix	Remark
1	Sonmez et al. (2018)	An adaptive neuro-fuzzy inference system (ANFIS)	Filyos River, Turkey	The concentration of Fe, Cu, Mn, Zn, Ni, Cr/Cd concentration	The mean absolute deviation (MAD), mean squared error (MSE), root mean square error (RMSE), mean absolute percentage error (MAPE), Nash-Sutcliffe efficiency (E), and coefficient of determination (R^2).	ANFIS methodology for Cd metal prediction found better than conventional data processing method with high correlation. Authors suggested ANFIS model can be dependable for another heavy metals predication.

the fuzzy logic, ANN, and ANFIS models are presented in this section. These models have been used for Pb ion adsorption prediction (Jana et al., 2018; Rahmanian et al., 2011, 2012). They typically used S/M and pH/flux or rejection ratio as input parameters. The first study used the BBD of RSM to optimize the data for the Mamdani model's structure of the fuzzy logic system along with the *triangle* membership function as the input and max–min aggregation and centroid defuzzification methods to calculate the reliability and accuracy of prediction.

Rahmanian et al. (2011) addressed the FFD to distinguish all the important factors of the experimental process of Zn(II) rejection estimation, permeate flux, and its prediction. Given that factorial designs produce many curvatures, the Mamdani fuzzy model network applied a fuzzifier, a defuzzifier, and a fuzzy inference engine to capture the curvature of the response. The authors concluded that the result of the model was qualitatively and quantitatively consistent with actual data.

Two intensive studies on Cu(II) ion removal were reported in 2013. Bingöl et al. (2013) compared the ANFIS and MLR prediction models for date palm adsorption. The ANFIS model was designed with an FFNN in which each layer was a neurofuzzy layer with 27 rules and *gaussmf* to achieve a prediction accuracy better than that of the MLR model. Turan and Ozgonenel (2013) stated that the ANFIS (pi-shaped MF) model was better than the full-factorial mathematical design in predicting clinoptilolite adsorption capacity from real industrial wastewater (i.e., effluent of ETI Copper Works in Samsun, Turkey).

In another study, Jafari and Jafari (2014) applied three different AI approaches (i.e., ANN, ANFIS, and RSM), to simulate and predict Hg(II) removal. CCD, LM, and Gaussian MFs were selected to design the RSM, ANN, and ANFIS models because of their low error terms. All three models showed potential in predicting Hg(II) removal. However, researchers conducted a verification test to produce the sequencing of the model by obtaining low to high percentage errors (ANN < ANFIS < RSM). The ANN model exhibited the most accurate predictability in mercury removal.

Mandal et al. (2015b) investigated the predictability of the batch and column experimental process of As(III) and Cr(VI) removal percentage prediction by using the neurofuzzy method to reduce the cost of experimental efforts. A hybrid (combination of the gradient descent and least squares methods) learning rule (i.e., the Sugeno type fuzzy model) with Gaussian MFs used 81 and 32 rules for the batch and column experiments, respectively, to achieve remarkably high in terms of predicting both ions.

Rebouh et al. (2015) used two predictive models—an intelligent modeling system (i.e., ANFIS) and a conventional mathematical isotherm model (i.e., Langmuir, Freundlich, and Redlich–Peterson), to predict the Cu(II) and Cr(VI) removal process. ANFIS was proven to be a better predictive model compared with traditional isotherm models in terms of evaluating interpolated and extrapolated data. ANFIS used the bell-shaped function at the first layer for exhibition, the t-norm to "AND" membership grades at the second layer, the ratio calculation for the firing strength at the third layer, and the TS fuzzy design at the fourth layer. Researchers proposed this model for use in predicting other HMs, dyes, and organic solvents separately or in groups.

In another study, Ronda et al. (2015) used two models (i.e., ANFIS and FFD) to predict Pb(II) ion adsorption. The second-order equation (i.e., the 27 (3^3) of the FFD method) illustrated all factors that considerably influence the response. The Gaussian member function stood out with the best modeling architecture of the ANFIS model for predicting Pb(II) ion adsorption. The effect of chemicals follows the order NaOH > H_2SO_4 > HNO_3 > untreated olive stone (OS) as per their adsorption improvements of OS biosorption (Table 3 (a)).

Javadian et al. (2017) studied an intelligent architecture-based fuzzy technique (i.e., Mamdani-type of fuzzy inference) that comprises 26 rules with eight levels of triangular membership functions. The technique indicated a R^2 value and exhibited its potential in predicting Pb(II) sorption.

Lashkenari et al. (2018) conducted a comparative study of an intelligent modeling system (i.e., ANFIS) and empirical models (i.e., Thomas and Yoon methods). Among the various membership functions utilized, *gbelmf* was the best, followed by *trapmf* and *gaussmf*, as per the high *R* value, the Nash–Sutcliffe (N–S) coefficient, and low MAE and RMSE. The results of ANFIS revealed more matches with the experimental value compared with those of the empirical models for Zn ion adsorption using a nanocomposite (γ-Fe_2O_3/polyrhodanine) in a fixed-bed column experiment.

Sonmez et al. (2018) explored five layers of the learning process of the hybrid learning algorithm and used *gaussmf* to design a TS-type fuzzy inference system for the prediction of Cd ion concentration of the Filyos River in Turkey. ANFIS displayed a high degree of reliability and robustness, as indicated by performance evaluators.

2.3. Kernel models (support vector machine (SVM), support vector regression (SVR), SVM–GA

Since 1995, the support vector machine (SVM) has been used in the development of the science and engineering fields (Vapnik, 2013). However, it has not been explored much for solving environmental issues. For HM removal, minimal research has been conducted in the past two decades, as illustrated in Table 4. The generalizing capacity of SVM makes SVM superior to many AI models due to its prompt high convergence response and because it overcomes the overfitting phenomenon and ignores the local minima (Parveen et al., 2017a; Solgi et al., 2017). The comprehensive theoretical and mathematical concepts of kernel-based learning methods have been discussed in previous studies (AK, 2002; Cristianini and Shawe-Taylor, 2000). In general, the proper kernel function of SVM called support vector regression (SVR) is used to rectify regression issues, which is utilized to construct nonlinear data-driven models for small samples, local minima, and high-dimensional space (Aryafar et al., 2012; Solgi et al., 2017). In recent years, several studies have investigated SVM. Salehi et al. (2016) proposed the intelligent least squares SVM (LS-SVM) method to predict the equilibrium adsorption of Cu(II). The LS-SVM method obtained optimized data from coupled simulated annealing (CSA). Then, the nonlinear and linear equations (Lagrange multipliers) were separated using the appropriate kernel function (i.e., RBF). The authors evaluated the performance of the model through an advanced $R^2{}_m$ matrix along with five performance indicators and found a high agreement between the predicted and actual values.

On the basis of Shur River's downstream HM detection, prediction, generation, release, and transportation, two exclusive studies are reviewed in this section. Both studies compared two data-driven models (Gholami et al., 2011). compared the SVM and BPNN models for predicting Ni and Fe metals, whereas (Aryafar et al., 2012) compared the SVM and GRNN models for Cu, Fe, Mn, and Zn. The robust intelligent system (the SVM) is trained with the early stopping and automated Bayesian regularization method most of the time, whereas the leave-one-out (LOO) cross-validation technique is used to estimate the optimum procedure for the radial basis Gaussian function (RBGF) kernel technique, which is used to build the model effectively. The BPNN was trained with the early stopping and automated Bayesian regularization method by (Gholami et al., 2011), whereas the trial-and-error method with an optimum smooth factor (SF) was utilized by (Aryafar et al., 2012) to construct the GRNN model. Overall, statistical learning theory (SLT) (i.e., SVM) outsmarts the BPNN and GRNN models due to its high degree of accuracy, reliability, and consistency with the experimental data. The other models also alternative options after SVM as per their evaluator indicators. A reviewed study also reveals that Ni metal prediction was more accurate than Fe metal prediction, and another study reported an HM removal sequence of Mn, Zn, Cu, and Fe from high to low prediction accuracy.

Aya et al. (2016) studied the removal rate of Fe(II), Mn(II), fulvic acid, and iron hydroxide from drinking water, which has been modeled for selecting optimal parameters for the best prediction value using the unified SVR model. A grid search with 10-fold cross validation was used with the RBGF kernel technique to generalize and enhance the performance of the SVR model.

A team of researchers compared the predictability of SVR against an MLR model for Pb(II) ion sorption in the first study and analyzed the Cu(II) ion biosorption capacity in another study (Parveen et al., 2017b, 2016). In both studies, the SVR model was developed with a hyperparameter and an RBGF kernel parameter, thus providing optimized data from the grid search methodology with 10-fold cross validation. The problem of kernel function and bias parameters was rectified using single Karush–Kuhn–Tucker conditions. The SVR model outperformed the MLR model as indicated by various evaluation indicators (Table 4).

González Costa et al. (2017) conducted a comprehensive research on five toxic metals (i.e., Cd, Cu, Ni, Pb, and Zn) as a response and 15 explanatory variables to characterize soils using SVM, MLR, and regression trees. LM multiple regression was found to be a remarkable model. MLR exhibited more affinity for Cr, Cu, and Pb which are associated with a humified organic matter (OM), and hematite. To overcome the challenge of noise, the SVM model utilized the maximum parsimony principle. Most explanatory inputs were clay among 15 predictors followed by the percentage of vermiculite and slime where these were same in case of Cd and Cr adsorption as well. Furthermore, these two metals illustrated remarkable performance by both MLR and SVM regression. Marginal adsorption and retention have been reported between Cr and Cd and Cu and Zn in multiple regression and between Cr and Cd in SVM regression. Ni adsorption was estimated to have the highest number of variables.

In 2017, Cr(VI) sorption prediction was studied by using and comparing the SVR, MLR, and ANN models (Parveen et al., 2017a). The RBGF kernel function was constructed in the SVR model to generalize, optimize, and predict efficiency, and SVR outperforms MLR and ANN in terms of predictability accuracy, and generalization.

Two studies based on a hybrid model (i.e., SVM-GA) have been conducted. Hlihor et al. (2015) used GA for adaptive crossover and mutation rates to enhance the rate of model performance. RBGF was used for the structural risk minimization (SRM) principle for the SVR algorithm (SVM for regression) to build a robust intelligent system and capture the pattern easily for Cd(II) biosorption prediction. Meanwhile, Solgi et al. (2017) proposed the combination of SVM and GA and compared it with the ANN model in terms of predicting Cr(VI) removal. GA is popular for its usefulness in the global search of complex search spaces. Hence, GA was used to optimize the input data for the RBGF constructed for the SVR model. In the model, LM was used to train the MLP network of the ANN model, which used the same variable and was evaluated by various indicators. The SVR model outperformed the ANN model.

2.4. Evolutionary models

Evolutionary models (e.g., differential evolution (DE), genetic programming (GP), GA, PSO, etc.) have emerged recently in HM removal modeling due to their high capability of reducing global optimization issues by using different genetic functions (i.e., cross over and mutation) and search algorithms, thereby addressing overfitting problems, especially in cases of GA and GP (Danandeh Mehr et al., 2018; Esmaeili and Hashemipour, 2018; Kinnear et al., 1999). GP is famous for being less problem-dependent while computing with an intelligent approach (Okhovat and Mousavi, 2012). GA is also popular for its application of mutation and crossover to a population of encoded input data spaces and addressing many optimization issues (Cao et al., 2017). Information on detail theory and the mathematical approaches of evolutionary

Table 4
The summarized details (calibration approach, predictive models, input/output variables, performance metrics and research remark) of the reviewed researches on heavy metal variables using the feasibility of kernel models over the period (2000–2020).

Sl No	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
1	Okhovat and Mousavi (2012)	Filtration by nanofilter(NF)/ Aqueous solution	Genetic programming	Feed concentration and TMP/ions rejection (As, Cr, Cd)	R^2, SSE, MSE, RMSE, NB%	GP used as a predictable tool to assess the performance of NF process for each HMs removal separately, in line to ion rejection as a function of TMP and feed concentration. GP exhibited as an empirical model which promptly acted as a less problem-dependent model
2	Curteanu et al. (2014)	Adsorption by ash and modified ash	SNN-GA (neuro-evolutionary optimization methodology)	type of adsorbent, pH, adsorption time, solid/liquid ratio, and the initial ion concentration in solution/process yield for Cu(II)	R, APE, MSE	SSN entails of three different neural structure of MLP and fetched optimal data design by GA of ANN to optimize the best output. Authors performed to optimize the removal process to give best process yield, mostly.
3	Mandal et al. (2014a)	Adsorption by cerium oxide tetraethylenepentamine (CTEPA) hybrid material/ Aqueous solution	GP, LS-SVM	Temperature, time, concentration, pH and dose/As(III) removal	R^2, MSE, RMSE, MAPE, AARE, NB, SD (σ), chi-square ($\chi 2$)	GP method performed better predictively for As (III) than the LS-SVM model and showed 97.2% maximum removal by the hybrid adsorbent.
4	Yasin et al. (2014)	Adsorption (by intercalated tartrate-Mg-Al layered double hydroxides)/Aqueous solution	ANN and Genetic algorithm (GA)	time, solution pH, adsorbent dosage, and lead ion concentration/Removal of Pb ions	R^2	Levenberg-Marquardt (LM) of ANN used to develop a predictive model to achieve the best determination coefficient (R^2) value, whereas, ANN model used with GA to utilize the simulation and optimization of the lead ions removal.
5	Mohan et al. (2015)	Adsorption by cupric oxide nanoparticles (CuONPs)/ Aqueous solution	ANN-GA, RSM	initial Cr(VI) concentration, pH, adsorbent (CuONPs) dose, and temperature/Cr(VI) removal	R^2, MSE	CCD of RSM optimized the best coherency between variables and target and then followed by ANN-GA model to predict the Cu (VI) removal.
6	Patil-Shinde et al. (2016)	Adsorption by tannin-formaldehyde (TFA) and tannin-aniline formaldehyde (TAFA) resins/Aqueous solution	computational intelligence (CI) such as genetic programming (GP) and genetic algorithm (GA)	Moles of tannin, aniline and formaldehyde, and reaction pH/ adsorption (%) of arsenite [As (III)] and arsenate [As (V)] ions on TFA and TAFA	RMSE, R	Proposed 'GP-GA' hybrid model is for modeling and optimizing the adsorption reaction data without detailing of physiochemical properties of reaction. The very first time this hybrid model introduced in Environmental Engineering
7	(Zafar et al., 2017)	Adsorption by Zn-loaded pinecone Biochar/stock solution	RSM, ANN, Hybrid Artificial RSM_GA	As(III) concentration, EtOH concentration, and pH/As(III) adsorption capacity	SEP, PE, RMSE	This study depicted RSM-GA was perfect to predict a better optimal solution than normal RSM with a high value of PE. ANN used to estimate the stimulating effect of EtOH followed by pH and As(III) concentration on the adsorption phenomena; whereas, the quadratic model showed the dull impact on the same variables.
8	Cao et al. (2017)	Adsorption by Reduced Graphene Oxide-Supported (Fe_3O_4/rGO) Composites/ Aqueous solution	ANN-GA, ANN, RSM	temperature, initial pH, initial Hg ion concentration and contact time/removal percentage of Hg	MSE, R^2	RSM and ANN used to optimize the variables for enhancing the response, whereas ANN-GA showed better agreement with experimental data than RSM model.
9	Fan et al. (2017)	Biosorption by Reduced graphene oxide-supported nanoscale zero-valent iron (nZVI/rGO) magnetic nanocomposites/Aqueous solution	RSM, ANN-genetic algorithm (GA), ANN-particle swarm optimization (PSO)	operating temperature, initial pH, initial concentration and contact time/removal efficiency (%) of Cu(II)	R^2, ABE, MSE	ANN-PSO reported the best model to optimize the biosorption process over RSM and ANN-PSO.
10	Hoseinian et al. (2017)	ion flotation/Aqueous solution	ANN, Hybrid neural-genetic algorithm (GANN)	pH, collector concentration, frother concentration, impeller speed and flotation time/removal percentage of Ni(II) ions and water during ion flotation	R, NRMSE	ANN predictive model reported better than GANN in line to NRMSE and R. Sensitive analysis has been done to raise up the best suitable input variable to maximize the removal efficiency and water removal.
11	Subashchandrabose et al. (2017)	Biosorption by soil microalga, *Chlorella* sp. MM3/Aqueous solution	ANN, GA, Factorial design	Interaction between the quaternary mixture of polyaromatic hydrocarbons (PAHs), phenanthrene and benzo[a]pyrene, and two heavy metals (Cd and Pb)/removal of PAH and uptake of heavy metals	RE	Use of ANN and GA is limited than factorial analysis. First-time factorial design with ANN and GA reported by researchers. This hybrid predictive model performed significantly for removal of PAH and uptake of heavy metals along with satisfactory RE.
12					R^2	

(continued on next page)

Table 4 (*continued*)

Sl No	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
	Esmaeili and Hashemipour (2018)	Adsorption by CNT/aqueous solution	Genetic Programming (GP)	adsorbent dosage, initial solution pH, initial concentration of Cr(VI), contact time and temperature/final concentration of Cr(VI)		GP showed its perfectness to predict more data to utilize for kinetic and equilibrium parameters.
13	Karri and Sahu (2018)	Adsorption by palm oil kernel shell/Aqueous solution	Differential evolution(DE) embedded neural network (ANN_DE), RSM_CCD	initial solution concentration, pH, AC dosage, residence time and process temperature/percentage Zn(II) removal	R^2, RMSE	Higher R2 and lower RMSE calculated in terms of ANN_DE, which depicted better optimization and predictive model than RSM-CCD.
14	May Tzuc et al. (2018)	Biosorption by clinoptilolite-rich tuffs/aqueous solutions	genetic programming (GP) model and Swarm Particle Optimization (SPO)	the contact time, pH value, initial concentration, and sorbent dosage/ Pb(II) removal	R^2, MAE, RMSE, MAPE	Genetic programming model focused on assessing the optimal input variable for best output i.e. Pb removal, whereas, SPO used to calculate the optimal values. Therefore, the coupled model found a reliable tool to optimize the input variables for the best output.
15	Nag et al. (2018)	Bioremediation by natural (leaves of jackfruit, mango and rubber plants) waste materials/Stock solution	Hybrid model (GA-ANN)	Number of Sorbent, pH, adsorbent dosage, time, and initial concentration/percentage removal of Cd(II)	MSE, R, AARE, SD, CCC, χ^2	This hybrid model used to slim down the optimized performance of the network. A low value of MSE showed excellent performance of the network analysis.
16	Sutherland et al. (2018)	Biosorption by banana floret/ aqueous solutions	ANN_GA	Agitation speed, particle size, pH, time/removal of Cu(II) ions	RE, MSE	ANN model used as a predictive and optimized by using GA. The ANN-GA prediction found a very less residual error.
17	Sadat Hoseinian et al. (2019)	Ion floatation/Synthetic wastewater	GANN, MLR	Time, collector concentration, frother concentration, pH of solution/Zn(II) removal	R, MSE	Hybrid model (GANN) predicted Zn (II) ion removal superiority then MLR as displayed by R ad MSE indicators.

model can be obtained from well-known references for DE (Feoktistov, 2006; Price et al., 2006), GP (Banzhaf et al., 1998; Koza and Koza, 1992), GA (Davis, 1991; Jang et al., 1997), and PSO (Chatterjee and Siarry, 2006; Eberhart and Shi, 2001). DE increases the robustness of AI by adjusting the weights and minimizing the biases of the neurons (Karri and Sahu, 2018). Despite its promising quality, few studies on DE have been conducted, as exhibited in Table 5 (a and b).

Okhovat and Mousavi (2012) proposed a novel robust intelligent model (i.e., GP), for As, Cr, and Cd removal prediction. GP was selected by the authors due to its minimal dependence on problem domain knowledge as input data to the concentration and trans-membrane pressure. Meanwhile, ion rejection was used as dependent data. GP showed a high degree of consistency between the predicted value and the experimental data through its various evaluators, as mentioned in Table 5.

Mandal et al. (2014a) presented a strong evidence of the ability of GP and the LS-SVM model for As(II) removal prediction. Further analysis revealed that the GP model exhibited minimal error in case of a large range between population size and number of generation values. The termination criterion was obtained after several mutations via the crossover approach, resulting in the higher correlation between the predicted value and actual data via GP compared with that via the LS-SVM model.

Mohan et al. (2015) exhibited the effective ability of a hybrid model (i.e., ANN-GA) for Cr(VI) removal prediction; the model was fed by optimized variables obtained by the CCD of the RSM model. GA was used to optimize the weight and bias of the feedforward MLP architecture of the ANN model, which was constructed by the BP algorithm to reach its maximum performance. ANN-GA was applied for Cr(VI) removal process optimization, which was 8.1% higher than that using RSM. In addition, ANN-GA exhibited a better prediction ability compared with RSM.

Cao et al. (2017) examined Hg removal prediction with various input variables by using a GA embedded in an ANN model. The solution of optimization issues and the enhancement of the adsorption rate through the ANN-GA model resulted in a 5% error between the predicted and actual values, which was significantly lower than the error deliberated by the RSM model in which BBD was used to calculate the response function and determine the coefficient.

Hoseinian et al. (2017) established a hybrid neural–genetic robust model for Ni(II) removal prediction. Compared with when the ANN model alone is used, the initial weights of the neurons and the threshold of the network features were adjusted for the hybrid ANN-GA model to escape the local minima and match the predicted data with the actual value. With only the ANN model, the CCD algorithm was applied to build the RSM model to optimize and then simulate the treatment procedure using the ANN model.

Esmaeili and Hashemipour (2018) proposed the GP model for Cr(VI) adsorption prediction. The major reason for selecting GP was to generate additional data for kinetic and equilibrium model prediction and precise estimation. The GP model uses an initial population by using the tree and max gene depth approach to show its potential.

Recently, Nag et al. (2018) presented a GA-ANN hybrid model for Cd(II) ion removal prediction. The authors used GA to optimize the treatment procedure, the input variable, and the number of neurons at the hidden layer and enhance the adsorption and performance of the AI model. GA was performed by utilizing the roulette selection rule along with the single point crossing over and uniform mutation rules. The performance of the GA-ANN model is superior to various conventional isotherm models.

Two rigorous scientific works are discussed in this section, focusing on the As(III, V) removal process. These processes were optimized and simulated by various computational intelligence approaches, such as GP, GA, RSM, ANN, and RSM-GA (Patil-Shinde et al., 2016; Zafar et al., 2017). The data-driven modeling strategy (i.e., GP) minimized the complication of assumptions regarding the form of the data fitting function and used the optimized input data acquired by the GA algorithm, thereby improving the adsorption of As(V) on tannin-aniline formaldehyde (TAFA) resin by 12.77% with

Table 5a
The summarized details (calibration approach, predictive models, input/output variables, performance metrics and research remark) of the reviewed researches on heavy metal variables using the feasibility of evolutionary models over the period (2000–2020).

Sl.No.	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
1	Hlihor et al. (2015)	Biosorption by dead and living biomass of *Trichoderma viride*/ Aqueous solution	SVR-GA	pH, biomass dosage, metal concentration, contact time and temperature/biosorption efficiency of Cd(II)	R^2	SVM-GA used to find the optimal working conditions and produce high prediction value by its performance indicators.
2	Aya et al. (2016)	Adsorbent by submerged reactor membrane/Stock solution	SVR	Fe(II), Mn(II), fulvic acid and iron hydroxide/membrane pressure change	R^2, RMSE	A unified SVR method used to estimate the performance of the membrane in terms of Fe and Mn ion removal.
3	Salehi et al. (2016)	Adsorbent by modified membrane [amino-functionalized multi-walled carbon nanotubes (MWCNT-NH_2)]/synthetic water	Least-Squares Support-Vector-Machine (LS-SVM)	Membrane adsorbent types, initial concentrations of Cu(II) ion and temperature/Equilibrium adsorption of Cu(II) ion	R^2, APRE, AAPRE, RMSE, STD, $R^2{}_m$	Authors used LS-SVM algorithm and got satisfactory confidence limits and correlation coefficients to predict adsorption efficiency of modified MWCNT which was prepared and studied holistic approach of adsorption process in their previous work (Salehi et al., 2016)
4	Parveen et al. (2016)	Adosrption by tree fern/Aqueous solution	SVR, MLR	Initial lead concentration, pH, temperature and contact time/ sorption capacity of Pb (II)	AARE, R, RMSE, SD, MRE	Hyperparameter(C, ε) and Kernel parameter (RBF, γ) kernel used to architect the RBF and the performance indicators of this model shows better than the SVR model predictability.
5	(González Costa et al., 2017)	Sorption by soils/Soil sample	SVM, MLR, regression trees (RT)	15 explanatory variables characterizing soils/Sorption and retention of Cd, Cu, Ni, Pb and Zn metals	R^2, MAD	Authors reported each of the metals adsorption and retention and grouping as a binary combination. Cr, Cu and Pb sorption and retention were exhibiting higher R^2 value.
6	Parveen et al. (2017a)	Biosorption by a litter of natural trembling poplar(*Populus tremula*)/Aqueous solution	SVR, MLR	Adsorbent concentration, pH, particle size, initial Cu(II) concentration, agitating speed and temperature/Cu(II) biosorption efficiency	R^2, R, AARE, RMSE, SD, MRE	Again the same authors used SVR and MLR with the same training and testing algorithm but different variables in input and output. Again, the author found SVR is superior in line to generalization and prediction ability.
7	Parveen et al. (2017b)	Adsorption by maize bran/ aqueous solutions	ANN, Support Vector Regression (SVR), MLR	contact time, initial sorbate concentration, pH of the medium and temperature/sorption capacity of Cr(VI)	R, AARE, RMSE, SD, MRE	SVR raised up in statistical evaluation parameters, higher generalization ability and accuracy than ANN and MLR, consecutively. ANN and MLR were based on empirical risk minimization (ERM).
8	Solgi et al. (2017)	Adsorption by Medlar seed (*Mespilus germanica*)/Aqueous solution	ANN, Support Vector Regression-Genetic Algorithm (SVR-GA)	pH, initial concentration of Cr(VI), adsorbent dosage and contact time/ % of Cr(VI) removal	R^2	Very first time Medlar seed used as an adsorbent to remove Cr (VI). Hybrid SVR-GA model predicted % of Cr (VI) removal better than ANN with more accurate of Regression correlation coefficient value.

Table 5b
The summarized details (predictive models, river or region, input/output variables, performance metrics and research remark) of the reviewed researches on heavy metal variables using the feasibility of evolutionary models over the period (2000–2020).

Sl.No.	Reference	Predictive models	River or region	Input/Output	Performance Matrix	Remark
1	Gholami et al. (2011)	SVM, back-propagation neural network (BPNN)	Shur River, southern Iran(Feb 2006)	pH, SO4, HCO3, TDS, EC, Mg, and Ca/Ni and Fe concentrations	The correlation coefficient (R) and RMSE	Inline to the high correlation coefficient and faster running time have been obtained by SVM than BPNN
2	Aryafar et al. (2012)	Support vector machine (SVM), General Regression neural network (GRNN).	Shur River, Sarcheshmeh copper mine, Iran (Feb 2006)	pH, SO4, Mg/Cu, Fe, Mn, Zn	RMSE, Correlation coefficient (R)	Both models are based on data-driven but SVM stood up in line to explicitly with RMSE reduction and quicker than GRNN.

a high degree of agreement with the actual data of As(II, V) adsorption (Patil-Shinde et al., 2016). In another study, GA-optimized data were simulated with the RSM model, showing a better performance compared with the BBD-optimized data. This RSM-embedded data along with a feedforward neural network trained by the LM BP algorithm performed well due to the applicability of the search algorithm and the global optimization solution (Zafar et al., 2017).

Two intellectual studies are reviewed in this section for Zn(II) removal prediction to develop an AI model, i.e., ANN-DE, RSM, GANN, and MLR (Karri and Sahu, 2018; Sadat Hoseinian et al., 2019). Delay in mode building occurred due to eight/bias issues, which were addressed by the hybrid model (i.e., DE entrenched with ANN), which outperformed the CCD-embedded RSM model (Karri and Sahu, 2018). In another study, GA was used to adjust the initial weight and threshold of the BP algorithm to improve the MLP model performance over MLR and RSM (Sadat Hoseinian et al., 2019).

Three exhaustive works on a hybrid intelligent model for Cu(II) removal prediction are examined (Curteanu et al., 2014; Fan et al., 2017; Sutherland et al., 2018). The first study proposed a neuro-evolutionary optimization methodology (i.e., single neural network

(SNN)-GA). An SNN comprises three combinations of MLP (8:20:1), MLP (8:25:1), and MLP (8:18:1), with optimized percentage contributions of 60%, 27%, and 13%, respectively. A stack composed of an MLP network processed with GA-optimized input data produced an effective prediction of Cu(II) as per the performance indicators (Curteanu et al., 2014). In the second study, two robust intelligent modeling systems were introduced (i.e., ANN-GA and ANN-PSO) and compared with each other and with RSM. The optimized value for procedure showed maximum model efficiency evaluated by ANN model than RSM, whereas BPNN (i.e., ANN-PSO) searching the optimization by updating the generations, found superior by 3.15% and 8.54% in case of ANN-GA and RSM, respectively. Last year, Sutherland et al. (2018) used a stochastic nonlinear optimization method (i.e., GA) to enhance the efficiency of the ANN model for Cu(II) removal prediction using different variables, and ANN-GA performed well.

Three scientific works on Pb(II) removal prediction using various statistical and intelligent predictive models are logically examined in this section (May Tzuc et al., 2018; Subashchandrabose et al., 2017; Yasin et al., 2014). Yasin et al. (2014) utilized the remarkable features of GA to optimize the experimental predictors and enhance the presentation of the model. Then, they used the LM-trained ANN model in the simulation process to produce the highest prediction value. Subashchandrabose et al. (2017) proposed the FFD for its typical advantages of easy and precise factorial analysis and used it in the ANN and GA models for predicting the uptake capacity of HMs. Therefore, improved input data were utilized in the embedded model, exhibiting a high degree of predictive robustness and consistency with the experimental data. May Tzuc et al. (2018) integrated GP with PSO for its well-known features that suited the experimental procedure of Pb(II) removal. The syntax tree of GP arranged the population (individuals), which was reproduced through generations, and obtained the mathematical equation through an iterative process by which PSO performed well on multivariable optimization problems to produce high-performance matrices.

2.5. Hybrid soft computing model application

Different types of data mining models, such as ANN, RSM, MLR, fuzzy logic, SVR, GA, and GP, have many advantages. However, various issues, such as the activeness of nonlinear regression data, the normalization conditioning of the variables, and the initial weight adjustment of the neural network, remain. A trend has progressed to host new mathematical or statistical methods broadly in environmental engineering for the complex nonlinearity of the experimental data of the HM removal process. The flexibility of improved or hybrid methods enables them to deal with the problems mentioned above. A hybrid or improved model is required to improve the robustness of the model for specific HM treatment techniques. Ignoring the variance issues to enhance the forecasting process (Quinlan, 1996), proposed BRT. Nonlinear equation performance can be enhanced by regression analysis and evaluated by different PMs (Yan et al., 2000). Hybrid models of AI have to go long way for HM removal prediction as the limited number of studied conducted so far which displays in Table 6 (a and b). The following models or algorithms could be learned comprehensively through theoretical and computational approaches, such as the dose response (DRM) and diffuse layer (DLM) models (Dobson and Barnett, 2008; McCullagh, 2019), SOM (Kohonen et al., 1999; Ritter et al., 1992), BRT (Friedman, 2002; Roe et al., 2005), distributed time delay (DTD) (Zhou, 2014), cascade forward (*cascade*) and Elman (*Elman*) neural networks (Cheng et al., 2002; Fahlman and Lebiere, 1990), quantitative ion character–activity relationship (QICAR) model (Le Faucheur et al., 2011), artificial bee colony optimization (ABCoptim) (Karaboga and Basturk, 2008), group method data handling (GMDH) (Farlow, 1984; Onwubolu and Onwubolu, 2015), and partial least squares regression (PLSR) (Abdi and Williams, 2013; Jang et al., 1997).

Two decades ago, Yan et al. (2000) presented a modified nonlinear regression model (i.e., DRM) that outperformed conventional isotherm models (i.e., Thomas or Bohart model and Adams model) for HM (Pb, Cd, Ni, and Zn) biosorption kinetics by (*Mucor rouxii*) column. The nonlinear least squares method was utilized to assess the parameters of the nonlinear regression model to obtain high R^2 values.

In 2001, a surface complexation model with DLM was proposed to understand the surface charge effects on adsorption and enhance the adequacy of the prediction of Cu(II) and Cd(II) removal (single or combination of HMs) from the dried waste slurry obtained from seafood-processing factories (Lee and Davis, 2001).

Lee and Scholz (2006) proposed an SOM model to predict two HMs (i.e., Cu and Ni), in wetlands. SOM can be utilized with complete domain knowledge. The Euclidian distance was used to measure the weight vectors of SOM, and those near the best matching unit (BMU) were selected. Furthermore, the BMU result in the map for each dataset was used to predict the HM removal in urban runoff and evaluated by the low mean absolute scaled error and high R^2. The quantization (QE) and topographic (TE) errors were obtained for the mean distance between each data and BMU and for a proportion of all data.

Khajeh et al. (2013) conducted a comparative study between RSM and ANN-PSO for the prediction, simulation, and optimization of the Mn and Co metal extraction process by using a tea waste adsorbent. The BBD algorithm was used to optimize the experimental variables for the ANN and RSM models. PSO typically adjusts the initial weight by searching a large area of neurons to enhance the robustness of the ANN model, thus facilitating HM prediction with a higher consistency with the experimental data compared with the conventional statistical model (i.e., RSM).

Thomas breakthrough equations and the ANN model were applied for two commercial bone chars (i.e., BCM and BCB) to analyze the potential and challenges of hybrid models and determine the dynamic adsorption of fluoride contamination (Tovar-Gómez et al., 2013). The input value of the Thomas model for calculating the F_i/F_o ratio was used as the output of the ANN model to ignore its negativity restrictions. Another input value of ANN was estimated by the Thomas breakthrough curves.

An ensemble approach (i.e., CCD of the RSM and desirability function approach (DFA)) was applied to optimize the BRT, ANN, and RSM models (Mazaheri et al., 2017) for Cd(II) and MB dye removal from walnut carbon. CCD was used to minimize the number of experimental trials, which was essential to obtaining the main effect of each parameter and its interactions. In general, the CCD algorithm was used with the DFA to optimize the input variables and increase the removal percentage of HM and dyes. By contrast, LM was used to train the ANN model and optimize the grouping parameters (i.e., lr, tc, and nt) to obtain the smallest values of lr for the best predictive performance of the BRT model with the minimum error. BRT showed a better parsimonious model compared with ANN and RSM by evaluating the performance indicators.

Moreno-Pérez et al. (2018) introduced surrogate modeling embedded with ANN, DTD, *cascade*, and *Elman* for the multicomponent dynamic adsorption of ternary and quaternary HM ((i.e., Cd(II), Ni(II), Zn(II), and Cu(II) ions)) systems onto biochar. FFBP is a common network aggregated with DTD (FFBP-DTD), which is famous for its time dependency along with the tap delay line associated with the input weight for obtaining the finite dynamic output. *Cascade* has ensemble weights which comes from the input

Table 6a
The summarized details (calibration approach, predictive models, input/output variables, performance metrics and research remark) of the reviewed researches on heavy metal variables using the feasibility of hybrid soft computing models over the period (2000–2020).

SL. No	References	Treatment Technique/source of heavy metal	Proposed predictive models	Input/output variables	Performance indicators	Research finding
1	Yan et al. (2000)	Biosorption by *Mucor rouxii*/ Metal solution	Modified dose-response model (non-linear regression model)	Flow rate, influent pH and influent concentration of metals (Pb, Cd, Ni and Zn)/Biosorption of metals (Pb, Cd, Ni and Zn) and breakthrough curve	Random error	The modified model represented better suited for prediction and estimation of biosorption result than conventional models like Thomas model and Bohart–Adams model with the low error value.
2	Lee and Davis (2001)	Adsorption by a dried waste slurry of seafood processing factories/Aqueous solution	Diffuse layer model (DLM)	pH, bed volume, the ratio of Cu(II) and Cd(II)/% adsorbed of Cu(II) and Cd(II)	NA	A surface complex model with DLM showed significate tool to optimize and predict the Cu and Cd removal process by adsorption technique.
3	Lee and Scholz (2006)	Biosorption by wetlands consists of gravel and sand substrate and native Phragmites australis/Urban runoff	self-organizing map (SOM)	conductivity, pH, temperature and redox potential, DO, Outflow temperature/Ni and Cu concentration	R^2, MASE, QE, TE	The SOM model showed the best performance especially for Ni and Cu in water flow. Correlation established to set the best relation of input to each output.
4	Khajeh et al. (2013)	Adsorption by solid-phase tea waste extraction	Hybrid of artificial neural network particle swarm optimization (PSO_ANN), RSM	pH, amount of tea waste, the concentration of PAN (complexing agent), effluent volume, the concentration of eluent, and sample and eluent flow rates/extraction percent Manganese (Mn) and Cobalt (Co)	RMSE, MPE, SEP, R	Authors used ANN_PSO and RSM predictive model to assess the removal efficiency of the adsorption process of Mn and Co. Hybrid ANN_PSO showed better prediction fittings with a maximum correlation coefficient.
5	Tovar-Gómez et al. (2013)	Fixed or packed bed adsorption by bone(BCM from Carbones Mexicanos and BCB from Brimac Carbon Services) char/ aqueous solution	Hybrid ANN-Thomas model	Feed fluoride concentration, the operation time of packed bed column and the feed flow/break through the curve of fluoride adsorption	R^2, MSE	The first time, traditional linear regression of Thomas breakthrough equations of vibrant adsorption process upgraded by application of ANN with about unity of determination coefficient.
6	Mazaheri et al. (2017)	Adsorption by walnut wood/ Aqueous solution (Binary)	BRT, ANN, RSM	Stirring time, pH, adsorbent mass and concentrations of MB and Cd^{2+} ions/ percentage removal of MB and Cd^{2+}	R^2, AAD, MAE, RMSE	Variables importance on response and their respective places for it measured by BRT. RSM used to analysis of variance. CCD and DFA algorithm of ANN used to optimize the variable for effective response. BRT illustrated obviously better than others in line to performance indicators did for Cd and MB removal process.
7	Moreno-Pérez et al. (2018)	Biochar (bone char)/Aqueous solution	ANN surrogate model [FFBP, FFBP-DTD, Cascade forward neural network (Cascade), Elman neural network (Elman)]	feed composition (C0), feed composition (C0)/concentration profile (C_t/C_0) of Cu ion and multi-metallic solution	R^2, eM %, RE	The authors revealed that Cascade was the best model for multi-metallic adsorption breakthrough curve modeling against FFBP, FFBP-DTD and Elman.
8	Salahinejad and Zolfonoun (2018)	Adsorption by multi-walled carbon nano tubes (MWCNTs)/ stock solution	Quantitative ion character-Activity Relationship (QICAR)	Boiling point, Electronegativity atomic number, covalent index, effective nuclear charge, square of ionic radii with coordination number/q_{max} of 25 HMs [Ag(I), Al(III), As(V), Ba(II), Bi(III), Cd (II), Co(II), Cr(III), Cs(I), Cu(II), Fe(III), Ga(III), Hg(II), In(III), Mn(II), Ni(II), Pb(II), Rb(I), Se(VI), Sr (II), Ti(IV), Tl(I), V(V), Zn(II) and Zr(IV)]	r^2_c, r^2_p, Q^2_{loo}, Q^2_{lmo}, RMSEC, RMSEP, r^2_m, MAE, CCC	QICAR used GA, ERM, SPA and ERM–OSC–PLS to optimize the best variables of out of 200. ERM–ISC–PLS Model revealed the best response for prediction of the removal capacity over others. ERM searches with a full landscape including local minima, whereas, GA restricted with an initial set of variables.
9	Ferreira et al. (2019)	Biosorption by emulsion liquid membrane of biosurfactant [(ELMB), chelating agents and biosurfactant produced in loco]/Aqueous solution	artificial neural network (ANN) and ABCoptim	concentrations of EDTA, D2EHPA, NaCl, and H2SO4, and the contact time/removal of Mn (II)	R^2, RMSE	Hybrid model (ABCoptim) successfully satisfy the optimization of variables for better yield and the fast process of predication reported by ANN of Mn (II) ion removal by the low cost of the process i.e. ELMB techniques.
10	Sekulić et al. (2019)	Membrane filtration techniques/Synthetic wastewater	PNN_GMDH, MLR	Characteristic parameters (molar mass of heavy metals, molar mass of metallic solution, molar mass of complexing agent) and Operational parameters [pH, initial concentration of heavy metals {Zn(II), Pb(II), Cd(II)} ions, concentration of complexing agent, and pressure on flux]/flux prediction	R^2, RMSE, MAE, MAPE, d_r	PNN is non-physical and self-synthesis ANN architect model used GMDH and MLR algorithm to understand the complexity of the relation between flux (output) and multivariable (input). This model showed the perfect result with different evaluator indicators. Authors also reported published ANN work showed incapability to understand this experimental design relationship.

Table 6b
The summarized details (predictive models, river or region, input/output variables, performance metrics and research remark) of the reviewed researches on heavy metal variables using the feasibility of hybrid soft computing models over the period (2000–2020).

SL.No.	Reference	Predictive models	River or region	Input/Output	Performance Matrix	Remark
1	Yu et al. (2001)	Multivariate linear regression (MLR), Correlation analysis (CA), Principal component analysis (PCA)	Five rivers (Yenshui river, Tsengwen river, Chishui river, Potzu river, Peikang river) of southern Taiwan. (spring and summer of 1998)	Zn, Cu, Pb, Ni, Cr, Co/ correlation of binding fractions between any two heavy metals along with its oxides and organic matter(OM)	Correlation coefficients (R), Coefficients of determination (R^2)	These three statistical methods used to find the correlation between the metals, oxides, sediments matrices and OM. CA and PCA used to find a binding fraction of any two heavy metals along with its clarification. MLR method also used to evaluate the enslavement of such a correlation.
2	Xia et al. (2007)	A four univariate regressions model (linear, logarithmic, power, exponential regression models), Partial least-square regression (PLSR)	Yangtze river of Bagua zhou island, China (October 2004)	Cd concentration, spectral variables/sensitive wavelength for Cd concentration.	Pearson correlation coefficients (PCC), RMSE, Root-mean-square error of cross-validation (RMSECV)	This research revealed the theoretical approach to predict Cd concentration and its binding types based on its spectral data. PCC was evaluated to fix the sensitive wavelength for Cd concentration by using CD concentration and spectral variables. The univariate model used to predict Cd concentration by using its relation with bands; whereas, PLSR used to compare the univariate model result and validated with RMSECV.
3	Wang et al. (2015)	Linear regression model (LRM), Principle component analysis (PCA), correlation coefficient analysis (CCA)	Huaihe River sediments, China (July 2013)	Concentration of Cu, Pb, Zn and Ni/Enrichment factor(EF) distribution, cumulative distribution function (CDF)	Pearson correlation coefficients, the Correlation coefficient	The concentration of Zn estimation went up among all by using LRM and PCA. Researchers studied the geo-accumulation index (Igeo) and modified geo-accumulation index (Igeom) and compare with the heavy metal profile of regional background along with the suggestion to the next research is needed to confirm this.
4	Bhuyan and Bakar (2017)	PCA, Correlation matrix, ANOVA	Halda river, Bangladesh	Eigenvalues/Pb, Cd, Cr, Cu, Hg, Al, Ni, Co, Zn, Mn,	p for ANOVA	PCA used to evaluate the best relation between the heavy metals; whereas, Correlation matrix found the set of the relation between the variables. ANOVA found no significant variation between the site and HM.

and others antecedent. *Elman* has a context layer at the hidden part for the familiarization of the time-varying characteristics of a structure. The FFBP-DTD model exhibited improved multimetallic adsorption breakthrough curve modeling and prediction performance. The authors mentioned that the model failed to simulate the zone of the breakthrough point. Therefore, the accuracy must be improved by reducing the error for a packed bed column.

Salahinejad and Zolfonoun (2018) evaluated the performance and challenges of the QICAR model for the absorption capacity of 25 HMs using multiwalled carbon nanotubes. QICAR is associated with quantitative structure activity and inadequate with definable and accessible descriptors for metal ions and an insufficient number of metals. Each sample was optimized with GA (along with partial least squares (PLS)), enhanced replacement method (ERM), and successive projection algorithm (SPA). The orthogonal signal correction (OSC) approach minimized the variation from input variables. The SPA was used to ignore the variable collinearity issues of the model. ERM was performed for the global search to reduce the standard deviation of the linear model. The PLS-GA method was applied to construct the QICAR model and secure maximum adsorption. Lastly, the authors reported that the ERM–OSC–PLS model exhibited the best performance in terms of understanding the behaviors of asymmetric relation and statistical prediction performance.

Ferreira et al. (2019) proposed the ABCoptim algorithm to improve the performance of the ANN model for Mn(II) removal procedure. ABCoptim was used to search the global optima of the landscape by self-organization and the division of task as its basic feature. The ANN-ABCoptim model's performance was consistent with the experimental data compared with that of the ANN model alone.

Sekulić et al. (2019) studied the competency of the GMDH and MLR algorithms in understanding the complex behaviors of Pb(II), Zn(II), and Cd(II) flux values through the membrane filter technique. A polyneural network is an auto-organizing ANN and a nonphysical model that ignores the representative validation set; it is superior to MLR or other conventional models due to its different classes, such as linear, quadratic, and cubic, that suit the relationship between the presented variables and the model response as flux prediction.

Four studies are reviewed on the basis of different intelligent models (i.e., regression, CA, and PCA) to estimate the HMs from different river sediments in Asia (Bhuyan and Bakar, 2017; Wang et al., 2015; Xia et al., 2007; Yu et al., 2001). The first study compared the correlation analysis (CA), PCA, and linear regression analysis (LRA) models to establish the relation of HM binding and sediment matrices (Yu et al., 2001). CA and PCA revealed their ability to strengthen the binary combination within HMs or with sediment metrics, such as Cr–Fe oxides, Zn–OM, Pb–carbonates, and Cu–OM/Fe oxide, which are stronger than three HMs (i.e., Co, Ni, and Mn). In addition, PCA and LRA showed their capability in other binary combinations, such as carbonate-bound Ni and Cr, Fe-oxide-bound Ni and Cr, and Mn-oxide-bound Cu and Cr (Xia et al., 2007). utilized four univariate regression models (i.e., linear, logarithmic, power, and exponential regression models) and PLSR to understand the complex behavior of Cd contamination in the Yangtze River sediment of the Bagua Zhou Island, China. The regression models revealed the quantitative and qualitative analyses of Cd ions in river sediment. PLSR was used for spectral analysis by using different data transformations (i.e., Ref, nRefVIS, and FD) for comparison with the univariate prediction models. In addition, PLSR was utilized by the one-out cross-validation technique for the calibration set to achieve the unscrambler behavior. In the third study, Wang et al. (2015) reported the statistical relationship of four HMs (i.e., Cu, Pb, Zn, and Ni) and their combinations, and a reference element was observed from the sediment from the Huaihe River, Anhui, China. Geochemical normalization and linear regression were applied to predict HM concentration. PCA and correlation coefficient analysis were applied to determine the HM source. A modified geoaccumulation index (I_{geom}) was utilized for generalization. However, a higher value was observed by I_{geom} compared with I_{geo}. A linear regression model was used to analyze Cu, Pb, Zn, and Ni concentrations; Zn exhibited the highest amount. Recently, Bhuyan and Bakar (2017) performed PCA and built a correlation matrix to understand the behavior variation of HMs in the sediment and water of the Halda River in Bangladesh. The spatial and temporal distributions of resultant factors were determined using PCA tools and applied to determine the standard features of dataset variations along with generalization and unification.

3. Treatment techniques for HM removal

Clean water access declined with increasing globalization and industrialization, which have also released various HM effluents in freshwater systems (Le Vo, 2007; Molden, 2013). Fig. 4 shows the most toxic and accessible HMs used for various studies in the past 20 years. The high toxicity of HMs and their accumulation and retention in water bodies have highlighted the need for HM removal studies over the past couple of decades. Fig. 4 illustrates that the Cu ion is the most interesting HM to be treated because it is the most toxic to living organisms and available globally due to industrial effluents, such as metal cleaning, plating baths, pulp, paper board mills, wood pulp production, and the fertilizer industry (Özer et al., 2009; Shanmugaprakash et al., 2018). In addition, Cd, Pb, Zn, and Cr were observed in all reviewed studies in terms of interest among researchers. The availability of Cd in soil due to anthropological activities is toxic to animals and humans (Mendoza-Castillo et al., 2018; Rossi et al., 2019). Pb has typical disadvantages of long-term stability in an ecosystem and causes many human health issues, such as cancer, nausea, and renal failure (Dil et al., 2017c; Fiyadh et al., 2017). The Zn ion is one the most disposed HMs from various industries and causes many hazardous problems to nature (Shanmugaprakash et al., 2018; Yildiz, 2017). Meanwhile, Cr(III) and Cr(VI) ions can harm aquatic life after a certain range (Ashan et al., 2017; Tümer and Edebali, 2019). In the case of As, Co, Hg, Fe, and Mn, interest among environmental scientists has declined, as displayed in Fig. 4, despite their high toxicity to the ecosystem. As(III) is more harmful than As(V), and both revealed toxicity in terms of various human health problems (e.g., melanosis, edema, keratosis, cancer, enlargement of liver, kidney, and spleen problems). Hence, WHO does not recommend their use of above 10 mg/L concentration (Gnanasangeetha and SaralaThambavani, 2014; Mandal et al., 2014a). Despite the great link of B_{12} vitamin with Co, it leads to neurotoxicological disorders due to the high affinity of various chemical reactions that increase the degree of toxicity (Dil et al., 2017a; Hymavathi and Prabhakar, 2017; Khajeh et al., 2013). The inclination of Hg ions may lead to severe long-term ecosystem issues, as reported in the priority list of pollutants by the USEPA and the European Union (Cao et al., 2017; Elektorowicz and Qasaimeh, 2004). Industrial effluents considerably contribute to the release of Fe into water bodies. These effluents may alter the taste and condition of water, stain clothes, and weaken plumbing fixtures, rather than raise major health issues (Aya et al., 2016; Oguz, 2014). Mn is important for the structure and qualitative function of cell enzymes in controlling various metabolic activities within the range decided by WHO (Aya et al., 2016; Khajeh et al., 2013). Fig. 4 illustrates that Sb and Ce are the least important HMs for removal studies. Majority of the reviewed study worked in group of HMs removal by single treatment method. These HMs affect soil microbial activity, leading to the alteration of crop yield (Zhu et al., 2018). Furthermore, the accessibility of Sb and Ce increased in the environment due to mining and smelting processes in recent years (Aydin et al., 2010; Dar et al., 2012; He et al., 2012). Therefore, various treatment techniques play an important role in protecting the environment from the toxic HMs in water or wastewater; these techniques are categorized in Fig. 1. Various types of sorption materials, such as indigenous (IM) and modified indigenous materials (MIM) for different HM removal processes, have been extensively applied; these materials are presented in Fig. 6 to elucidate their application percentage in each category of treatment technique.

3.1. Biosorption process

The biosorption technique has received considerable critical attention. Biosorption is an indigenous way of protecting the environment with less effort. The application of different bacteria, such as *Mucor rouxii*, revealed collective resistance to Pb, Cd, Ni, and Zn (Yan et al., 2000). *Vibrio parahaemolyticus* has a high resistance capacity in different contaminations and exhibits a promising sorption of Hg(II) ions (Jafari and Jafari, 2014), The *Trichoderma viride* species plays a vital role in Cd(II) removal (Hlihor et al., 2015). The immobilized *Bacillus subtilis* bead demonstrates a high capacity for Cd ion removal (Ahmad et al., 2014; Ahmad and Haydar, 2016), and the details of bacteriological remediation are presented in Tables 2–6 The sunburst chart typically illustrates that the natural use of biosorbent materials is approximately 80%, as shown in Fig. 6. Therefore, further research should be conducted to understand the potential of HM sorption and sorbent regeneration by

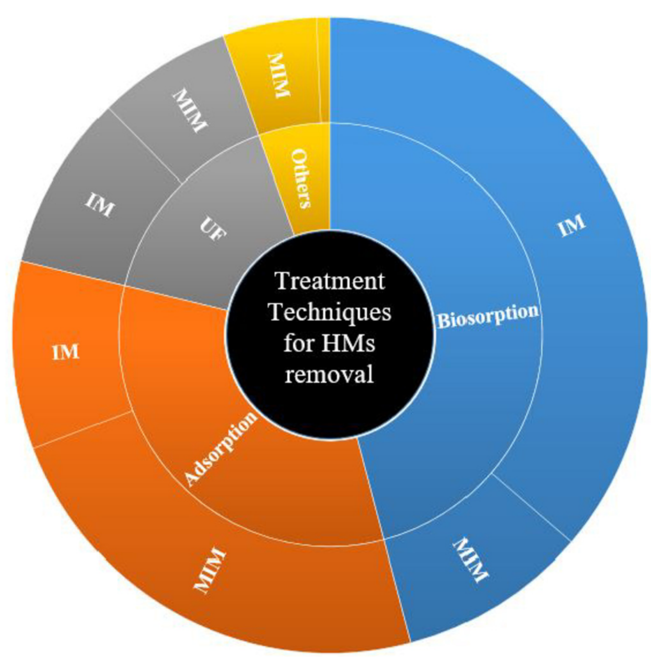

Fig. 6. Sunburst chart of Treatment techniques with indigenous material (IM) and modified indigenous material (MIM).

modifying the IMs, as reported by research on modification (Ahmad et al., 2014; Ahmad and Haydar, 2016; Khandanlou et al., 2016). Another example of modified biosorbents demonstrated 98.31% As(II) removal (Gnanasangeetha and SaralaThambavani, 2014). However, Cu ion removal also increased due to the addition of sodium dodecyl sulfate (SDS) as a surface-active agent for the biosorbent material (Abdulhussein and Alwared, 2019). In the case of Cd removal, modified seafood waste and engineered nanoparticles enhance the sorptive capacity of the biosorbent (Lee and Davis, 2001; Rossi et al., 2019). Both studies on Mn removal showed an improved performance when chemicals, such as chelating and complexing agents, were used (Ferreira et al., 2019; Khajeh et al., 2013).

3.2. Adsorption process

The adsorption process is common in HM removal techniques and characterized by the use of IMs or MIMs. During the past 20 years, many applications of natural materials, either direct or modified, as an adsorbent have been studied. In the composition of the biosorption process, the MIM applied was approximately 70% higher than the IM to enhance the efficiency of sorption potential (Fig. 6). However, complications in the adsorbents' surface structure were observed, increasing the cost of and the time required by the process and requiring skilled supervision (Debnath et al., 2016; Mandal et al., 2014b; Ramazanpour Esfahani et al., 2014; Tümer and Edebali, 2019). These demands may require further studies to address the complication of the treatment method. This process should focus on IM adsorption studies to minimize cost and time, e.g., the simplification of the process for Cu(II) ion removal and the grouping of Pb(II), Cd(II), Ni(II) ion removal (Kabuba et al., 2014; Reynel-Avila et al., 2014). Clinoptilolite materials exhibited the most promise as adsorbent, with minimal effort to remove Pb(II) (May Tzuc et al., 2018) and Cu(II) (Turan and Ozgonenel, 2013). In addition, ignimbrite and hematite ores demonstrated a promising result for Fe and Cd removal, respectively (Oguz, 2014; Singh et al., 2006). Some studies demonstrated the promising result of mining products and HM concentration drainage (Rooki et al., 2011; Turan et al., 2011b). The recent trends for adsorbent selection, such as modified membrane (ELMB), CNT or modified CNT, clinoptilolite or modified clinoptilolite, and chitosan or modified chitosan, are increasing due to its potential for HM removal (Allahkarami et al., 2017; Debnath et al., 2016; Esmaeili and Khoshnevisan, 2016; Kavosi Rakati et al., 2019). Tovar-Gómez et al. (2013) also reported that BCM has a higher adsorption capacity compared with BCB because it has more hydroxyl groups. Cu(II) ion reportedly has a higher adsorption capacity compared with Cd(II), Ni(II), Zn(II), and Cu(II) ions onto biochar (Moreno-Pérez et al., 2018). The tea waste adsorbent Co metal exhibited a higher percentage in adsorbate compared with the Mn metal (Khajeh et al., 2013). Lee and Scholz (2006) showed that Ni exhibits a higher tolerance against salt compared with Cu in wetland soil. All details can be found in Tables 2–6.

3.3. Ultrafiltration (UF) process

UF is an important treatment technique in wastewater engineering and plays a key role in HM removal. In the past two decades, various UFs and improved UFs have been applied to remove different HMs or HM mixtures. Micellar-enhanced ultrafiltration (MEUF) is recognized as a promising HM removal technique. MEUF was applied thrice for Pb ion removal, and the process was explained explicitly, that is, SDS was used as an anionic surfactant to alleviate the power of MEUF in terms of ion exchange (Rahmanian et al., 2012). As soon as the surface of MEUF interacted with the pollutant, the surfactant monomers were converted into micelles through combination; then, micelles lubricated the organic particles or bound the metal ions on the surface of the oppositely charged micelle through electrostatic approaches to remove HMs (Jana et al., 2018; Rahmanian et al., 2011a). The S/M and L/M ratios of MEUF were demonstrated well on Zn removal (Rahmanian et al., 2011; Rahmanian et al., 2011b). Nine comprehensive studies were reviewed to enumerate the soil retention and filtration capability along with various soil properties due to either runoff or mining drainage issues throughout the world (i.e., Spain, Germany, Iran, Taiwan, China, and Bangladesh). In Spain, Fe, S, Cr, Cu, and Pb showed a positive relation with humified OM and hematite (González Costa et al., 2017; Kemper and Sommer, 2002). In Germany, Cu and Zn demonstrated a high affinity with soil retention capacity during water flow (Anagu et al., 2009). In Iran, Ni, Fe, Mn, Cu, Pb, and Fe were detected due to AMD activity (Aryafar et al., 2012; Gholami et al., 2011). However, these high metal concentrations have been explained a decade ago by (Yu et al., 2001) who reported that Fe oxide and the carbonates of soil have a promising binding ability, followed by Mn oxide. In China, the presence of Cd with Fe oxide revealed by Xia et al. (2007) and the order of Zn > Pb > Cu > Ni in terms of amount presented by Wang et al. (2015), they also explained that Zn and Pb may be due to automobiles (ships), coal combustion, and flue gas deposition, whereas Cu and Ni availability can be attributed to anthropology activity. Recently, various toxic metals have been determined in Bangladesh where the concentrations of Pb, Cd, Cr, Cu, Hg, Al, Ni, Co, Zn, and Mn in water and Pb, Cu, Al, Ni, Co, Zn, and Mn in sediment exceeded the acceptable range, especially after monsoon, thereby altering the ecosystem (Bhuyan and Bakar, 2017). The details are presented in Tables 2–6.

3.4. Other processes

Over the last decade, a few studies have been conducted to find alternate options for HM removal to overcome the general issues of the conventional treatment process. The electrocoagulation approach exhibited potential for Cr and Cu removal from aqueous solutions (Aber et al., 2009; Bhatti et al., 2011). Sabonian and Behnajady (2014) proposed a photocatalytic process to remove Cr ions from a solution. Floatation and leaching techniques were applied to remove the mixture of ash and sulphur with good sorption efficiency (Vasseghian et al., 2014). Nano filter tools were used for the removal of HM combinations (i.e., As, Cr, and Cd), demonstrating the potential capability of filters (Okhovat and Mousavi, 2012). Recently, two intensive works were conducted to evaluate the efficiency of the ion flotation technique for Ni and Zn ion removal and yielded encouraging results (Hoseinian et al., 2017; Sadat Hoseinian et al., 2019). Sekulić et al. (2019) applied microfilter treatment for a group of HMs (i.e., Zn, Pb, and Cd) with molar characteristics to enhance the filtration capacity. However, with a limited number of studies, these types of HM removal techniques are expensive and time consuming and require a standard procedure and skilled supervision. Therefore, further research must be conducted to find additional alternative options that are comparable to conventional approaches. The details are presented in Tables 2–6.

4. Research assessment, evaluation, and prospective research possibilities

Although all AI models can be used to optimize and simulate HM removal techniques successfully, the selection of optimization and predictive models for individual HM removal techniques is highly essential. Many of the reviewed papers explained in detail how these two characteristics help obtain a high modeling performance. In most of the reviewed works, MATLAB software was used to design the AI models. In general, 45–55 observations were used to build the model. The following subsections summarize the critical points observed in the reviewed works.

4.1. Superiority of AI models

The application of each AI model is illustrated in Fig. 3, which shows the selection and value of each model among respected researchers. This figure also reveals the gap which would be the prospective models (less used models) for future research to have more conceptual understanding the building process of AI to achieve high performance. ANN as a predictive model for HM removal from aqueous solutions has been conducted by most researchers for improved generalization, optimization, and prediction of HM treatment techniques (Fig. 3). Fig. 8 illustrates the relevant models used for each HM, indicating the importance of each model among the researchers. In general, ANN reported the importance and consequence of both sorbent and sorbate characteristics of the metal sorption along with its kinetics and isotherms. Training and testing processes were used to address the number of hidden layers by minimizing the error (Altowayti et al., 2019); the number of hidden layers was selected by trial and error to design the best NN structure (Fiyadh et al., 2017; Mandal et al., 2014b). In most cases where the ANN model was used, 10 or approximately 10 hidden layers exhibited the lowest MSE value, including the breakthrough curve and the coefficient of adsorption isotherm model as output. In most cases, relevant input variables were optimized using the RSM model; then, ANN was used for prediction. In addition, the prediction values of RSM and ANN were compared. ANN was found superior to RSM with respect to predictability performance. In most works, the RSM model used CCD, FFD, and BBD for simplification in terms of producing optimized data for the ANN model. The potential of RSM could be increased if it is precisely designed in accordance with the experimental design parameters. In most cases, the BP and LM algorithms suited the MLP network with 10 neurons allocated for the hidden layers to build an improved predictive model. Overall, ANN shows a marginally lower predictive error compared with the RSM and MLR models. ANN has also become a benchmark for developing various AI models.

Despite the numerous capabilities of the ANN model, ANN has some limitations, such as the need for a large amount of experimental data for training, overfitting, local minima, the selection of relevant variables, and divergence. ANN also exhibits either incorrect prediction or low robustness in the case of wrongly selected dependent variables, such as the zone of the breakthrough point and the grouping of HMs. ANN-based model simulation can further contribute to the further understanding of the dynamic behavior of the process in which some unfathomable phenomena occur (Esfandian et al., 2016). Modeling enhancement procedures have been introduced to overcome the above issues. The isotherm mathematical equation was used as an additional data producer for HM removal and was optimized using RSM prior to AI model implementation. Various hybrid AI models (e.g., ANN-GA, ANN-DE, ANN-PSO, ANN-DTD, ANN-IPS, and ANN-Coptim) have been applied to increase the robustness of standalone AI models. The BFGS optimization function of ANN has been demonstrated as one of the principal approaches for adjusting the weight and bias of the network. The IPS and two-fold cross-validation methods are well known for determining the lowest error of the network and avoiding the overfitting problem of the network (Anagu et al., 2009).

However, to overcome these challenges and validate the suggested algorithm's efficiency, further research must be conducted for different categories of HM removal techniques. The Mn removal study conducted by the ELMB adsorbent resulted in $R^2 = 0.76$, using only the ANN and ABCoptim models (Ferreira et al., 2019). Thus, this is the potential work to use another model to evaluate the better value of R^2.

The fuzzy logic model offers simplification in terms of pattern understanding between the investigational data and the feedback by using the linguistic expression to present uncertainties. ANFIS is known for minimizing the complexity of the mathematical model for a system (i.e., Mamdani-type and TS-type fuzzy inference systems). However, in the case of Hg(II) removal techniques, ANFIS showed a marginally higher error compared with the other AI models. Fig. 6 illustrates that the application of the fuzzy model to different HM removal techniques requires further attention to assess its performance. Furthermore, the surveyed fuzzy logic performance for grouping HMs and the breakthrough curve data for different treatment techniques have not been investigated.

The kernel model is preferred due to its high convergence, prompt response, minimizing the overfitting phenomenon and local minima ignorance (Abdulwahab et al., 2019). The Bayesian regularization method and RBGF are mostly used, but few studies have applied the hybrid model (i.e., SVM-GA) to highlight the efficiency of the model. Approaches, such as SLT, SRM, RBGF kernel function, LOO, and SF, have been used with SVR to improve the performance of the model compared with different neural networks, such as BPNN and GRNN. However, among other models, SVM has been applied in a limited number of studies (Fig. 3); thus, SVM and the application of kernel model for various HM treatment techniques must be investigated in future research. Ni metal prediction had higher accuracy compared with Fe metal prediction using SVR and BPNN (Gholami et al., 2011). However, Mn > Zn > Cu > Fe revealed the order of predictive accuracy (Aryafar et al., 2012).

The important features of evolutionary models include the self-adjustment of the weight and bias of the neurons, which tend to minimize the global optimization problem, the auto search of the algorithm, and robustness against overfitting issues (Salih, 2019; Salih et al., 2018; Yaseen et al., 2019). GA is increasingly recognized as the best optimizer for input data. GP and PSO are also alternate options in terms of the nonlinearity of the HM removal process. GP is used to generate additional data to feed the modeling for improved performance (Esmaeili and Hashemipour, 2018). Fig. 5 shows that the evolutionary model requires further studies to assess its performance based on different biosorption and adsorption processes with the grouping of HMs in a solution.

Recently, various hybrid model applications for different HMs removal techniques have been observed. ANN outperformed other AI models after combining with different optimization algorithm to sort out the optimal range of variables to gain maximum removal efficiency. The result is promising, exhibiting less network noise and minimal error. This was observed in another research scope of environmental engineering (Afan et al., 2016; Fahimi et al., 2016; Yaseen et al., 2018, 2015). The efficiency of the hybridization of another AI model must also be validated by using the ANN hybrid model as a benchmark for future types of HM removal techniques.

The complex biosorption experimental design must focus on selecting variables, algorithms, and functions to achieve excellent performance. Mostly, PM showed a marginal difference while comparing two models for one experimental design. Fig. 5 shows that the ANN model may be a benchmark for the further advancement of AI model intervention in the HM removal process.

4.2. Importance of optimization algorithm in AI modeling

In the case of the complicated process of HM removal, the construction of AI models depends mainly on three features: a) nature of the predictors and target data; b) optimization of the weights, bias, numbers of neurons—nodes and hidden layers of the processing units; and c) feeding of the model with generalized and optimized input data (Al-Musawi et al., 2018; Al Sudani et al., 2019). These features can improve the maximum output value. These features become more difficult in terms of grouping HMs and derivative variables. The following models could reduce the above issues:

i. FFD was highlighted for its S/M, L/M, and pH/flux simplification process for AI models (Dil et al., 2017a; Turan et al., 2011a).
ii. The CSCF technique was used for optimization by improving the data points between the minimum and maximum removal efficiency (%) due to its ease of implementation and to yield a curve that appears to be unified. Moreover, this technique also ignored the alterations near the first and last samples by using least squares curve fitting (Turan et al., 2011a).
iii. The BFGS optimization function of ANN adjusted the weight and bias of the network successfully in terms of the breakthrough curve, equilibrium concentration, and adsorption capacity parapets as output.
iv. The LOO cross-validation technique was used to estimate the optimum procedure for the RBGF kernel technique of the SVM (Aryafar et al., 2012).
v. The trial-and-error method and the optimum SF were utilized to construct the GRNN model and calculate the optimum processing unit of the model (Aryafar et al., 2012)
vi. The IPS and two-fold cross-validation methods were used to determine the lowest error of the network freely and to avoid the overfitting problem of ANN, respectively.
vii. The GP-integrated algorithm showed a higher data pattern-capturing capability for HM removal techniques compared with LS-SVM (Mandal et al., 2014a).
viii. GA optimization was applied to adjust the noise of the processing unit and the predictors. The roulette selection rule, along with the single-point crossing-over and uniform mutation rules, enhanced the GA optimization power against various isotherm models.
ix. The OSC approach minimized the variations from predictors.
x. SPA was used to ignore the variable collinearity issues of the corresponding model.
xi. ERM was performed for the global search to reduce the standard deviation of the linear model.
xii. The PLS-GA method was applied to construct the QICAR model for securing the maximum adsorption for many HM groupings of 25 metals.
xiii. I_{geom} was utilized for generalization; however, a higher value was observed in I_{geom} compared with that in I_{geo} (Wang et al., 2015).
xiv. The PS method was the best method in terms of ignoring the local minima and the speed of convergence for a feasible optimizing power.
xv. CSA was applied after using the appropriate kernel function (RBF) to separate the nonlinear equation from the linear equation (Lagrange multipliers).
xvi. Single Karush—Kuhn—Tucker conditions were used to minimize the problem of the kernel function and bias parameters (Parveen et al., 2017b, 2016).
xvii. The parsimony principle was used to overcome the challenge of SVM model noise.
xviii. DFA was applied in the optimization of input variables in the groupings of HMs for the BRT, ANN, and RSM models.

4.3. Trend of AI model intervention in HM removal performance

The major advancement of AI modeling was observed in the implementation of new algorithms, functions, and optimization techniques to maximize the performance of the model as per the individual characteristics of the HM removal techniques. Fig. 2 illustrates that the trend of AI model development aids in the HM treatment techniques over the last 20 years. Fig. 2 shows that in the last 7 years, the simulation and prediction of targets have attracted research interest. In 2014 and 2017, research shifted toward SC contribution to cut the cost, skilled supervision, large space requirement, and time required by complex HM removal experimental processes. Fig. 8 shows the importance of each model application in each major HM removal. Figs. 1, 4 and 6 demonstrate that HM removal process simulation should be developed to understand various HM treatment techniques in terms of different HMs and materials used for HM adsorption. In addition, Fig. 6 shows that the reduced MIM of biosorption and reduced IM of adsorption treatment techniques have been conducted in the past two decades. However, the UF process tends to be equal in IM and MIM. Fig. 4 reveals the interest in popular HM selection among the esteemed researchers, revealing the seriousness of HM (more time used) and prospective HM (less time used) removal prediction techniques, which should be tested using different AI models to explore the reliability of the models as per the target and variables. Fig. 5 presents the number of studies for each model per year, illustrating the development of various AI models for HM removal prediction. Moreover, it reveals how the new model has the same purpose and how its importance to researchers varies (e.g., ANN scored maximum times selection in the last decade, followed by RSM). However, hybrid and other newly developed models have been applied in recent years for HMs removal prediction.

4.4. Performance matrix used in various AI models with their merits and demerits

The application of PM was examined to evaluate model performance in terms of the prediction of HM removal efficiency. PM is the mathematical approach to weighing the quality of various AI models. Approximately 30 types of PMs, such as R, R^2, ME, MSE, RMSE, SEP, AAD, MAD, F-value, P-value, EF, MRE, RC, ARPE, AARE, r, E_r, intercept and slope, SDR, MAR, MAPE, SD, AE, eM%, ei%, adjusted R^2, MAE, and SSer, have been applied in all the reviewed works. Fig. 7 shows that 12 out of the 30 PMs have attracted increased interest from the researchers. Fig. 7 also illustrates that the trend line of the graph presents an exponential decline in terms of the

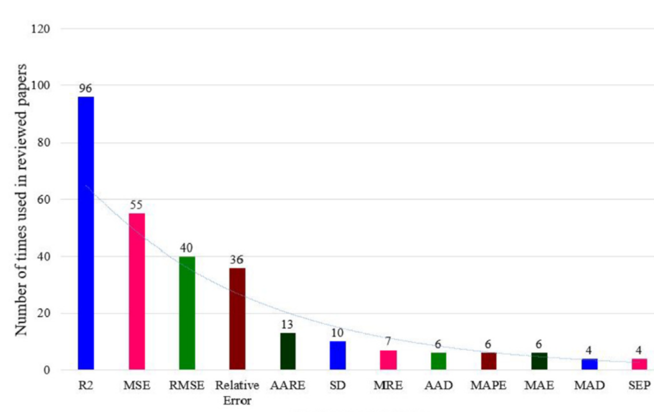

Fig. 7. Number of each performance matrix used among all reviewed papers.

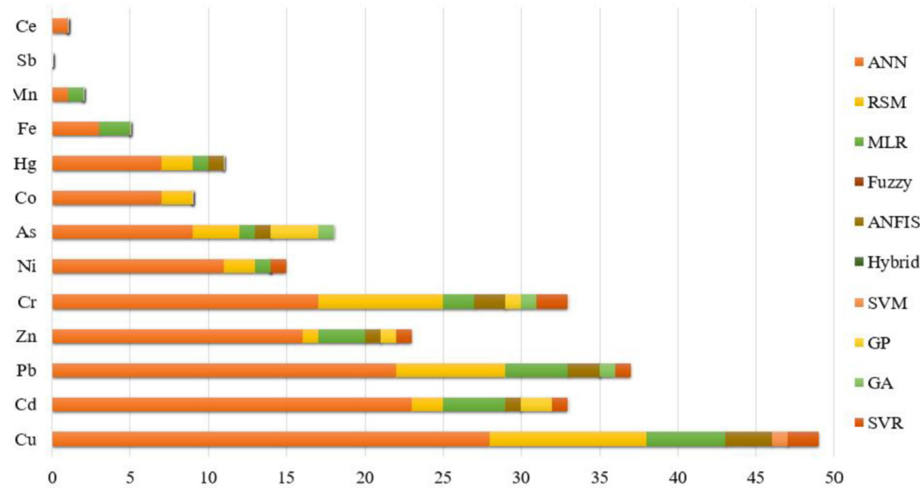

Fig. 8. Various models used for each distinct HM removal.

selection of PM by the researchers, where R^2 was the most selected in many studies, followed by MSE, RMSE, and RE. AARE, SD, and MRE were used 13, 10, and 7 times, respectively. AAD, MAPE, and MAE were applied in six studies, followed by MAD and SEP, which were used four times each. A total of 18 different PMs was of interest for a specific and limited number of studies, as shown in Tables 2–6. These PMs were applied many times and compared with traditional mathematical evaluators, but the selection of the correct PM is depicted in the model performance.

The presentation of the PM based on the AI model followed by HM removal techniques may clarify the optimization, simulation, and prediction performance. ANOVA has also been used many times to validate the model data, followed by enumerating the suitability of AI models using the p- and f-values (Dil et al., 2017a). The following assessments have been evaluated by this study:

i. R^2 or R measures the degree of collinearity of the ANN model simulation, which is used to achieve the efficiency and effectiveness of single HM removal. By contrast, other AI and hybrid models and HM removal experiment combinations require additional PMs to compare the results of the reviewed papers. These PMs are sensitive to extreme values and less sensitive or insensitive to the additional and proportional difference between the model results and the actual data (Chai and Draxler, 2014; Legates and McCabe, 1999; Moriasi et al., 2007).
ii. MSE and RMSE show the basic features for measuring the error between the model output and actual data when a single AI model is applied. RMSE has a marginal sharpness in the overall calculation process while calculating the performance of a specific model. However, they are limited in the case of the breakthrough curve data produced by a hybrid model. In recent years, these models have been used with other newly developed error evaluators, such as QE and TE, which reveal promise in reporting the performance of the model, especially in BMU measurement.
iii. Relative error and AARE are mostly applied for combined AI models (i.e., ANFIS and UF removal techniques). AARE has been recognized for its high sharpness in terms of overall evaluation. However, its use with three to four other evaluators indicates low confidence among the researchers.
iv. In general, SD used in case of ANFIS model to measure the deviation from the mean line in terms of performance of the model. By contrast, SD has a limitation when used for a single model.
v. In most cases, MRE is utilized by the ANN model for the biosorption process (i.e., phytofilter and chitosan) as a sorbate and showed promise with either R or R^2. However, it has been evaluated against R^2 often.
vi. AAD has been mostly utilized for ANN, followed by RSM and BRT. It measures minute deviation but must compare the calculation with other evaluators.
vii. MAPE is applied to assess the single to hybrid model performance. It is sensitive with a high variation in the scatter plot and used with other PMs.
viii. MAE aims to compare the result among other applied PM matrices. It has potential application for hybrid models to check the row error at the testing phase (Yaseen et al., 2016).
ix. MAD is based on the row error value for HM removal of the hybrid model testing phase evaluator. MAD performs better than the standard deviation in terms of outlier data (Leys et al., 2013).
x. SEP is applied in a hybrid model and indigenous adsorbate. If the bias is low, then the SEP can be performed to evaluate the calibration and validation processes precisely (Büning-Pfaue, 2003).

In addition, the remaining PMs used the least number of times in the reviewed works must be applied to HM removal prediction modeling to assess their precision and reliability.

4.5. Assessment of the treatment techniques

Various treatment techniques have been performed for HM removal and integrated with computer aids. Biosorption and adsorption have been applied many times (Fig. 6) with IMs and MIMs and have been proven to be a low-cost approach. Adsorbent pretreatment, such as wheat straw pacified with acidic and alkaline pretreatment, exhibited a good removal result and considerably promoted Cu(II) and Cr(VI) adsorption, respectively (Rebouh et al., 2015). However, Cr comes with low removal percentage during the treatment of HM combinations. In combined HM removal (i.e., dyes and HMs), the effects of pH on HM removal and adsorbent dose on dye removal have been observed (Mazaheri et al., 2017). Most batch experiments executed for the adsorption process are rather continuous; therefore, further research on continuous removal techniques must be conducted to achieve real wastewater treatment requirements effectively. The modified indigenous biosorption process must focus further on computer aids in the future to enhance the removal process and promote the cost reduction of the treatment technique in the case of the indigenous adsorption process.

The high removal efficiency of HMs has been observed by membrane filtration, but expensive and membrane fouling, along with low permeate flux, limit its use. In addition, the difficulties in building proper AI models with these input and output variables are increasing. In the polymer assisted ultrafiltration (PAUF) process, few studies on the flux decline in the dead-end filtration process were found. UF requires further investigation to overcome these challenges. Other expensive HM treatment techniques, such as nanofilter, microfilter, and electrocoagulation techniques with high-efficiency and low-cost sorption processes, such as the photocatalytic process, have been developed. However, these methods experience some challenges in the proper fitting to AI models and in the implementation of the experimental process.

In another study, sodium dodecyl sulfate polyethylene glycol aggregates were adopted to modify the MEUF to enhance the Cu removal process (Xiarchos et al., 2008). PEG has the advantages of water solubility and biodegradability. Khajeh et al. (2013) conducted a comparative study of the Mn and Co metal extraction processes using tea waste adsorbent, where Co showed a better adsorbate percentage compared with Mn. Two bone chars (i.e., BCM and BCB) were utilized to remove the F contamination and revealed that BCM is superior because it has more hydroxyl groups (Tovar-Gómez et al., 2013). The treatment of the combination of dye and HMs from an aqueous solution by using the activated carbon of a walnut wood shell showed a higher removal rate of HMs compared with that of dye (Mazaheri et al., 2017). The correlation analysis indicates that treatment techniques (wetlands) have a high pH effect in winter and on conductivity in terms of Ni removal. Meanwhile, in the case of Cu prediction, redox and temperature are the most effective (Lee and Scholz, 2006). In the case of Cr(VI) removal, CuONPs showed up to 98% removal under the optimized condition, such as initial metal concentration, pH, CuONP dose, and temperature (Mohan et al., 2015). In another study, chicken feathers showed a promising sorption of Pb and Cd ions (Reynel-Avila et al., 2014). Fig. 6 typically illustrates that the use of natural biosorbent materials is significantly higher. Therefore, further research should be conducted to improve the understanding on the HM sorption and regeneration potential (using 0.1 M HCl) of sorbents by modifying IMs, as exhibited by some of the modified works (Ahmad et al., 2014; Ahmad and Haydar, 2016; Khandanlou et al., 2016). Another example of modified biosorbent demonstrated 98.31% As(II) removal (Gnanasangeetha and SaralaThambavani, 2014). Moreover, the Cu ion removal also increased due to the addition of SDS as a surface-active agent to the biosorbent material (Abdulhussein and Alwared, 2019). In the case of Cd removal, modified seafood waste and engineered nanoparticles also enhance the sorptive capacity of the biosorbent (Lee and Davis, 2001; Rossi et al., 2019). Two studies on Mn removal reported an improved performance in the case of adding chemicals, such as chelating and complexing agents (Ferreira et al., 2019; Khajeh et al., 2013).

Each experimental design revealed different efficiencies in terms of the specific HM removal process. The following critical assessments were observed:

i. Physical, chemical, and biological parameters have a remarkable effect on the treatment process, but only few of the reviewed works presented actual wastewater treatment. Therefore, in future works, the experimental design's efficiency must be verified with actual wastewater. Majority of the cases revealed that pH 5 is one of the most sensitive predictors to achieve a process with high efficiency.
ii. The Cr(VI) removal by the biosorption process needs $CaCl_2$ pretreatment to reduce the effect of pH prior to estimation and then followed by simulation process by using BBD of RSM to achieve the substantial improvement of removal and accuracy of prediction (Cobas et al., 2014).
iii. In another study, Ronda et al. (2015) addressed Pb(II) ion adsorption onto chemically treated (with HNO_3, H_2SO_4 and NaOH) and untreated OS. Their result demonstrated that the treatment using this three chemically treated OS sorption was good.
iv. Given that HM selection greatly affects the treatment design and simulation mode, a standard criterion for selecting the valance of HMs should be set for researchers in terms of the feasibility of industrial wastewater treatment (Yetilmezsoy and Demirel, 2008).
v. The assessment of the binding strength between HMs and OM has been studied and reported that Cr bound to Fe oxides, Zn bound to OM, Pb bound to carbonates, and Cu bound to either OM or Fe oxides were stronger than three HMs, namely, Co, Ni, and Mn.
vi. Other binary combinations, such as carbonates bound to Ni and Cr, Fe oxides bound to Ni and Cr, and Mn oxides bound to Cu and Cr, have been mentioned (Yu et al., 2001). HM adsorption has a particular affinity toward specifically adsorbed bed configuration (Hernández-Hernández et al., 2017).
vii. The binding behavior requires further research to enhance removal process efficiency.
viii. Mn removal is often observed in HM mixtures. Thus, Mn removal must be examined alone to understand the nonlinear behavior of Mn.
ix. To the best of the authors' knowledge, the removal of the combination of As(II), Cu(III), Pb(IV), and Cr(V) and simulation models require further investigation because the mixtures of these HMs are the typical effluents of different industries (Aziz et al., 2008; Li et al., 2007; Papandreou et al., 2011).
x. Research on desorption or adsorbent regeneration must be conducted to develop reusable techniques.
xi. The changes in a model (hybridization), in an adsorbent (by combining two adsorbents in a specific ratio/modified product), and in HMs (a combination of different HMs/combination of different ions of the same HM/HM pretreatment) must focused on in future research.
xii. The oscillatory trend of adsorption process parameters must improve the model to improve the residual plots (Gomez-Gonzalez et al., 2016).
xiii. A few studies based on the nonlinear relationship between the properties of sorbent and sorbate have been conducted for HM ion removal. The acidic functional group, the lignin composition of tested biomasses, and pollutant molecular characteristics affect HM sorption (Mendoza-Castillo et al., 2014). Therefore, additional sorbent and sorbate characteristics must be studied.
xiv. In another removal process, Sekulić et al. (2019) applied microfilter treatment for a group of HMs (i.e., Zn, Pb, and Cd) with molar characteristics to enhance the capacity of filtration. However, with a limited number of studies, these types of HM removal techniques are expensive and time consuming and require a standard procedure and skilled supervision. Therefore, effort must be exerted to find alternative options to overcome these issues.

xv. Only one study focused on 25 HMs to reveal real-time process challenges that can be replicated by minimizing the listed challenges during the selection of HMs and other research variables; in this manner, the understanding of the nonlinear relationship between the HMs was enhanced (Salahinejad and Zolfonoun, 2018).

5. Conclusion

The current research reviewed all research papers on HM removal modeling using soft computing methodologies from 2000 to 2019. The main objective of the current research was to provide an integrated viewpoint of various AI models to help experts in decision making and guide researchers who want to contribute to this area. The reviewed works were categorized in accordance with the commonly applied predictive models and subclassified in accordance with the specific HM removal targets, and majority of the reviewed works reported that pioneering or hybrid models outperformed classical ones. This review indicated that several key topics on AI methodologies have yet to be applied to HM removal prediction. These topics included different ANN algorithms, deep learning, unsupervised methods, various metaheuristics, and ensemble models. Furthermore, the ANN for various HM removal prediction techniques is excellent but selecting a single method as the best remains challenging. In addition to the AI models reviewed, single HM removal technique was adopted more frequently than multiple HM prediction techniques in rivers. In terms of the HM removal process, three major categories, namely, biosorption, adsorption, and UF, were recognized. The effect of multiple HMs and the adsorbent characteristics on the HM removal process was not reported comprehensively. Although several measures were used (such as EDA) to determine the prediction accuracy, analyzing the merits and demerits of each applied measure in terms of the nature of the prediction issue could still be an area of prospective research. Most of the reviewed works considered the data of the aqueous solution of HMs. However, real wastewater with the actual presence of various contaminants (i.e., combination of HMs and synthetic organic carbon) with high-accuracy HM prediction is an interesting research direction. In some of the cases, the pretreatment techniques of the HM removal process increased the removal accuracy along with the prediction value of the AI models after few remarkable EDA processes. However, the same cannot be said for the combination of contamination (i.e., for real wastewater and different adsorbent characteristics). Therefore, additional accurate models for HM prediction must be cultivated with various valued EDA steps, and the full potential of different AI algorithms must be utilized in this field.

Declaration of competing interest

The authors have no conflict of interest to any party.

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Abbreviation

Absolute error (AE), Absolute percent error (APE), Absolute relative percentage error (ARPE), Acid mine drainage (AMD), Adjusted coefficient of determination (adjusted R2), Alginate-based composite bead (ABCB), Artificial bee colony optimization (ABCoptim), Average Absolute Deviation (AAD), Average absolute percent relative error (AAPRE), Average absolute relative error (AARE), Adaptive neural fuzzy interference (ANFIS), Average percent relative error (APRE), Average relative error (ARE); Back propagation neural network (BPNN), Batch Back Propagation (BBP), Batch gradient descent (BGD), Batch gradient descent with momentum (BGDM), Best-matching unit (BMU), Boosted regression trees (BRT), Box-Behnken (BB), Box-behnken Design (BBD), Broyden−Fletcher−Goldfarb−Shanno (BFGS); Carboxylate-functionalized walnut shell (CFWS), Cascade forward neural network (Cascade), Charge coupled device (CCD)/Center composite design (CCD), chi square (χ2), Coefficient of determination of calibration (r2c), Coefficient of determination of prediction (r2p), Coefficient of determination/Regression coefficient/R-square (R2), Coefficient of efficiency (CE), Concordance correlation coefficient (CCC), Coupled simulated annealing (CSA), Cubic spline curve fitting (CSCF), Cubic spline curve fitting technique (CSCFT); Defatted Pongamia oil cake (DPOC), Design of experiment (DOE), Desirability function approach (DFA), Differential evolution optimization (DEO); Electrolyte concentration (CNaCl), Elman neural network (Elman), Enhanced replacement method (ERM), Enhanced replacement method−orthogonal signal correction−partial least squares (ERM−OSC−PLS), Evolutionary algorithm (EA), explanatory data analysis (EDA); Feed forward back propagation (FFBP), Feed forward back propagation neural network with distributed time delay (FFBP-DTD), Feed forward neural networks (FFNN), Fisher test (F-test), Fletcher−Reeves conjugate gradient backpropagation (FRCGBP), Fractional factorial design/Full factorial design (FFD); General regression neural network (GRNN), Genetic algorithm (GA), Gradient descent (GD), Group method data handling (GMDH); Implicit finite difference method (IFDM), Incremental Back Propagation (IBP), Index of model performance (dr); Least square curve fitting (LSCF), Leave many-out cross-validated coefficient of determination (Q2lmo), Leave one-out cross-validated coefficient of determination (Q2loo), Levenberg-Marquardt (LM), Levenberg-Marquardt back propagation (LMBP), Ligand−zinc ratios (L/M); Mean absolute deviations (MAD), Mean Absolute Error (MAE), Mean absolute percent error (MAPE), Mean error (ME), Mean modeling errors (eM, %), Mean absolute scaled error (MASE), Mean relative error (MRE), Mean square error (MSE), Median absolute error (MEDAE), Micellar-enhanced ultrafiltration (MEUF), Modeling efficiency (EF), Modified geo-accumulation index (Igeom), Modular neural network (MNN), Multi-layer perceptron (MLP), Multiple linear regression (MLR or MnLR), Multiple Regressions Analysis (MRA); Nano filtration (NF), Nash-Sutcliffe coefficient (N−S), Network prediction (r), Network/genetic algorithm (GANN), Nonlinear multi-variable regression (MNLR), Normalized bias (NB), Normalized root mean square error (NRMSE); One step secant backpropagation (OSSBP), Organic matter (OM), Pattern search (PS), Partial least squares (PLS), Partial least-square regression (PLSR), Pearson correlation coefficients (PCC), Pearson product-moment correlation coefficient Or Correlation coefficient (R), Performance matrix (PM), Polak−Ribi'ere conjugate gradient backpropagation (PCGBP), Polyaromatic hydrocarbons (PAHs), Polymer assisted ultrafiltration (PAUF), Polynomial neural network (PNN), Powell−Beale conjugate gradient backpropagation (PCGBP); Principal component analysis (PCA), Quantitative ion character−activity relationships (QICAR), Quantization error (QE), Quasi-Newton backpropagation (QNBP), Quick propagation(QP), r2 metrics (rm2); Radial basis function (RBF), Regression coefficient (RC), Relative error/Residual error (Er or RE)/percentage error (Er), Relative root mean square error (RRMSE), Residuals analyses (RE), Resilient backpropagation (RP/Rprop), Response surface methodology (RSM), Root mean square error (RMSE), Root mean square error of calibration (RMSEC), Root mean square error of prediction (RMSEP), Root-mean-square error of cross-validation (RMSECV); Scaled conjugate gradient backpropagation (SCGBP), Self-organizing map (SOM), Simulated annealing (SA), Sodium dodecyl sulfate (SDS), Standard deviation (SD), Standard Deviation (σ), Standard deviation error (STD), Standard error of prediction (SEP), Standard error of prediction (SEP), Standard squared error (SSE), Statistical learning theory (SLT), Structural risk minimization (SRM), Successive projection algorithm (SPA), Sum of squared errors (SSer), Support Vector Regression (SVR), Surfactant to metal molar ratio (S/M); Tannin-aniline formaldehyde (TAFA), Topographic error (TE), Trans membrane pressure (TMP), Transmembrane pressure (TMP); United States Environmental Protection Agency (USEPA), Unsteady of advection-dispersion adsorption equation (UADAE); Variable learning rate backpropagation (VLRBP); Zeolite prepared from fly ash (ZFA).

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