Comparison of Neural Networks and Kalman Filter for the Modeling of Ion Exchange Process

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Abstract: This paper compares the performance of time delayed neural network (TDNN) with that of the Kalman filter for the up-take of copper during an ion-exchange process. Since the ion-exchange process is a complex and nonlinear process, the modeling based on time related empirical equations is simplistic and difficult to account for all the concomitant processes influencing the process variables. Thus, the time delayed neural networks and the Kalman filter is used to model this process because of its ability to model complex nonlinear systems without fully understanding the system. The minimum square error (MSE) minimization technique is used to determine the optimal neural network architecture for the process. TDNN is simpler to implement since it does not require a model for the system. The simulation results show that the performance of the Kalman filter for the modeling of the ion-exchange process is superior to TDNN.

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1. Introduction

In many countries including South Africa, mining and metallurgical operations are the main sources of ground water pollution. Since huge amounts of contaminated mine and metallurgical operations waters are produced, and ground and surface waters are main sources of drinking water, there is the need to remove metal pollutants from metallurgical industrial waste prior to their disposal. The ion exchange process is one of the popular water treatments for water purification [1]. Ion-exchange reaction occurs between at least two phases one of which is liquid. The ion exchanger may be organic (such as activated carbon, resin) or inorganic such as (zeolites, clays, β-FeOOH, $ZrO2$). In our experiment an activated natural zeolite i.e clinoptilolite is used.

The up-take mechanism of the ion-exchange is a difficult process to model since it is nonlinear and all the factors affecting the process are not known. In this work, we compare the effectiveness of neural networks and the Kalman filter to model the ion exchange process. Time delayed neural network (TDNN) has been applied successfully to many problems involving time series prediction and modeling of non-linear systems [2]-[3]. TDNN is a feed forward neural network capable of using a fixed number of previous system inputs to predict the following output of the system. The TDNN has been used extensively used for speech recognition and has been shown to perform quite well. The Kalman filter is also a popular recursive technique for parameter estimation [5], [6]. It provides an efficient way to estimate the states of a process in a way that minimizes the mean square error. The Kalman filter does not only work well in practice but it can be shown that of all possible filters, it is the one that minimizes the variance of the estimation error.

In this paper, the performance of the Kalman filter and TDNN for the modeling of ion-exchange process is compared. Experimental results show that the Kalman filter provides improved performance over TDNN in several cases.

2. Time Delayed Neural Network

TDNN consists of feed forward network with tap delay line at the input which is very useful for time series predictions. In this work a one hidden layer TDNN with two delayed inputs is used.

Fig. 1 shows the implemented TDNN. The optimal TDNN is also determined by MSE minimization. Each neuron in the hidden layer is presented with delayed inputs in addition to the current one. For a time delay of τ the neural network is presented with $y(t), y(t-1) \dots y(t-\tau)$ inputs. A mapping by TDNN produces an output z(t) at time t as:

$$z(t) = f\left(y(t), y(t-1), \dots y(t-\tau)\right) \quad . (1)$$

TDNN is trained by using part of the dataset and adjusting the weights until an acceptable minimum square error is attained [7]. In this work, we used the backpropagation as the optimization algorithm. TDNN has been used successful in prediction because of its ability to capture the dynamics of the system after been trained.

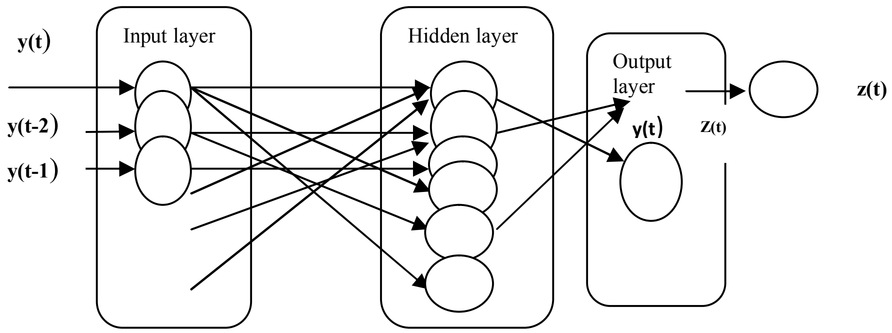

Fig 1. TDNN with two delayed inputs and one hidden layer

3. Kalman Filter

The Kalman filter addresses the general problem of estimation of the state of a discrete-time controlled process by the linear stochastic difference equations

$$x_t = Ax_{t-1} + Bu_{t-1} + w_{t-1} \quad (2)$$

with measurement z_t,

$$z_t = Hx_t + v_t \quad (3)$$

where w_{t-1} and v_t represent the process and measurement noise respectively. They are assumed to be white noise with normal probability distributions and zero-mean noise vectors. The covariance matrix of w_{t-1} and v_t are Q and R respectively. In our work, we assume that Q is very small or negligible and the measurement is corrupted by 0.1 mg/l white Gaussian noise (R = 0.01). Since there is no control input, u_t=0. The measurement z_t is also taken directly from the state, thus H=1.

4. Experiment

The preparation of the synthetic solution used for the experiment is described in [4]. The natural zeolite clinoptilolite-type used in this study was sourced from the Vulture Creek, KwaZulu-Natal Province of South Africa. The clinoptilolite was crushed and milled into powder with average particle sizes of approximately 75µm. The powder was then examined using an X-ray powder diffractometer (XRD) Phillips X'pert Model 0993 to determine its mineralogical and crystalline composition. Its elemental composition was determined using X-ray fluorescence spectroscopy (XRF, Phillips Magix Pro) while the surface area was analyzed using BET (Tristar 3000). The measurements were done under a nitrogen atmosphere. Prior to porosity and surface area analysis, 2g of sample was first degassed and nitrogen gas was flushed through for 4 hours at 120^{o}C. Clinoptilolite grains of sizes in the range of 2.8 mm to 5.6 mm were used for adsorption studies. A fraction of these grains was treated in HCl at concentration of 0.02M and 0.04M at room temperature over a period of 8 hours. The clinoptilolite was then washed in deionized water to remove the fine fractions and thereafter dried in the oven at 50^{o}C for 24 hours. The copper solution was prepared by dissolving CuSO4.5H2O in deionizer water at pH 6.5. The synthetic wastewater at three different Cu2+ ion concentrations, i.e. 0. 840, 0. 410, and 0. 460 g/l were prepared in a one liter flask and stirred at 300, 200 and 120 rpm respectively. The Cu removal from the aqueous solution through the ion-exchange process on the clinoptilolite was conducted at room temperature. The solution was assayed using atomic absorption spectroscopy (AAS), (Model Varian Spectra (20/20)).

Tab. 1. Experiment and corresponding estimation error

Experiment	Concentration of Cu 840 mg/l and stirring: 300rpm	Concentration of Cu 410 g/l and stirring: 200rpm	Concentration of Cu 460 mg/l and stirring: 120rpm
Average root mean square error (mg/l) using TDNN	11.1	3.1	1.3
Average root mean square error (mg/l) using Kalman filter	4.4	1.1	0.4
Average Percentage Error using TDNN	4%	1%	0.3%
Average Percentage Error using Kalman Filter	0.7%	0.4%	0%

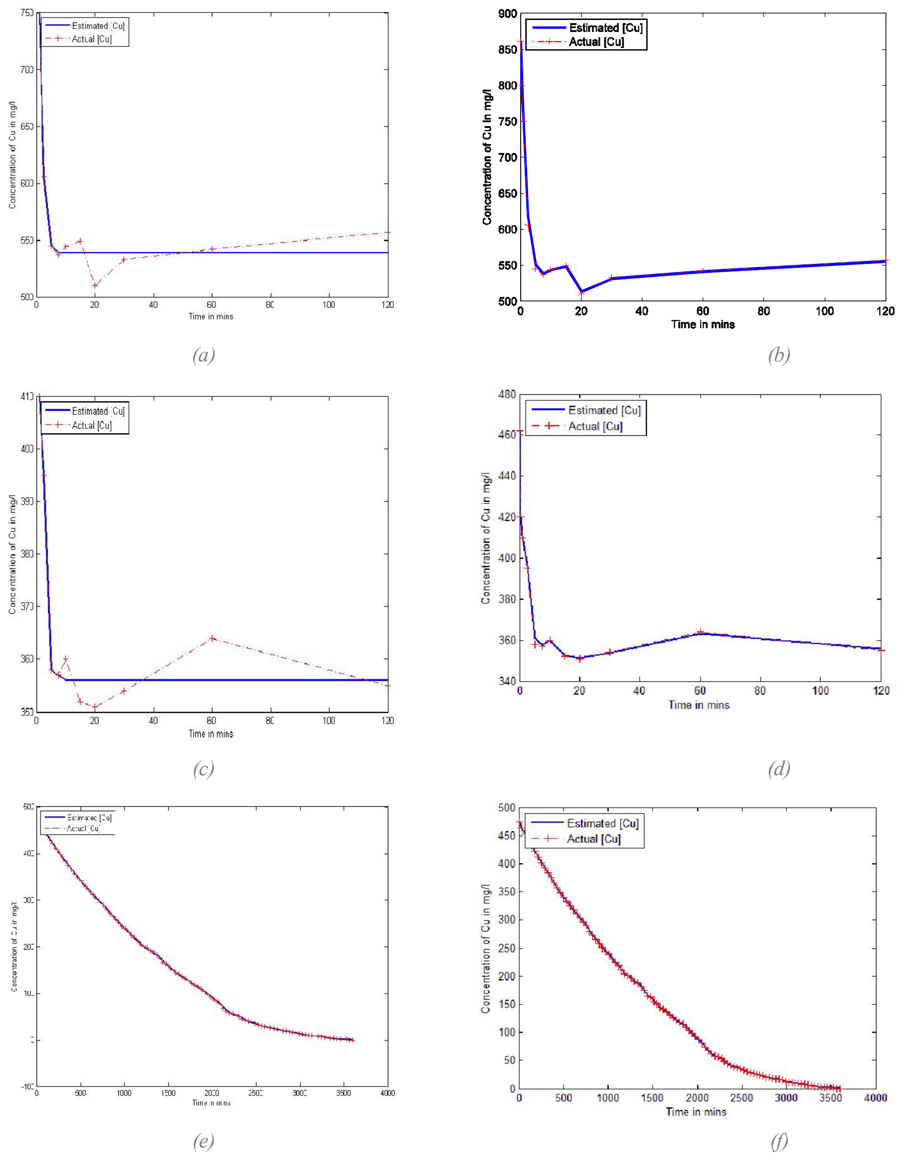

Fig. 2. The prediction of copper up-take during the ion exchange process from (a) solution with initial Cu concentration of 840m g/l and stirring of 300rpm using TDNN (b) solution with initial Cu concentration of 840m g/l and stirring of 300rpm using Kalman filter (c) solution with initial copper concentration of 410m g/l and stirring of 200rpm using TDNN (d) solution with initial copper concentration of 410m g/l and stirring of 200rpm using Kalman filter (e) solution with initial Cu concentration of 460m g/l and stirring of 120 rpm using TDNN filter (f) solution with initial Cu concentration of 460m g/l and stirring of 120 rpm using the Kalman filter

5. Results

Fig.2 shows the results of predicted values plotted against the ground truth of three experiments using TDNN and the Kalman filter. A visual comparison of the plots of the estimation by the Kalman filter in Fig.2 (b) and (d) and the plots of estimation by TDNN in Fig.2 (a) and (c) shows that the performance of the Kalman filter is better.

Tab. 1 also shows the average root mean square errors and average percentage errors of the estimated copper concentrations of each experiment. The overall average root mean square error and average percentage error for the prediction using TDNN are 5.17 mg/ l and 1.3 % respectively. The overall average root mean square error and average percentage error for the prediction using the Kalman filter are 1.8 mg/ l and 0.4 % respectively. The results in Tab.1 also show that the performance the Kalman filter for the prediction of the up-take of copper from an aqueous solution during ion-exchange can be superior to TDNN.

6. Summary

In this work, we compared the performace of a basic Kalman filter with TDNN for the modeling of the up-take copper from aqueous solution during ion-exchange. The results from the Kalman filter is better than TDDN with one hidden layer and two delayed inputs. The Kalman filter however requires a good knowledge of the process to be modeled making it more difficult model than TDNN. Neural networks (TDNN) requires no models. The main challenge for neural networks is the need to provide the network with data for training. This work is only the beginning, there is still more work to be done to test the potential of the prediction systems. Future work includes using multilayer networks, longer delayed inputs and the extented Kalman filter.

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