Modelling a rotating biological contactor treating heavy metal contaminated wastewater using artificial neural network

M. Gopi Kiran, Raja Das, Shishir Kumar Behera, Kannan Pakshirajan and Gopal Das

ABSTRACT

The performance of a continuously operated laboratory-scale rotating biological contactor (RBC) was assessed for the removal of heavy metals viz. Cu(II), Cd(II) and Pb(II) from synthetic wastewater using artificial neural networks (ANNs). The RBC was inoculated with Sulfate Reducing Bacteria consortium (predominantly Desulfovibrrio species), and the performance was evaluated at different hydraulic retention times (HRTs) and inlet heavy metal concentrations. A feed-forward back-propagation neural network model was developed using 90 data sets obtained over a period of three months, to predict the removal of heavy metal (HMRE) and COD (CODRE). The predictive capability of the model was evaluated in terms of the coefficient of determination ($R^2$) and mean absolute percentage error between the model fitted and actual experimental data, whereas sensitivity analysis was performed on the input parameters by determining the absolute average sensitivity (AAS) values. The higher AAS value of the HRT compared with that of inlet heavy metal concentration suggested that the change of HRT has a significant influence on HMRE and CODRE. Overall, the results obtained from this study demonstrated that ANNs can efficiently predict RBC behaviour with regard to heavy metal and COD removal characteristics under the prevailing operational conditions.

Key words | COD removal, heavy metal removal, modelling, neural network, rotating biological contactor

HIGHLIGHTS

- Development of a feed-forward back propagation neural network model for an RBC.
- Prediction of heavy metal and COD removal.
- Evaluation of predictive capability in terms of coefficient of determination and mean absolute percentage error.
- Sensitivity analysis by determining the absolute average sensitivity values.
INTRODUCTION

Heavy metals are released into the environment from different industries, such as metallurgy, tanneries, mining, electroplating industries, etc. (Kikot et al. 2010). Heavy metals such as Cu, Cd, and Pb discharged from industrial wastewater are toxic at high concentration and, thus, pose serious risk to both human health and the environment. Hence, removal of heavy metals from wastewater before their discharge into the environment is mandatory (Kiran et al. 2015).

Compared with the physico-chemical methods, biological methods have been proven to be cost-effective and environmentally friendly technology for heavy metal removal from wastewater (Bai et al. 2013; Yang et al. 2016a, 2016b; Yajun et al. 2019). Different kinds of bioreactor systems have been employed to treat heavy metals present in wastewater. For example, wastewater containing heavy metals (e.g. Cd, Cu, Cr, Zn, Pb and Ni) were treated in suspended growth bioreactors, viz. Continuously Stirred Tank Reactors (Gola et al. 2020), and Membrane Bioreactor employed for the treatment of textile industry wastewater containing chromium (VI). On the other hand, attached growth bioreactors, viz. Packed Bed Bioreactor was employed for the treatment of acid mine drainage containing a variety of heavy metals (Dev et al. 2017), and Rotating Biological Contactors (RBCs) for heavy metal removal from synthetic wastewater (Kiran et al. 2017a).

In the recent past, RBCs have received great attention due to their capability to treat various types of refractory wastewaters, e.g., coloured industry wastewater (Pakshirajan & Kheria 2012), agrochemical industry wastewater (Vasiliadou et al. 2016) and gold mine wastewater (Guadalima & Monteros 2018). The advantages of RBCs over other attached growth systems include but are not limited to: (1) handling specific contaminants viz. hydrocarbons, heavy metals, xenobiotics and pharmaceuticals/personal care products, (2) handling high organic loadings and resistance to toxic shocks, (3) requiring low land area, maintenance, energy and start-up costs, and (4) energy generation along with wastewater treatment (Hassard et al. 2015).

Recently, the application of artificial neural networks (ANNs) to model and predict the operational efficiency of various biological systems, including wastewater and waste gas treatment systems, has gained remarkable attention (Nair et al. 2016; López et al. 2017; Antwi et al. 2018; Baskaran et al. 2019; Lin et al. 2020). A neural network can be used to simulate the non-linear input/output dynamics of any process based on the time-series datasets (Menhaj 1998; Chen et al. 2019). The primary advantage of ANN over phenomenological/conceptual models is that it does not require information about the complex nature of the underlying process to be explicitly described in mathematical form (Sahoo
The ANN model, in this study, was developed using the most widely employed feed-forward back-propagation (BP) algorithm, which uses a gradient descent procedure to minimize the objective function (Rumelhart et al. 1986). In other words, in the BP algorithm, the weights between input, output and hidden layers are modified and the process is repeated until the error between the output of the neural network and the desired output is minimized.

López et al. (2017) used a two-stage biological waste gas treatment system consisting of a first-stage biotrickling filter (BTF) and second-stage biofilter (BF) for the removal of a gas-phase methanol (M), hydrogen sulphide (HS) and α-pinene (P) mixture. The performance of the gas treatment system was modelled using two multi-layer perceptrons (MLPs) employing the back-propagation algorithm, in order to predict the removal efficiencies of methanol (RE_M), hydrogen sulphide (RE_HS) and α-pinene (RE_P). An MLP with the topology 3-4-2 was able to predict RE_M and RE_HS in the BTF, while a topology of 3-3-1 was able to approximate the RE_P in the BF. In another study, a three-layered feed-forward back-propagation ANN model was developed to evaluate the performance of an upflow anaerobic sludge blanket reactor in terms of COD removal while treating industrial starch processing wastewater. The proposed Levenberg–Marquardt algorithm based ANN model demonstrated very satisfactory performance during COD removal predictions and simulation (Antwi et al. 2018). Baskaran et al. (2019) developed an ANN model to predict the performance of a compost biofilter in terms of trichloroethylene (TCE) removal under continuous operation mode. The ANN model used a three-layer feed-forward-based Levenberg–Marquardt algorithm with a topology 3-25-1 to predict the TCE removal with $R^2$ greater than 0.99 during the model training, validation, and testing. The performance of a laboratory-scale anaerobic bioreactor was modelled by using the feed-forward back-propagation algorithm to optimize the CH₄ content of 60%–70% in biogas obtained from digestion of the organic fraction of municipal solid waste (Nair et al. 2016). As evident from the aforementioned reports, ANNs have shown their capability to accurately predict the behaviour of various biological systems by establishing the correspondence between input and output domains. Thus, it is clear that ANN models can be developed for bioreactors with a definite objective and adequate training of time-series data collected from such reactors. However, modelling the performance of RBC or any other reactor for heavy metal removal from wastewater has not been reported so far. This is mainly important considering the non-biodegradable and toxic nature of heavy metals in wastewater such as acid mine drainage (AMD), characterized by its low pH and high sulphate content along with heavy metals.

Hence, this study focused on the feasibility of an ANN model to estimate, predict and simulate experimental results obtained from an RBC treating heavy-metal-contaminated-synthetic wastewater. The objectives of this study were formulated as follows: (i) to create an MLP, by varying the internal network parameters, that would predict the HMRE in the RBC used for heavy metal removal from synthetic wastewater (Kiran et al. 2017a), (ii) testing the developed model with data that was not presented to the ANN during training, (iii) to perform sensitivity analysis, analyze and determine the most influencing input parameters (HRT and inlet heavy metal concentrations) for each output (HMRE and CODRE), and (iv) to emphasize the application of ANNs for control of bioreactor input parameters and to address the potential advantages of ANNs for predicting bioreactor performance. To the best of the authors’ knowledge, this is the first report that has used ANN to model an RBC treating heavy-metal-contaminated wastewater.

**MATERIALS AND METHODS**

**Experimental**

**Microorganism and chemicals**

Mixed Sulphate Reducing Bacteria (SRB) consortium (predominantly consisting of Desulfovibrio species) used in the RBC was acquired from a laboratory-scale upflow anaerobic packed bed reactor treating sulphate-rich wastewater (Kiran et al. 2015). During the experiments, sulphate and COD concentration in the influent were adjusted to maintain a COD/SO₄²⁻ ratio of 0.67 ± 0.08. The pH of the solution was adjusted to 7 using 1 N NaOH. The stock solutions of Cd(II), Cu(II), and Pb(II) prepared using Cd(NO₃)₂·4H₂O, CuCl₂·2H₂O, and Pb(NO₃)₂, respectively were procured from...
Alpha Chemika Co. Ltd, India, Euclid Co. Ltd, India, and Karni Chemicals Co. Ltd, India. All the chemicals used for experiments were of reagent grade and were used without further purification (Kiran et al. 2017a).

**Reactor set-up and operation**

The operational protocol of the laboratory-scale anaerobic RBC (total working volume = 3 L) made up of polymethyl methacrylate material is described elsewhere (Pakshirajan & Kheria 2012). The RBC consists of two identical stages connected in series. Each stage had a working volume of 1.5 L and was equipped with seven discs enclosed with polystyrene mesh and polyurethane foam in which the SRB consortium was immobilized. The disc diameter was 0.16 m with a thickness of 0.0056 m and they were spaced at 0.02 m distance. The submerged surface was 40% (Kiran et al. 2017a).

The RBC was operated under continuous mode and was maintained at a temperature of 25 ± 2°C. The suspended biomass was measured in terms of mixed liquor volatile suspended solids. Samples collected at regular intervals were centrifuged at 8000 × g for 5 min, and the supernatant obtained was analysed for metal, sulphate, sulphide and COD concentrations (Kiran et al. 2017a). The metal stock solutions of Cd(II), Cu(II), and Pb(II) of 10,000 mg/l concentration each were prepared using Cd(NO₃)₂·4H₂O, CuCl₂·2H₂O, and Pb(NO₃)₂, respectively. The phase-wise (three phases) inlet concentrations of the metals Cd(II) and Pb(II) were chosen as 50, 75 and 90 mg/l, whereas for Cu(II), the concentrations were 100, 150 and 175 mg/l. All these inlet metal concentrations were chosen based on the studies conducted earlier using the same anaerobic biomass containing SRB (Kiran et al. 2015, 2017b). Reactor performance in terms of REHM was evaluated at two different HRTs (24 and 48 h). Each experiment was carried out for a period until three steady-state values of effluent heavy metal concentration at the respective HRT were obtained. All the results presented are averages of duplicate sample analyses. The combined effect of inlet metal and COD concentration and HRT on removal was examined by calculating the RE as given in Equation (1):

\[
\%\text{Removal efficiency} = \frac{C_i - C_o}{C_i} \times 100
\]  

where \(C_i\) and \(C_o\) are the inlet and outlet concentrations (mg/l), respectively.

**Analytical methods**

The heavy metal concentration in the samples was determined using an atomic absorption spectrometer (Varian, AA240, The Netherlands). The COD and sulphate concentration was determined by following the closed reflux method and standard turbidimetric method, respectively (APHA 2005). The dissolved sulphide concentration in the liquid samples was determined as per the method described elsewhere (Cord-Ruwisch 1985).

**ANN model development**

The back-propagation neural network (BPNN) is composed of layers of neurons. The input layer of neurons is connected to the output layer and the training process is undertaken by changing the weights in order to establish a desired input-output relationship. A schematic diagram showing the BPNN with two input nodes, two output nodes, and a single hidden layer of 12 nodes is given in Figure 1. The experimental values did not show any advantage of a double hidden layer over a single layer network. Therefore, a single hidden layer network is used in this work and all the connections have multiplying weights associated with them.
The input nodes have a transfer function of unity and the activation functions of the hidden and output nodes are sigmoidal and linear, respectively. The data required for developing a representative and reliable ANN model consisted of the parameters, viz., inlet concentration (mg/l), HRT (h), HMRE (%) and CODRE (%) obtained from steady-state operation of the RBC. The data was normalized and scaled to the range of 0–1 using Equation (2) so as to suit the transfer function in the hidden (sigmoid) and output layer (linear):

\[ \hat{X} = \frac{X - X_{\text{min}}}{X_{\text{max}} - X_{\text{min}}} \]  

(2)

where \( \hat{X} \) is the normalized value, and \( X_{\text{min}} \) and \( X_{\text{max}} \) are the minimum and maximum values of \( X \) respectively.

From the steady-state RBC operation data, the set of 90 data points were divided into training and testing sets; 70% (NTr: 63) of the data points were used for training the network while the remaining 30% (NTe: 27) were used for testing the developed model. An MLP was formulated to predict the output parameters, HMRE (%) and CODRE (%) using inlet concentration and HRT as the input parameters. Table 1 describes the basic statistical information about the training and test data sets for the RBC. The data used as input are transmitted through the network and a set of output data are obtained. The obtained outputs are compared with the desired output values, and the difference between the desired output and calculated output (error) is used to adjust the weights of the network in order to reduce the magnitude of the error. After training, the ANN accepts new ‘unknown’ data as input and predicts the corresponding output based on its training. The best values of network parameters, i.e., training count \( (T_c) \), number of neurons in the hidden layer \( (N_H) \), learning rate \( (\eta) \), momentum term \( (\alpha) \) and epoch size \( (\epsilon) \) were selected by trial and error. These values are shown in Table 2. The predictive capability of the model was evaluated in terms of the coefficient of determination \( (R) \) and the mean absolute percentage error \( \text{(MAPE)} \). Further details pertaining to the effect of these network parameters and neural network modelling can be found elsewhere. Sensitivity analysis in the form of absolute average sensitivity \( \text{(AAS)} \) value was computed to determine the most influential input parameter affecting the output of the ANN (Maier & Dandy 1998; Rene et al. 2009, 2011).

The predictive modelling work using ANN was carried out using the shareware version of the NN and multivariable statistical modelling software, MATLAB® (Version 9.2.0.538062 [R2017a], Neural Network Toolbox). The specification of the computer used to perform the simulation had the following configurations: Operating system – Windows 8.1 Single Language; processor – Intel(R) Core(TM) i5-4200 CPU @ 1.60 GHz 2.30 GHz; 8.00 GB system memory.

RESULTS AND DISCUSSION

Effect of network parameters and best network topology

The input and output parameters in ANN modelling are usually selected on the basis of the objective of the modelling and the data availability. In order to develop the ANN model for the laboratory-scale RBC in this study, the selection of input parameters viz., HRT and inlet concentration and that of output parameters viz., HMRE (%) and CODRE (%) were decided on the basis of system knowledge and real-life requirements.

The first step of this modelling task was to identify a suitable network topology for the MLP through proper optimization of the network parameters (Maier & Dandy 1998; Sahinkaya 2009). Towards this, \( T_c \) and \( N_H \) were varied from 0 to 100 by keeping other network parameters such as \( \eta \) (0.75) and \( \alpha \) (0.75) at their constant values. The best values of \( \eta \) and \( \alpha \) for the developed model were determined by keeping some training parameters constant at their default values (suggested by MATLAB®), and by gradually changing values of the parameters from 0.1 to 0.9, with a step-size increment of 0.1 for each parameter. It was observed that increasing the number of neurons \( (N_H) \) from 6 to 12 increased the \( R \) value. The optimized values of network parameters for the model are shown in Table 2. The best network topology for the RBC was found to be 2-12-2 (i.e. two input parameters, 12 neurons in one hidden layer and two output parameters). After obtaining the best network topology for the RBC, the connection weights and
Table 1 | Basic statistics of the data used for ANN model development: (a) Cu, (b) Cd, and (c) Pb

### (a) Cu

**Basic statistics of the training data**

| Variable          | N    | Mean  | Std Dev | Minimum | Maximum | Sum Sq   |
|-------------------|------|-------|---------|---------|---------|----------|
| HRT (h)           | 63   | 36.57 | 12.08   | 24.00   | 48.00   | 13,606.29|
| Concentration (mg/l) | 63   | 173.28| 11.89   | 150.00  | 191.31  | 241,569.85|
| HMRE (%)          | 63   | 95.61 | 2.31    | 91.31   | 99.28   | 72,675.62 |
| CODRE (%)         | 63   | 53.53 | 15.96   | 13.73   | 94.38   | 28,158.88 |

**Basic statistics of the test data**

| Variable          | N    | Mean  | Std Dev | Minimum | Maximum | Sum Sq   |
|-------------------|------|-------|---------|---------|---------|----------|
| HRT (h)           | 27   | 35.56 | 12.22   | 24.00   | 48.00   | 8,582.21 |
| Concentration (mg/l) | 27   | 166.19| 10.10   | 151.00  | 186.00  | 145,067.91|
| HMRE (%)          | 27   | 95.54 | 1.87    | 92.10   | 98.78   | 47,486.59|
| CODRE (%)         | 27   | 56.26 | 12.19   | 28.66   | 85.43   | 18,582.62 |

### (b) Cd

**Basic statistics of the training data**

| Variable          | N    | Mean  | Std Dev | Minimum | Maximum | Sum Sq   |
|-------------------|------|-------|---------|---------|---------|----------|
| HRT (h)           | 63   | 35.43 | 12.08   | 24.00   | 48.00   | 13,046.11|
| Concentration (mg/l) | 63   | 78.10 | 14.67   | 54.78   | 101.60  | 53,185.95|
| HMRE (%)          | 63   | 85.44 | 8.30    | 70.19   | 95.86   | 59,522.24|
| CODRE (%)         | 63   | 47.95 | 14.82   | 17.50   | 79.25   | 23,078.86 |

**Basic statistics of the test data**

| Variable          | N    | Mean  | Std Dev | Minimum | Maximum | Sum Sq   |
|-------------------|------|-------|---------|---------|---------|----------|
| HRT (h)           | 27   | 40.00 | 11.53   | 24.00   | 48.00   | 9,926.60 |
| Concentration (mg/l) | 27   | 76.52 | 13.81   | 58.10   | 102.90  | 33,259.98|
| HMRE (%)          | 27   | 89.41 | 8.35    | 66.23   | 97.38   | 42,497.02|
| CODRE (%)         | 27   | 54.40 | 18.34   | 18.18   | 79.38   | 19,480.24 |

### (c) Pb

**Basic statistics of the training data**

| Variable          | N    | Mean  | Std Dev | Minimum | Maximum | Sum Sq   |
|-------------------|------|-------|---------|---------|---------|----------|
| HRT (h)           | 63   | 36.95 | 12.06   | 24.00   | 48.00   | 13,787.95|
| Concentration (mg/l) | 63   | 76.12 | 14.93   | 53.35   | 106.00  | 51,246.11|
| HMRE (%)          | 63   | 86.39 | 3.88    | 78.76   | 92.74   | 59,578.72|
| CODRE (%)         | 63   | 56.95 | 22.73   | 9.85    | 95.87   | 35,290.53 |

**Basic statistics of the test data**

| Variable          | N    | Mean  | Std Dev | Minimum | Maximum | Sum Sq   |
|-------------------|------|-------|---------|---------|---------|----------|
| HRT (h)           | 27   | 31.11 | 11.17   | 24.00   | 48.00   | 6,983.63 |
| Concentration (mg/l) | 27   | 77.94 | 15.79   | 53.35   | 105.00  | 33,161.19|
| HMRE (%)          | 27   | 85.12 | 4.79    | 78.74   | 92.79   | 37,990.46|
| CODRE (%)         | 27   | 46.28 | 21.02   | 11.47   | 83.20   | 16,624.63 |
bias term were obtained for the interconnections between different neurons in different layers of the MLP (Table 3). These connection weights determine which input neuron dominates the contribution to a specific hidden neuron, while the sign (+, −) suggests the nature of correlation between an input to a neuron and the output from the neuron. Detailed information on the interpretation of connection weights for neural network models have been discussed in Garson (1991). The biases, which are essentially constant, are an additional input into the next layer and are not influenced by the previous layer but they do have outgoing connections with their own weights. The bias unit ensures that even when all the inputs are zeros, there will still be an activation in the neuron.

### Predictive capability of the developed model

The performance of this trained ANN model was assessed by comparing the prediction of the ANN model with that of the experimental values of output parameters. The results were evaluated in terms of the most commonly used error measurement index, MAPE values for HMRE (%) and CODRE (%) during training and testing (Table 4). The measured and model-fitted profiles of HMRE (%) and CODRE (%), during model training and testing, are shown in Figures 2 and 3, respectively. As observed from Figures 4 and 5, the ANN model developed for the RBC showed high R values during both training and testing. The model gave R values between 0.95–0.96 and 0.93–0.96 for heavy metals, and 0.91–0.98 and 0.92–0.98 for COD, respectively, during training and testing. Thus, overall, only <10% of the total deviations could not be mapped by these models during the training and testing process, indicating a strong correlation between predicted and measured values. This phenomenal performance could be attributed to the ability of the BPNN model to capture complex behaviour or trend that existed among the variables obtained from the RBC. The slightly fluctuating heavy metal and COD removal profiles that are usually governed by the microbial activity in the RBC cannot be interpreted by the neural network unless it is integrated with a process-based model. Therefore, any unexpected variations in the removal profiles can affect the ANN’s learning capability, eventually leading to a decline in performance of the model (Zamir et al. 2011).

Similar results on successful application of ANN models for predicting removal of pollutants in different bioreactors are reported in the literature (Antwi et al. 2018; Baskaran et al. 2020). Overall, the ANN model developed in this study is found to be well applicable for predicting the HMRE and CODRE of the RBC.

For the RBC under investigation in this study, ANN-based models can provide adequate information on different safe operational regimes in terms of inlet concentrations of the different heavy metals and HRT to reach high HMRE (%) and CODRE (%). These regimes can be represented by two-dimensional contour plots as shown in Figures 6 and 7. These contour plots can be interpreted as follows:

(a) To achieve high HMRE (>90%), the values of independent parameters should be within a specific range, mentioned herein: (i) the allowable inlet heavy metal concentration can be up to 160 mg/l and HRT should be 48 h for Cu (Figure 6(a)), (ii) the allowable inlet heavy metal concentration can be up to 90 mg/l and HRT should be 48 h for Cd (Figure 6(b)), and (iii) the allowable inlet heavy metal concentration can be up to 75 mg/l and HRT should be 48 h for Pb (Figure 6(c)).

(b) To achieve high CODRE (>60%), the various conditions are: (i) the allowable inlet heavy metal concentration can be up to 160 mg/l and HRT should be 48 h for Cu (Figure 7(a)), (ii) the allowable inlet heavy metal concentration can be up to 80 mg/l and HRT should be 48 h for

### Table 2 | Best values of network parameters used for training the network: (a) Cu, (b) Cd, and (c) Pb

| Parameters                      | Cu  | Cd  | Pb  |
|---------------------------------|-----|-----|-----|
| Training count                  | 10  | 29  | 9   |
| Number of neurons in input layer| 2   | 2   | 2   |
| Number of neurons in hidden layer| 12  | 12  | 12  |
| Number of neurons in output layer| 2   | 2   | 2   |
| Learning rate                   | 0.1 | 0.1 | 0.1 |
| Momentum term                   | 0.1 | 0.1 | 0.1 |
| Error tolerance                 | 0.001 | 0.001 | 0.001 |
| Training algorithm              | LM  | LM  | LM  |
| Number of training data set     | 63  | 63  | 63  |
| Number of test data set         | 27  | 27  | 27  |

Note: LM – Levenberg-Marquardt.
Table 3 | Connection weights and bias terms of the developed neural network model (2-12-2): (a) Cu, (b) Cd, and (c) Pb

**Input to hidden layer**

| Variable | HID1 | HID2 | HID3 | HID4 | HID5 | HID6 | HID7 | HID8 | HID9 | HID10 | HID11 | HID12 |
|----------|------|------|------|------|------|------|------|------|------|-------|-------|-------|
| (a) V1   | 7.82 | 8.21 | 9.09 | 2.11 | – 0.79 | 5.37 | 5.52 | – 3.58 | – 5.74 | – 10.43 | 5.97 | 6.02 |
| V2       | – 9.11 | 3.43 | 4.46 | – 9.03 | – 10.47 | 10.05 | – 8.48 | 8.57 | 5.36 | – 5.28 | – 4.53 | – 9.20 |
| Bias     | – 8.93 | – 8.24 | – 5.78 | 5.20 | 4.04 | 2.38 | 4.59 | – 2.97 | – 5.83 | – 2.04 | 10.94 | 8.19 |

**Hidden to output layer**

| V3 | V4 |
|----|----|
| HID1 | – 0.57 | 0.92 |
| HID2 | – 0.85 | 2.49 |
| HID3 | 1.07 | – 0.10 |
| HID4 | 0.30 | – 1.30 |
| HID5 | 0.12 | 0.68 |
| HID6 | 0.19 | – 1.38 |
| HID7 | 0.05 | 1.15 |
| HID8 | 0.40 | – 0.85 |
| HID9 | – 1.24 | 1.09 |
| HID10 | – 0.09 | – 0.03 |
| HID11 | 0.59 | 1.63 |
| HID12 | – 0.54 | – 1.38 |
| Bias | – 0.33 | – 0.60 |

**Input to hidden layer**

| Variable | HID1 | HID2 | HID3 | HID4 | HID5 | HID6 | HID7 | HID8 | HID9 | HID10 | HID11 | HID12 |
|----------|------|------|------|------|------|------|------|------|------|-------|-------|-------|
| (b) V1   | – 4.85 | – 4.84 | 1.25 | 4.39 | 4.78 | – 4.67 | 1.04 | – 1.04 | – 5.59 | – 1.20 | – 4.81 | 3.59 |
| V2       | – 1.41 | – 0.60 | – 4.94 | 1.71 | – 3.31 | 1.62 | 6.43 | 3.49 | 0.88 | – 4.25 | – 1.92 | 3.05 |
| Bias     | 4.43 | 3.97 | – 2.72 | – 2.36 | – 0.94 | 0.22 | 1.10 | – 1.12 | – 1.44 | – 2.41 | – 2.95 | 4.08 |

**Hidden to output layer**

| V3 | V4 |
|----|----|
| HID1 | – 0.11 | 0.27 |
| HID2 | – 0.17 | 1.46 |
| HID3 | 0.22 | 0.05 |
| HID4 | – 1.28 | 0.26 |
| HID5 | 0.11 | 2.09 |
| HID6 | 0.42 | 1.19 |
| HID7 | 0.20 | 0.12 |
| HID8 | – 0.07 | 0.01 |
| HID9 | – 0.34 | 0.89 |

(continued)
Cd (Figure 7(b)), and (iii) the allowable inlet heavy metal concentration can be up to 80 mg/l and HRT should be 48 h for Pb (Figure 7(c)).

Metal removal and COD removal were observed to be the maximum at HRT of 48 h rather than at 24 h. This is because a long HRT allows the SRB to reduce sulphate to a greater extent by efficient utilization of the carbon source, thereby precipitating the metals as their respective sulphide salts. Compared with cadmium and lead, the higher RE of copper at a higher inlet concentration range can be attributed to its low solubility product value with sulphide, i.e., copper sulphide is least soluble compared with cadmium sulphide and lead sulphide (Kiran et al. 2017a). At a low initial metal concentration, precipitation of the insoluble metal due to sulphide produced by the SRB avoids any toxic effect of the metal on the SRB. However, high initial metal concentration level has resulted in a reduced activity of the SRB, leading to low sulphate reduction efficiency and metal removal (Kiran et al. 2017b). At a low concentration combination of these metals, the removal of all the metals was the maximum,

| Variable | HID1 | HID2 | HID3 | HID4 | HID5 | HID6 | HID7 | HID8 | HID9 | HID10 | HID11 | HID12 |
|----------|------|------|------|------|------|------|------|------|------|-------|-------|-------|
| HID10    | 0.62 | 0.60 |      |      |      |      | V3   |      |      |       |       |       |
| HID11    | 1.78 | 1.93 |      |      |      |      |      | V4   |      |       |       |       |
| HID12    | 1.13 | 1.20 |      |      |      |      |      |      |      |       |       |       |
| Bias     | 0.53 | 0.13 |      |      |      |      |      |      |      |       |       |       |

Table 3 | continued

Input to hidden layer

| Variable | HID1 | H1-D2 | HID3 | HID4 | HID5 | HID6 | HID7 | HID8 | HID9 | HID10 | HID11 | HID12 |
|----------|------|-------|------|------|------|------|------|------|------|-------|-------|-------|
| HID10    | 0.38 | 3.91  | 7.26 | 0.85 | 3.65 | 0.99 | 0.24 | 0.13 | 10.13 | 6.83  | 9.76  | 5.73  |
| HID11    | 9.74 | 8.40  | 6.29 | 9.43 | 8.24 | 9.58 | 9.99 | 7.75 | 6.75  | 0.29  | 7.59  |       |
| Bias     | 0.02 | 2.03  |      |      |      |      |      |      |       |       |       |       |

Hidden to output layer

| V3 | V4 |
|----|----|
| 0.57 | 0.62 |
| 0.05 | 1.18 |
| 0.02 | 2.03 |
| 0.09 | 0.37 |
| 0.54 | 0.79 |
| 0.10 | 0.52 |
| 0.85 | 0.59 |
| 0.57 | 0.38 |
| 1.12 | 3.90 |
| 0.20 | 1.06 |
| 0.29 | 1.94 |
| 0.53 | 0.47 |
| 0.78 | 0.70 |
and at a high concentration combination of these metals, the metal RE was slightly lower. Owing to the increase in the metal sulphide (M/S²⁻/C⁰) ratio, reduction in the metal RE can be observed at a high concentration combination of metals. In contrast, at a lower value of the M/S²⁻/C⁰ ratio (<1), sulphide formed due to sulphate reduction is high, which ensures a high metal sulphide precipitation for the metal removal (Villa-Gomez et al. 2015).

Sensitivity analysis

To identify the most influential input parameter of the developed model, sensitivity analysis is usually performed by estimating the absolute average sensitivity (AAS) (Maier & Dandy 1998; Rene et al. 2009, 2011). The AAS values for CuRE,% were 0.40 and 1.71, respectively, for inlet concentration and HRT and the AAS values for CODRE,% were 0.77 and 1.71, respectively. Similarly, the AAS values for CdRE,% were 0.60 and 1.62, respectively, for inlet concentration and HRT and the AAS values for CODRE,% were 1.37 and 3.74, respectively. And, the AAS values for PbRE,% were 0.17 and 0.60, respectively, for inlet concentration and HRT and the AAS values for CODRE,% were 1.63 and 1.97, respectively. In all these cases, when compared with inlet concentration, the higher value of HRT has a significant influence on HMRE and CODRE. Sensitivity analysis has been applied to select the key variables affecting the performance of a bioreactor (Rene et al. 2009, 2011). Rene et al. (2009) examined the performance of a perlite biofilter inoculated with a mixed microbial culture for styrene removal from contaminated air based on two input parameters viz., concentration and flow rate. After sensitivity analysis they found the performance of the biofilter to be largely influenced by the flow rate. In another study, the performance of a monolith bioreactor for styrene removal from contaminated air was examined on the basis of various input parameters viz. concentration, G/L (gas/liquid) ratio, and pressure drop. However, after sensitivity analysis they found the performance of the monolith bioreactor to be significantly affected by the concentration followed by the G/L ratio and pressure drop (Rene et al. 2011).

Practical implications of ANNs for performance evaluation of different bioreactor systems

Table 5 provides a detailed summary of the different literature reports where neural networks have been used to evaluate the performance of different bioreactor systems, though no serious effort has so far been made to implement this technique for real-time systems. In industrial wastewater treatment plants, ANNs have successfully been implemented for fault detection and diagnosis, plant and instrument monitoring, dynamic forecasting and robust process control (Boger 1992). The models developed based on the laboratory-scale experimental data, where input parameters to the RBC such as inlet heavy metal concentration and HRT were systematically controlled and other physico-chemical and environmental parameters were adequately maintained, might not accurately predict the removal efficiency of a full-scale RBC. Therefore, for full-time applications, the wastewater treatment system should be fitted with online measurement devices to monitor the parameters at a regular interval. This information can be stored in a large database, and the system can be equipped with an automatic control system to maintain the desired values of these process parameters. The trained neural network model can then be integrated with a programmable logic controller (PLC) to ascertain and control the process variables, thereby evaluating the reactor performance on a regular basis. The data obtained from real-time bioreactor operation can be merged with the already existing database, and the ANN model can be trained in offline/online mode, and the connection weights can be updated before integrating it with the PLC. The ANN models, when combined with more prominent applications like genetic algorithms, multi-objective

Table 4 | Observed mean absolute percentage error (MAPE) during training and testing: (a) Cu, (b) Cd, and (c) Pb

| Outputs | HMRE (%) | CODRE (%) |
|---------|----------|-----------|
| (a)     |          |           |
| Training| 0.52     | 10.71     |
| Testing | 0.52     | 7.32      |
| (b)     |          |           |
| Training| 1.93     | 10.45     |
| Testing | 1.89     | 11.98     |
| (c)     |          |           |
| Training| 0.84     | 14.24     |
| Testing | 1.37     | 16.31     |
Figure 2 | ANN model predictions of heavy metal removal during training and testing: (a) Cu, (b) Cd, and (c) Pb.
**Figure 3** | ANN model predictions of COD removal during training and testing: (a) Cu, (b) Cd, and (c) Pb.
Figure 4 | Comparison of predictions by ANN models with the experimental measurements for heavy metal removal during training and testing: (a) Cu, (b) Cd, and (c) Pb.
Figure 5 | Comparison of predictions by ANN models with the experimental measurements for COD removal during training and testing: (a) Cu, (b) Cd, and (c) Pb.
Figure 6 | Contour plots showing the effect of input parameters on the heavy metal removal after ANN training: (a) Cu, (b) Cd, and (c) Pb.

Figure 7 | Contour plots showing the effect of input parameters on the COD removal after ANN training: (a) Cu, (b) Cd, and (c) Pb.
optimization using evolutionary algorithm, multi-objective optimization based on ANN modelling, fuzzy-logic-based control systems, and fuzzy neural optimization softwares would allow better prediction and control of bioreactor performance (Venu Vinod et al. 2009; de Medeiros et al. 2019).

**CONCLUSIONS**

An ANN-based model was successfully developed and tested to predict the performance of RBC. The HMRE and CODRE were predicted using inlet concentration and HRT as the inputs to the model. After proper optimization of network parameters, and through vigorous training and testing, the network architecture 2-12-2 was obtained for the RBC. The results from sensitivity analysis showed that changes in HRT significantly affected the HMRE and CODRE of the model. Besides, the conditions to obtain high HMRE and CODRE, as a function of inlet heavy metal concentration and HRT, were also obtained from two-dimensional contour diagrams. The ANN model developed in this work for the RBC would yield more promising results when tested with online monitoring and control systems, thus allowing better access to control process variables and improving the performance of the bioreactor for heavy metal contaminated wastewater treatment.
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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest.

DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

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