Artificial neural network based model for evaluating performance of immobilized cell biofilter

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ABSTRACT

Artificial neural networks (ANNs) are powerful data driven modelling tools which has the potential to approximate and interpret complex input/output relationships based on the given sets of data matrix. In this paper, a predictive computerised approach has been proposed to predict the performance of an immobilized cell biofilter treating NH_3 vapours in terms of its removal efficiency (RE) and elimination capacity (EC). The input parameters to the ANN model were inlet concentration, loading rate, flow rate and pressure drop, while the output parameters were RE and EC respectively. The data set was divided into two parts, training matrix consisting of 51 data points, while the test matrix had 16 data points representing each parameter considered in this study. Earlier, experiments from continuous operation in the biofilter showed removal efficiencies from 60 to 100% at inlet loading rates varying between 0.5 to 5.5 g $NH_3/m^3.h$. The internal network parameters of the ANN model during simulation was selected using the 2^k factorial design and the best network topology for the model was thus estimated. The predictions were evaluated based on their determination coefficient values (R^2). The results showed that a multilayer network (4-4-2) with a back propagation algorithm was able to predict biofilter performance effectively with R^2 values of 0.9825 and 0.9982. The proposed ANN model for biofilter operation could be used as a potential alternative for knowledge based models through proper training and testing of the state variables.

1 INTRODUCTION

Ammonia is used extensively in the semiconductor industry, as the starting material for the manufacture of nitric acid and as a refrigerating fluid instead of chlorofluorocarbons. Malodors containing NH_3 are released from pulp and paper industry, wastewater treatment plants, night soil treatment plants and aerobic composting of low C/N material. Hence there arises a potential need to adapt suitable control techniques for the effective removal of these emissions from related process industries. Biofiltration is a cost effective technology for treatment of waste gases containing low concentrations of VOCs at large flow rates. The high removal efficiencies (REs) achieved along with uncomplicated flexible design, low operational and maintenance costs edges biofilters over other biological treatment techniques such as biotrickling filters and bioscrubbers (Kennes and Veiga, 2001). Biofilters have proved to remove NH_3 emissions effectively from gas streams using a bed of biologically active material such as compost, peat, wood bark, etc. In recent years, immobilization of microbes in support matrix such as alginate beads or suitable polymeric materials has gained popularity in the field of biofiltration. The main advantages of adopting immobilization techniques in biofiltration is to provide high cell concentrations, improve genetic stability, protection from shear damage and to enhance favorable microenvironment for microbes (nutrient gradients and pH). Chung *et al.* (1996) evaluated the effects of operational factors such as retention time, temperature and inlet concentration on the performance of a biofilter packed with *Thiobacillus thioparus* immobilized with Ca-alginate pellets and found an optimal S-loading of 25 g m^{-3} h^{-1}.

Traditionally the performance of biofilters has been modeled/predicted using process based models that are based on mass balance principles, simple reaction kinetics and a plug flow of air stream (Ottengraf and van Den Oever, 1983; Shareefdeen *et al.*, 1993; Deshusses *et al.*, 1995; Jin *et al.*, 2006). The main advantages of these process models are that they are based on the underlying physical process and the results obtained generally provide a good understanding of the system. However this depends on numerous model parameters and obligates information on specific growth rate of microbes, biofilm thickness and density, values of diffusivity, partition, yield and distribution coefficient, intrinsic adsorption etc. The accurate estimation of some of these parameters requires elaborate technical facilities and expertise, the absence of which hinders the preciseness of the model and limits the application and reliability of the model.

An alternate modelling procedure consists of a data driven approach wherein the principles of artificial intelligence is applied with the help of neural networks. It has been shown earlier that the performance of biofilters and biotrickling filters can be predicted from prior estimation of easily measurable operational parameters such as flow rate, unit flow, inlet loading rate, pressure drop and inlet concentration (Rene *et al.*, 2006; Elias *et al.*, 2006).

2 THE ANN BASED MODELING APPROACH

A multi layer perceptron (MLP) using the back propagation algorithm (Rumelhart *et al.,* 1986) is the most widely used neural network for forecasting/prediction purposes (Maier and Dandy, 2000). Neural networks acquire their name from the simple processing units in the brain called neurons which are interconnected by a network that transmits signals between them. These can be thought of as a black box device that accepts inputs and produces a desired output. MLP generally consists of three layers; an input layer, a hidden layer and an output layer. Each layer consists of neurons which are connected to the neurons in the previous and flowing layers by connection weights (W_{ij}). These weights are adjusted according to the mapping capability of the trained network. An additional bias term (θ_j) is provided to introduce a threshold for the activation of neurons. The input data (X_i) is presented to the network through the input layer, which is then passed to the hidden layer along with the weights. The weighted output ($X_i W_{ij}$) is then summed and added to a threshold to produce the neuron input (I_j) in the output layer. This is given by:

$$I_j = \Sigma\, W_{ij} X_i + \theta_j \tag{1}$$

This neuron input passes through an activation function $f\,(I_j)$ to produce the desired output Y_j. The most commonly used activation function is the logistic sigmoid function which takes the form;

$$f(I_j) = \frac{1}{1+e^{-I_j}} \tag{2}$$

3 MATERIALS AND METHODS

Experimental details pertaining to cultivation of micro organisms, media composition, preparation of immobilized packing media, experimental setup, biofilter operation and analytical techniques for data collection are given in our previously published work (Kim *et al.,* 2007).

4 MODELING METHODOLOGY

4.1 Model Input-Outputs

A neural network based predictive model was developed with flow rate, inlet loading rate, pressure drop and inlet concentration as the model inputs and elimination capacity and removal efficiency as the outputs.

4.2 Data Division

The experimental data was divided into training (N_{Tr}, 75%) and test data (N_{Te}, 25%). The test data was set aside during network training and was only used for evaluating the predictive potentiality of the trained network.

4.3 Error Evaluation

The closeness of prediction between the experimental and model predicted outputs were evaluated by computing the determination coefficient values computed by the following formulae (Elias *et al.,* 2006).

$$R^2 = \left[\frac{\sum_{i=1}^{N} \left(Y_{\text{model}_i} - \overline{Y_{\text{model}}} \right) \left(Y_{\text{observed}_i} - \overline{Y_{\text{observed}}} \right)}{(N-1) S_{Y_{\text{model}}} S_{Y_{\text{observed}}}} \right]^2 \tag{3}$$

4.4 Data pre-processing and randomization

Experimental data collected from the biofilter during the 67 days of continuous operation was randomized to obtain a spatial distribution of the data, which accounts for both steady state and transient steady state operation. The data was also normalized and scaled to the range of 0 to 1 using equation 4, so as to suit the transfer function in the hidden (sigmoid) and output layer (linear).

$$\hat{X} = \frac{X - X_{min}}{X_{max} - X_{min}} \tag{4}$$

Where, $\hat{X}$ is the normalized value, X_{min} and X_{max} are the minimum and maximum values of X respectively.

4.5 Network parameters

The internal parameters of the back propagation network namely epoch size, error function, learning rate (η), momentum term (μ), training count (T_c) and transfer function are to be appropriately selected to obtain the best network architecture that gives high predictions for the performance variables.

In this study the number of neurons in the input layer (N_I=4) and output layer (N_0=2) were chosen based on the number of input and output variables to the network.

A detailed study on the effect of internal network parameters on the performance of back propagation networks and the procedure involved in selecting the best network topology has been described elsewhere (Maier and Dandy, 1998). However in most instances, literature suggests the use of a trial and error approach where the performance goal is set by the user. In this study the best values of the network parameters were chosen by carrying out simulations performed using the 2^k full factorial design (Montgomery, 1991). The 2^k design is of particular significance in exploring the effect of many factors on the response variable for a particular system. It provides the smallest number of runs with which 'k' factors can be studied in a complete factorial design (In this study, k=4, Hence 16 simulations were done – *data not shown*). Determination coefficient (R^2) values were taken as the response variable and the setting that yielded the maximum R^2 value in the test data was taken as the best network parameter.

4.6 Softwares used

ANN based predictive modelling was carried out using the shareware version of the neural network and multivariable statistical modelling software, NNMODEL (Version 1.4, Neural Fusion, NY) and full factorial design was carried out by the statistical software MINITAB.

5 RESULTS AND DISCUSSIONS

5.1 Experimental

The performance of the immobilized cell biofilter was monitored by varying the flow rate and inlet concentration. A step increase from low to high loading rates to the biofilter caused a few days to adapt to the new concentration and reach a new steady state value shortly. The results from this study are shown in Figure 1 as a function of the operating time, loading rate, EBRT and RE. These removal profiles indicated that the immobilized cells possessed good activity with steady and consistent removal even during the beginning of the experiments. The loading rate of NH_3 was gradually increased to 2.5 g m^{-3} h^{-1} on the 14th day of continuous operation. The response was a sudden decline in the RE from 100% to 96% followed by a new steady state at the end of the 16th day where the RE was 98%. Hence, the loading rate was decreased to 1.7 g m^{-3} h^{-1} and subsequently increased in small time steps to a maximum of 4.5 g m^{-3} h^{-1}. The biofilter RE profiles displayed minor ameliorating fluctuations due to step increase in loading rate between 1 and 4.5 g NH_3 m^{-3} h^{-1}. It is also evident that the RE was nearly 100% (>95%) up to a loading rate of 4.5 g m^{-3} h^{-1}. However, after 60 days, when the ILR to the biofilter was increased significantly by varying both the concentration and flow rate to values as high as 7.5 g NH_3 m^{-3} h^{-1}, a noticeable decrease in the RE values from 100% to nearly 60% was observed. The critical NH_3

loading rate to the biofilter was considered as 4.5 g NH_3 m^{-3} h^{-1}. Pressure drop values were sufficiently low during the operational time (0.1 - 1.7 cms of H_2O) and did not cause any significant operational problem.

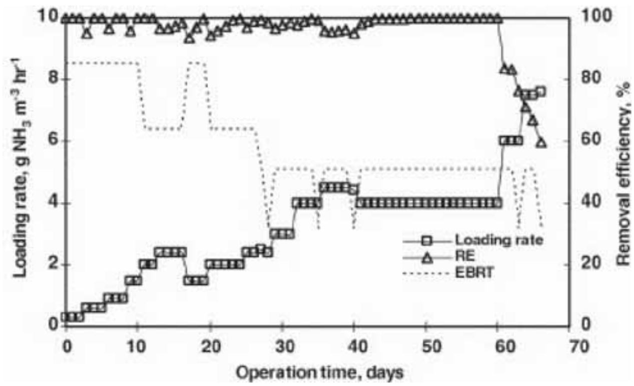

Figure 1. Time course profile of inlet loading rate and removal efficiency in the immobilized cell biofilter.

5.2 ANN based modeling

To model the performance of the biofilter, neural based simulations were carried out using the standard back error propagation network. The ranges of input and output parameters for the ANN model are given in Table 1. The experimental data collected from the biofilter was suitably divided into the training and test data set, pre-processed and randomized before carrying out simulations. The model was evaluated with the test data and the effect of network parameters on the R^2 value was used as a measure to choose the best network architecture.

Table 1.
Range of input and output parameters used for training and testing ANN model developed to represent biofiltration of NH_3 vapours

Parameter	**Training data, N_{Tr}-51**			**Testing data, N_{Te}-16**		
	Min	**Max**	**Mean**	**Min**	**Max**	**Mean**
Input						
Inlet concentration, ppm	10	150	63.3	20	150	74.1
Flow rate, m^3/h	6	16	9.25	6	16	9.13
Inlet loading rate, g/m^3.h	0.3	7.5	3.08	0.6	7.5	3.54
Pressure drop, cms of H_2O	0.1	1.5	1.1	0.2	1.5	1.16
Output						
RE, %	60	100	97.2	66.8	100	93.2
EC, g/m^3.h	0.3	5.3	2.93	0.5	5	3.18

5.2.1 Effect of Network Internal Parameters

The different values of network internal parameters used to train the network are given in Table 2. During simulations with different combinations of settings as given by the experimental design, the following interpretations were made; (i) increasing the number of neurons in the hidden layer decreases the R^2 value significantly (ii) an increase in the training count from low to high levels displays high R^2 value for the model (iii) the effect of learning rate did not play a major role in increasing the R^2 value, but it played a complementary role in speeding up the error convergence and (iv) the momentum term increased the R^2 value when increased from lower to high levels. The best network architecture was then selected by observing high R^2 value in the test data set (Table 3, For RE predictions, R^2 value – 0.9825, for EC, R^2 value – 0.9982).

Table 2.
Full 2^4 - factorial design for estimating the best network architecture.

Parameters	**Values**
Neurons, N_H	4 – 12
Training count, Tc	1000 – 16000
Learning rate, η_{ih}	0.1 – 0.9
Momentum term, μ	0.1 – 0.9
Best R^2	1
Error tolerance	0.0001

Table 3.
Best architecture obtained with different values of network internal parameters.

N_I	N_H	N_O	T_C	η	μ
4	4	2	16000	0.9	0.9

5.2.2 Predictive capability of the model

The RE and EC values predicted by the ANN model is illustrated in Figure 2 and 3 for the training data. It is quite apparent that, while predicting the RE and EC, the network was able to exactly map the data points. However, two or three data points were not adequately mapped by the network during training. This might have been caused by the step increase in loading rates where the microbes were reacclimatizing itself to attain new steady states. After training, the network was provided with the separate set of data for testing the developed model. The results presented as EC and RE is illustrated in Figure 4 and 5 respectively. A comparison between the EC and RE values predicted by the model with the experimental values reveals the predictive capability of the model. The model was able to adequately identify the low and high peaks in the EC and RE values. The R^2 values obtained during training and testing were greater than 0.98, which indicated that the predictions are accurate with best network architecture of 4-4-2.

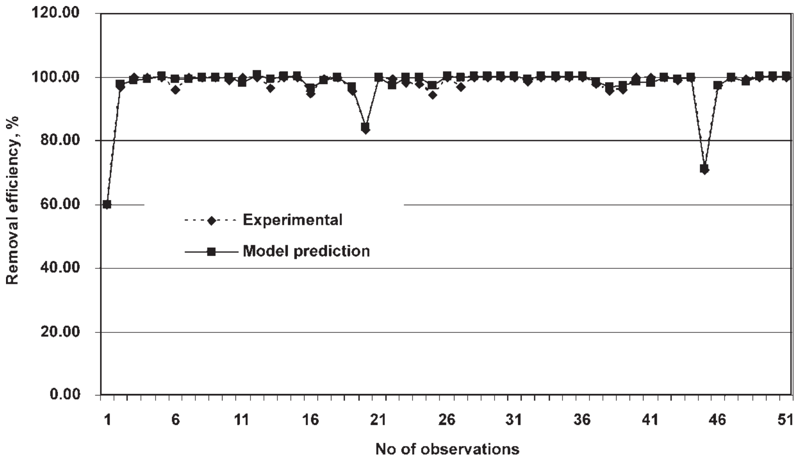

Figure 2. Comparison of experimental and predicted values of removal efficiency during model training (N_{Tr} -51).

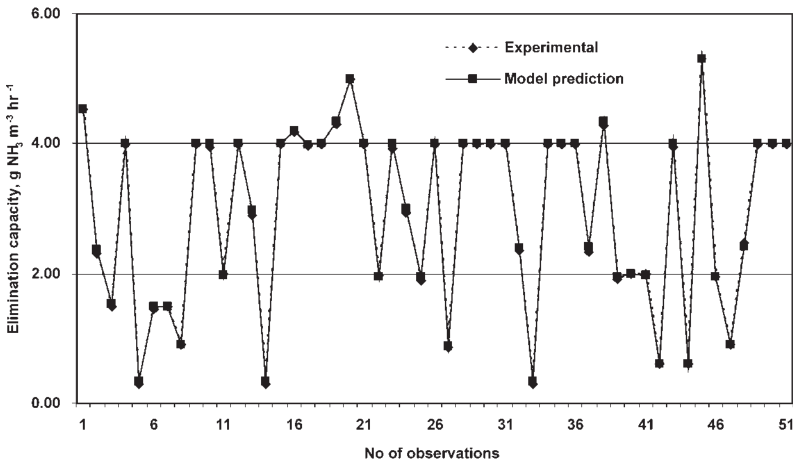

Figure 3. Comparison of experimental and predicted values of elimination capacity during model training (N_{Tr} -51).

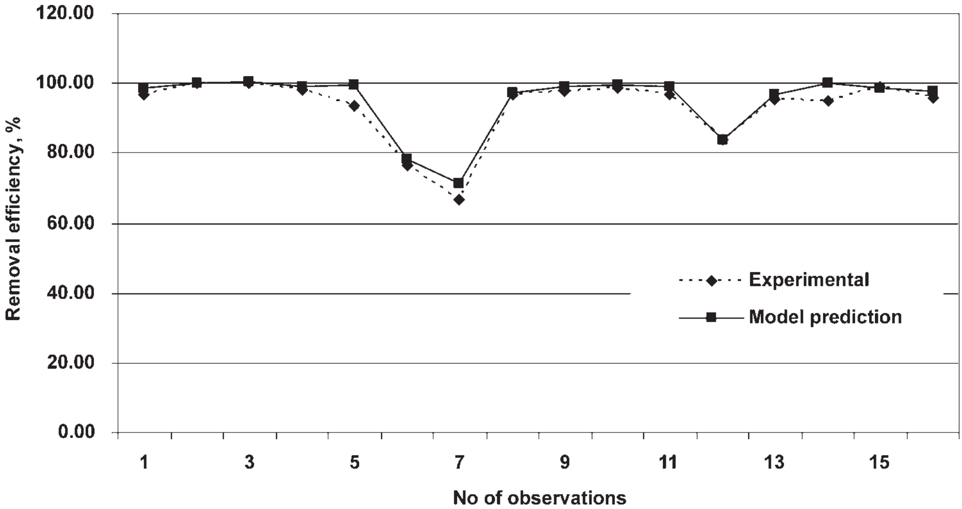

Figure 4. Comparison of experimental and predicted values of removal efficiency during model testing (N_{Tr} -16).

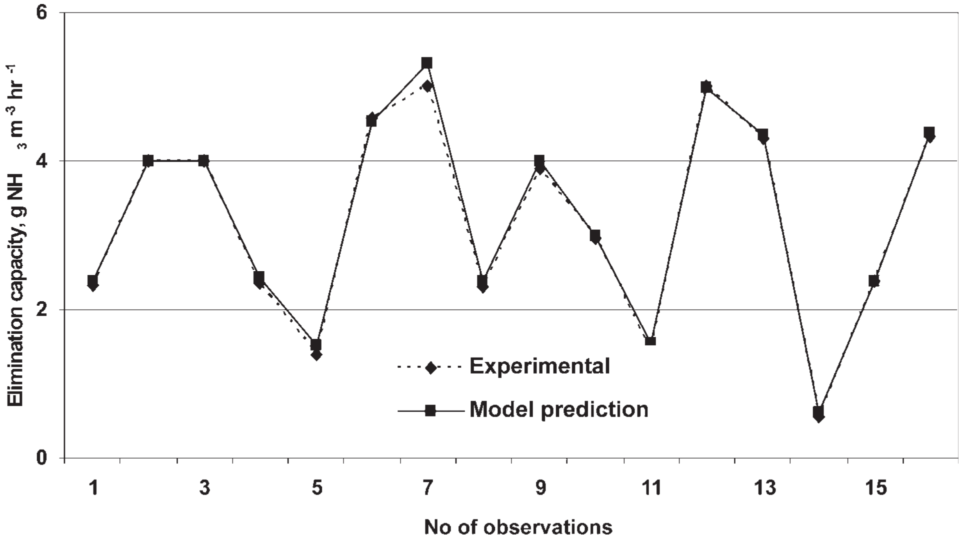

Figure 5. Comparison of experimental and predicted values of elimination capacity during model testing (N_{Tr} -16).

6 CONCLUSIONS

A laboratory scale immobilized cell biofilter evaluated to remove NH_3 vapours showed RE higher than 90% at loading rates less than 4.5 g NH_3/m^3 h. This study explores the application of ANN as a performance prediction tool for a biofiltration process. The ANN model showed the ability to predict the extreme operating conditions and address the performance with R^2 values greater than 0.98 for the training and test data set. The best network architecture (4-4-2) during effective training of the model was determined by 2^k factorial design. The results from this study suggest that neural networks can capture and extract complex relations among the easily measurable parameters in a biofiltration process and predict the performance.

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