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TECHNICAL ARTICLE

Artificial Neural Network Prediction of the Performance of Upflow and Downflow Fluidized Bed Reactors Treating Acidic Mine Drainage Water

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Abstract The performance of fluidized bed reactors treating synthetic acid mine drainage were predicted using an artificial neural network (ANN). The developed model gave satisfactory fits to the experimentally obtained sulfate, COD, alkalinity, and sulfide data; R-values were within 0.92 and 0.98. ANN can be effectively used to predict the performance of these complex systems and, with the proposed model-based applications, it is possible to reduce operational costs and risks.

Keywords Metal removal · Mine water · Reactor modeling · Sulfate reduction

Introduction

Artificial neural networks (ANNs) are a computational approach inspired by studies of the brain and nervous systems. The powerful functionality of biological neural systems has been attributed to the parallel distributed processing nature of neurons. An ANN emulates this structure by distributing computations to small and simple processing units, called artificial neurons, which are interconnected to form a network. Basically, ANNs are numerical structures inspired by the learning process in the human brain (Hamidi and Kayaalp 2008).

Researchers have established that anaerobic sulfate reducing fluidized bed reactors (FBRs) could be used to efficiently treat acidic mine drainage (AMD), assuming high biomass retention and dilution of the feed water with the recycling flow (Nevatalo et al. 2010; Sahinkaya et al. 2011; Sahinkaya and Gungor 2010). Biological processes taking place in a wastewater treatment plants are complex and not easily described by mechanistic models. The performance of aspects such as wastewater composition and operational parameters of the reactor and microbial community is very difficult to predict (Sahinkaya et al. 2007). ANNs can be used to provide information on process performance, either replacing a hardware sensor or complementing it (Aguadoa et al. 2009). When circumstances or processes are not understood well enough or parameter determination is impractical, there is a distinctive advantage for black-box models, like ANNs, since they do not require prior knowledge about the structure and relationships that exist between important variables. Moreover, their learning abilities make them adaptive to system changes (Sahinkaya 2009; Sahinkaya et al. 2007). ANN models have already been used to predict the performance of wastewater treatment plants (Mjalli et al. 2007), to simulate an industrial wastewater treatment plant (Gontarski et al. 2000), to model a submerged membrane bioreactor treating whey wastewater (Cinar et al. 2006), to assess wastewater reclamation potential (Chen et al. 2003), and to model biological water and wastewater treatment processes (Khataee and Kasiri 2011).

We modeled the performance of upflow and downflow FBRs using a popular neural network back-propagation (BP) algorithm in an attempt to predict reactor performance without using effluent parameters as input to determine if

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we could adequately predict reactor performance at different operational conditions without conducting experiments.

Materials and Methods

Fluidized Bed Reactors (FBRs)

The influent and effluent parameters of a laboratory-scale upflow fluidized bed reactor (UFBR) and two downflow fluidized bed reactors (DFBRs) inoculated with anaerobic digester effluent of a municipal wastewater treatment plant was used in this study. The methods for analyzing sulfate, soluble metal, sulfide, pH and alkalinity were described in Sahinkaya and Gungor (2010). The FBRs were maintained in a temperature controlled room at 35 °C. Zeolite particles (particle size 0.5–1.0 mm) were used as the biomass carrier for the UFBR (R1). The fluidization ratio in the UFBR was adjusted to 15–20 % with a high recycling rate, resulting in active fluidized bed volume of around 300 mL. Cubic sponge particles (for R2) and polyurethane material (for R3) with an average size of around 0.5 and 5 mm, respectively were the carrier materials for the DFBRs. The FBRs were fed with synthetic wastewater containing nutrients and varying concentrations of lactate and sulfate. Lactate was used as a carbon and electron source for the SRB. The ratio of lactate/sulfate (as COD/sulfate) was 0.67–1.0 for the UFBR and 0.67–1.25 for the DFBs. The feed solution, freshly prepared every day, was kept in a refrigerator at 4 °C. COD removal, Cu and Zn precipitation, and sulfate reduction was not observed in the feed container. The procedure given by Sahinkaya and Gungor (2010) was followed for the operational conditions of the FBRs.

Modeling

The procedure given by Sahinkaya (2009) was followed in the ANN modeling of FBRs. A feed-forward ANN, trained with a BP algorithm, was implemented using the MATLAB® 7.6.0 computer program. ANN algorithms attempt to mimic neurological performance, such as learning from past experience, making generalizations from similar situations,

Table 1 Input and output parameters in the modeling of the performance of FBRs for scenarios 1 and 2

	Scenario 1	Scenario 2
Input parameters [P]		
[P1]	Feed pH	Feed pH
[P2]	Effluent pH	Feed sulfate (mg/L)
[P3]	Feed sulfate (mg/L)	Feed metal (mg/L)
[P4]	Feed metal (mg/L)	Feed COD (mg/L)
[P5]	Feed COD (mg/L)	Operation time (day)
[P6]	Operation time (day)	
Output parameters [T]		
[T1]	Effluent sulfate (mg/L)	Effluent sulfate (mg/L)
[T2]	Effluent COD (mg/L)	Effluent COD (mg/L)
[T3]	Effluent alkalinity (mg $CaCO_3$/L)	Effluent alkalinity (mg $CaCO_3$/L)
[T4]	Effluent sulfide (mg/L)	Effluent sulfide (mg/L)

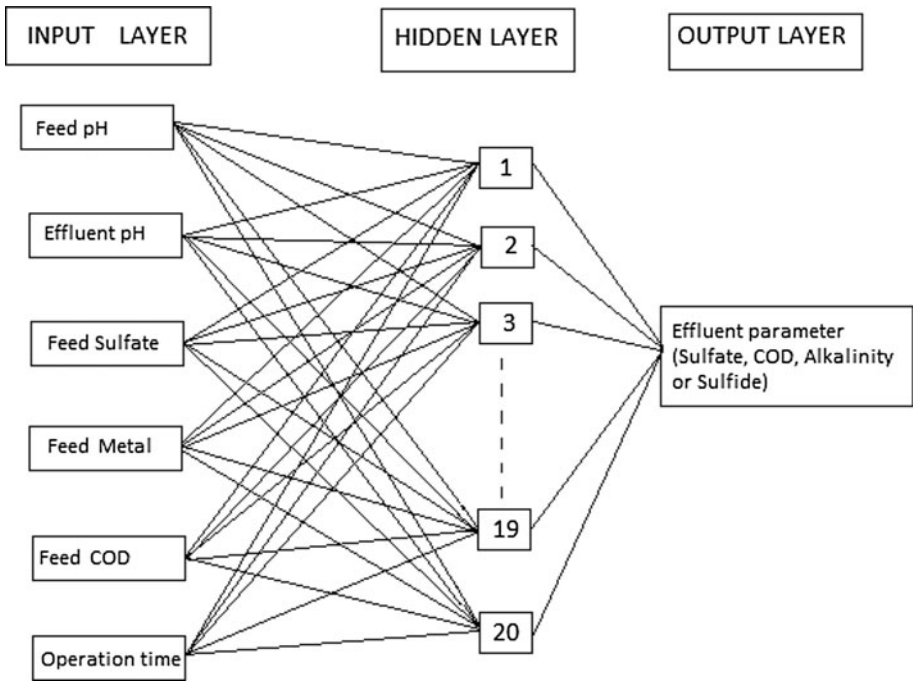

Fig. 1 ANN structure for prediction of reactor effluent parameters for scenario 1 (effluent pH was removed from the input parameters in scenario 2)

and producing decisions with incomplete knowledge, which involves great complexities and nonlinearities (Onkal-Engin et al. 2005). The BP neural network developed by Rumelhart et al. (1986) is the most representative ANN learning model. A feed-forward ANN consist of interconnected processing elements, called neurons, which are arranged in layers: an input layer, one or more hidden layers, and an output layer. Every unit contains a number of neurons, and these units are related to each other by weighted connections (Hamidi and Kayaalp 2008). Input for the network is normalized, and this normalized input data is randomly divided for training and validation (Purkait et al. 2009). BP algorithms use input vectors and corresponding target vectors to train ANN. ANN with a sigmoid and linear output layer are capable of approximating any function with a finite number of discontinuities (Ozkaya et al. 2008).

Table 2 Comparison of BP algorithms for predicting effluent sulfate, COD, alkalinity and sulfide of reactor 1, reactor 2, and reactor 3 (neuron number 20)

	Sulfate (mg/L)				COD (mg/L)				Alkalinity (mg $CaCO_3$/L)				Sulfide (mg/L)			
	*T-R	V-R	Tt-R	A-R	T-R	V-R	Tt-R	A-R	T-R	V-R	Tt-R	A-R	T-R	V-R	Tt-R	A-R
Reactor 1																
	BP algorithm trainrp				BP algorithm trainlm				BP algorithm trainrp				BP algorithm trainrp			
Scenario 1	0.98	0.94	0.91	0.94	0.99	0.85	0.93	0.95	0.99	0.94	0.96	0.97	0.99	0.95	0.96	0.98
	BP algorithm trainrp				BP algorithm trainrp				BP algorithm trainrp				BP algorithm trainrp			
Scenario 2	0.99	0.90	0.81	0.92	0.99	0.99	0.96	0.98	0.99	0.95	0.96	0.97	0.98	0.92	0.95	0.96
Reactor 2																
	BP algorithm trainrp				BP algorithm trainrp				BP algorithm trainrp				BP algorithm trainrp			
Scenario 1	0.99	0.90	0.90	0.95	0.99	0.98	0.94	0.98	0.99	0.97	0.95	0.98	0.99	0.91	0.94	0.96
	BP algorithm trainrp				BP algorithm trainrp				BP algorithm trainlm				BP algorithm trainrp			
Scenario 2	0.96	0.90	0.89	0.93	0.99	0.99	0.94	0.98	0.99	0.97	0.94	0.97	0.98	0.90	0.94	0.96
Reactor 3																
	BP algorithm trainlm				BP algorithm trainscg				BP algorithm trainlm				BP algorithm trainrp			
Scenario 1	0.99	0.77	0.92	0.92	0.99	0.97	0.96	0.97	0.99	0.91	0.94	0.95	0.97	0.87	0.9	0.94
	BP algorithm trainrp				BP algorithm trainlm				BP algorithm trainlm				BP algorithm trainlm			
Scenario 2	0.96	0.85	0.96	0.93	0.99	0.97	0.97	0.98	0.99	0.87	0.93	0.95	0.98	0.96	0.83	0.94

**T-R* training R-values, *V-R* validation R-values, *Tt-R* test R-values, *A-R* all R-values

Table 3 R-values of training, validation, test and all linear regressions at different neuron numbers for predicting effluent sulfate, COD, alkalinity and sulfide concentrations of reactor 1, reactor 2, and reactor 3

	Sulfate (mg/L)				COD (mg/L)				Alkalinity (mg $CaCO_3$/L)				Sulfide (mg/L)			
	*T-R	V-R	Tt-R	A-R	T-R	V-R	Tt-R	A-R	T-R	V-R	Tt-R	A-R	T-R	V-R	Tt-R	A-R
Reactor 1																
	Neuron number 20 (trainrp)				Neuron number 40 (trainlm)				Neuron number 20 (trainrp)				Neuron number 20 (trainrp)			
Scenario 1	0.98	0.94	0.91	0.94	0.99	0.86	0.94	0.94	0.99	0.94	0.96	0.97	0.99	0.95	0.96	0.98
	Neuron number 10 (trainlm)				Neuron number 20 (trainrp)				Neuron number 30 (trainlm)				Neuron number 30 (traingdx)			
Scenario 2	0.99	0.97	0.88	0.95	0.99	0.95	0.95	0.97	0.99	0.96	0.97	0.98	0.98	0.95	0.96	0.97
Reactor 2																
	Neuron number 20 (trainrp)				Neuron number 3 (trainrp)				Neuron number 10 (trainrp)				Neuron number 20 (trainrp)			
Scenario 1	0.99	0.90	0.90	0.95	0.99	0.99	0.95	0.98	0.99	0.97	0.97	0.98	0.99	0.91	0.94	0.96
	Neuron number 20 (trainrp)				Neuron number 10 (trainrp)				Neuron number 5 (trainlm)				Neuron number 20 (trainrp)			
Scenario 2	0.96	0.90	0.89	0.93	0.99	0.99	0.95	0.98	0.99	0.98	0.97	0.98	0.98	0.90	0.94	0.96
Reactor 3																
	Neuron number 20 (trainlm)				Neuron number 5 (trainscg)				Neuron number 20 (trainlm)				Neuron number 20 (trainrp)			
Scenario 1	0.99	0.77	0.92	0.92	0.99	0.97	0.97	0.98	0.99	0.91	0.94	0.95	0.98	0.87	0.90	0.94
	Neuron number 20 (trainrp)				Neuron number 20 (trainlm)				Neuron number 20 (trainlm)				Neuron number 20 (trainlm)			
Scenario 2	0.96	0.85	0.96	0.93	0.99	0.97	0.97	0.98	0.99	0.87	0.93	0.95	0.98	0.96	0.83	0.94

**T-R* training R-values, *V-R* validation R-values, *Tt-R* test R-values, *A-R* all R-values

Selection of the ANN Input Parameters

Modeling with ANN has two phases; the first phase involves determining network parameters (e. g. the number of layers and nodes in the hidden layer(s), the form and parameters of activation function) for training purposes, and the second phase tests the ANN parameters.

We used a two-layer ANN with a tan-sigmoid (neuron model) transfer function for the hidden layer and a linear transfer function for the output layer (Fig. 1). The input and output parameters are also depicted in Fig. 1. Two scenarios were modeled (Table 1). In addition to feed wastewater characteristics, effluent pH was also used as an input parameter in scenario 1 because pH is easy to measure. The effluent pH was not used as input in scenario 2 so that we could see how well the model could predict performance when experimental data are not available. Operation time was selected as an input parameter because biomass concentration and microbial community can change over time. Effluent sulfate, alkalinity, COD, and sulfide were selected as output parameters. Half of the data were used for training and one-fourth of the data was used for validation and then the other fourth for testing of the model.

Results and Discussion

Optimization of the Back-Propagation Algorithm and Neuron Number

Twelve BP algorithms were compared: trainlm (Levenberg–Marquardt back-propagation), traincgp (conjugate gradient back-propagation with PolakRibiere updates), traingd (gradient descent back-propagation), traingda (gradient descent with momentum and adaptive learning rate back-propagation), trainrp (resilient back-propagation), trainscg (scaled

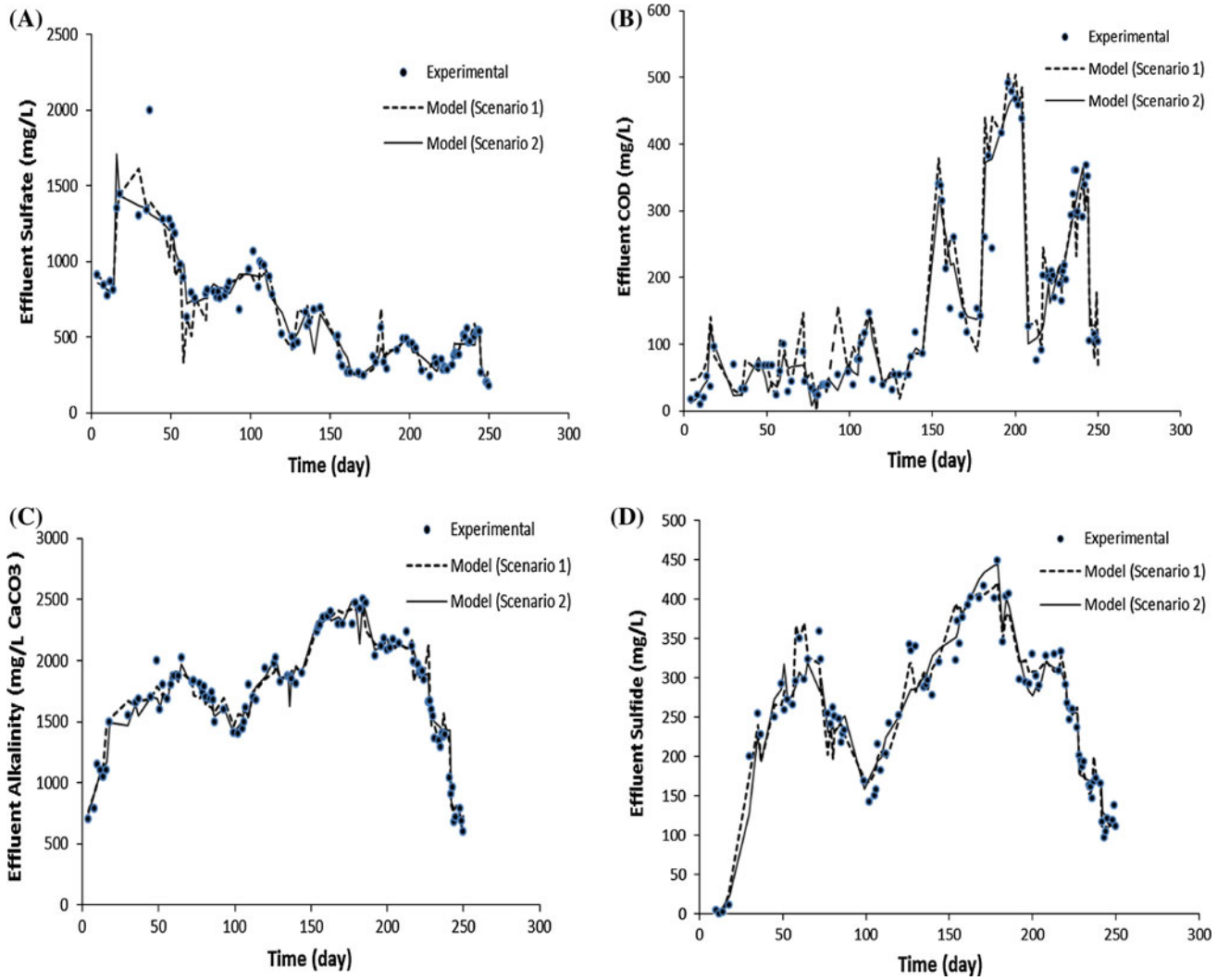

Fig. 2 Measured and neural network prediction of reactor 1 effluent sulfate (**a**), effluent COD (**b**), effluent alkalinity (**c**), and effluent sulfide (**d**) concentrations for scenarios 1 and 2 (mg/L $CaCO_3$:mg/L calcium carbonate alkalinity)

conjugate gradient back-propagation), trainoss (one step secant back-propagation), traincgf (conjugate gradient back-propagation with Fletcher-Reeves updates), trainbfg (BFGS quasi-Newton back-propagation), traingdm (gradient descent with momentum back-propagation), and traincgb (conjugate gradient back-propagation with Powell-Beale restarts) (Moral et al. 2008). In this comparison, the number of neurons was kept constant at 20. The performance of the BP algorithms was evaluated based on the root mean square error (RMSE) and determination coefficient (R) between the modeled output and measured data set. After selecting the best BP algorithm, the number of neurons was optimized by keeping all other parameters constant.

Predicting the Performance of UFBR and DFBRs

The applicability of ANN was investigated to predict the effluent sulfate, COD, alkalinity, and sulfide of a UFBR and two DFBRs. The training results are provided in Table 2. The performance of the BP algorithms was evaluated using the determination coefficient (R) of "Training", "Validation", "Test," and "All" data. The best fitting BP algorithms for predicting the different effluent parameters of the three reactors were trainlm, trainrp, trainscg, and traingdx (Table 2).

The optimum algorithm and neuron numbers for the three reactors for scenario 1 and 2 are shown in Tables 2 and 3, respectively. After selecting the best BP algorithms, the number of neurons was optimized, keeping all other parameters constant (Table 3). The neuron numbers for the two scenarios for the prediction of effluent parameters varied in the range of 3 and 40. The all-R values (representing the training, validation and test-R values) in the comparison of BP algorithms were observed in the range of 0.92 and 0.98.

Figures 2, 3, and 4 illustrate the time course variations of measured and predicted data for the UFBR and two DFBR reactors, respectively. The model data tracked the measured data closely for all of the effluent parameters. The developed ANN model satisfactorily predicted sulfate,

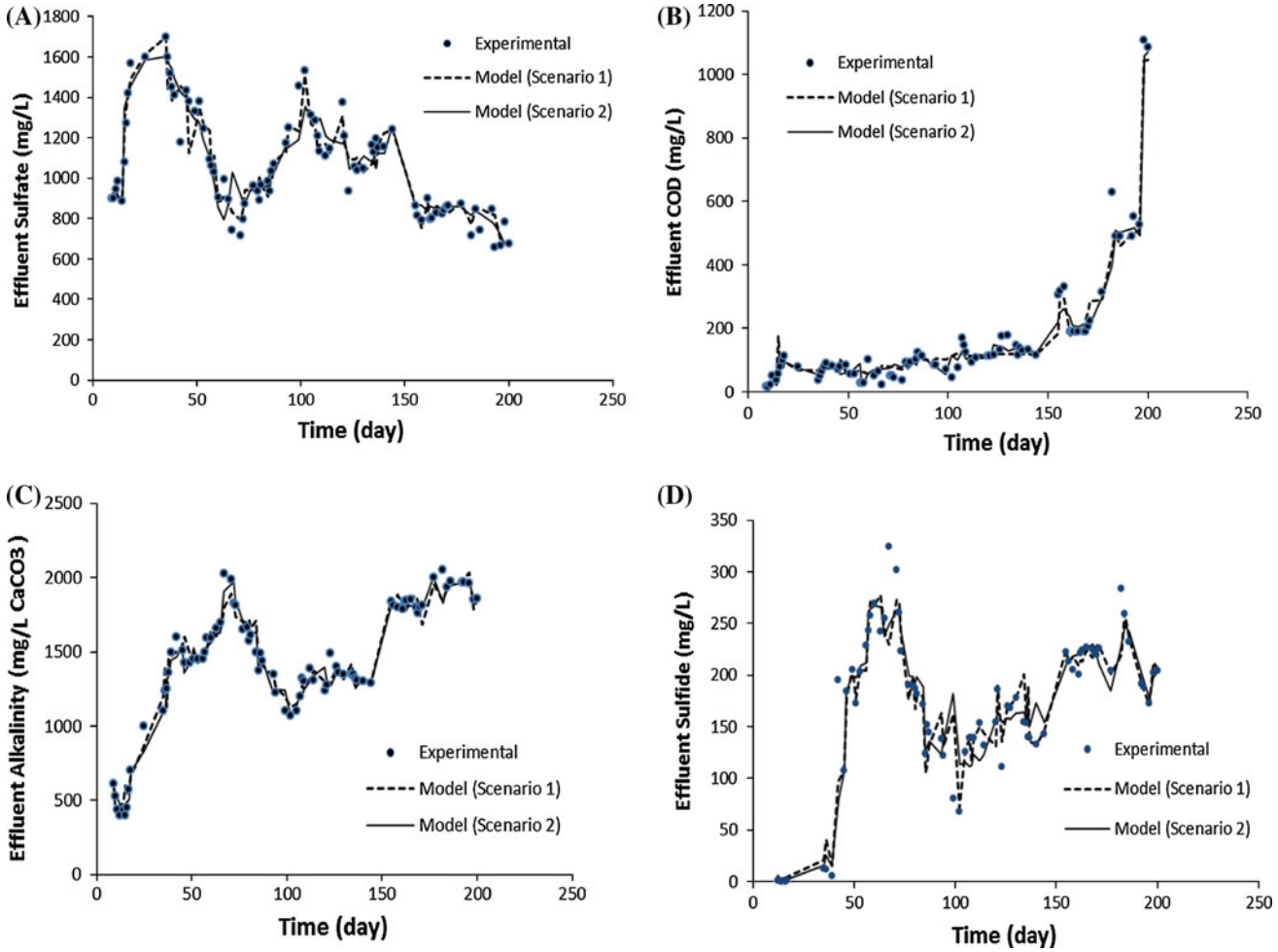

Fig. 3 Measured and neural network prediction of reactor 2 effluent sulfate (**a**), effluent COD (**b**), effluent alkalinity (**c**), and effluent sulfide (**d**) concentrations for scenarios 1 and 2 (mg/L $CaCO_3$:mg/L calcium carbonate alkalinity)

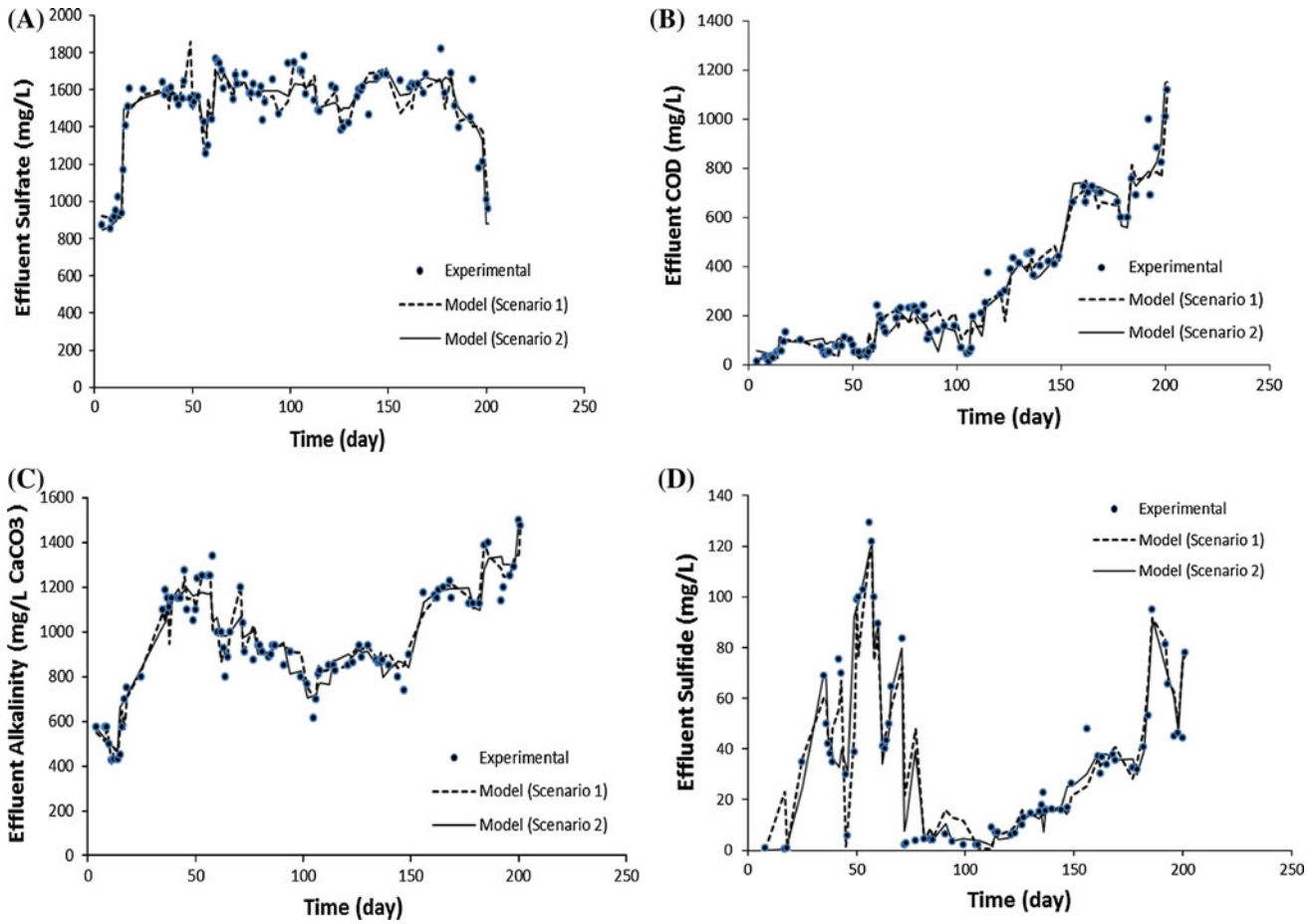

Fig. 4 Measured and neural network prediction of reactor 3 effluent sulfate (**a**), effluent COD (**b**), effluent alkalinity (**c**), and effluent sulfide (**d**) concentrations for scenarios 1 and 2 (mg/L $CaCO_3$:mg/L calcium carbonate alkalinity)

COD, alkalinity and sulfide at the reactor effluent, which allowed the fate of the externally added carbon and the electron source to be easily predicted.

Modeling of metal recovering bioprocesses is very important in optimizing reactor operational conditions. However, it is very difficult to predict the performance of such bioprocess using classical approaches, since performance depends on several factors, such as wastewater composition, operational parameters of the reactor, and the microbial community (Sahinkaya 2009). This study has shown that ANNs can be used to model the performance of metal recovering sulfidogenic upflow and downflow FBRs. In the second scenario, the reactor performance was successfully predicted, which would be useful during the reactor design phase (before processing). ANN can also be used to predict the response of the bioreactor to great variations in the composition of the incoming wastewater and unexpected overloads. This may allow an operation engineer to take measures to avoid possible process upsets due to unpredicted changes in the incoming wastewater. Using the ANN predictions, pre-treatments (such as neutralization) and metal precipitation can also be used to maintain good process performance during such overloading periods (Sahinkaya et al. 2007).

Conclusions

The designed, trained, and validated neural network model predicted the performance of the UFBR and DFBRs in the treatment of AMD. The developed model gave satisfactory fits to the experimentally obtained sulfate, COD, alkalinity, and sulfide data. The all-R values in the comparison of BP algorithms were observed as higher than 0.90. In the second scenario, the reactor performance was predicted without using effluent parameters as model input data, which may allow the prediction of reactor performance at different operational conditions without conducting experiments. The microbiology of anaerobic processes is complex as it depends on interdependent activity of a number of organisms. ANN can be effectively used to predict the performance of such complex systems. Thus, it

is possible to optimize operational costs to reduce the high expenses of chemicals with the proposed model-based applications.

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