Monitoring of sequencing batch reactor for nitrogen and phosphorus removal using neural networks

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Abstract

The information of nutrient dynamics is essential for the precise control of effluent quality discharged from biological wastewater treatment processes. However, these variables can usually be determined with a significant time delay. Although the final effluent quality can be analyzed after this delay, it is often too late to make proper adjustments. In this paper, a neural network approach, a software sensor, was proposed for the real-time estimation of nutrient concentrations and overcoming the problem of delayed measurements. In order to improve the neural network performance, a split network structure applied separately for anaerobic and aerobic conditions was employed with dynamic modeling methods such as auto-regressive with exogenous inputs. The proposed methodology was applied to a bench-scale sequencing batch reactor (SBR) for biological nutrient removal. The extrapolation problem of neural networks was possible to be partially overcome with the aid of multiway principal component analysis because of its ability of detecting of abnormal situations which could generate extrapolation. Real-time estimation of PO$_4^{3-}$, NO$_3^-$ and NH$_4^+$ concentrations based on neural network was successfully carried out with the simple on-line information of the SBR system only.

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1. Introduction

With increasingly stringent regulations of effluent quality, process monitoring and control have become more important. However, the lack of suitable on-line sensors for monitoring key process variables, such as nutrient concentrations, limits the effective control of effluent quality especially in biological wastewater treatment [1]. Although these nutrient concentrations can be measured by laboratory analyses, a significant time delay in a range of tens of minute to few hours is usually unavoidable. It is normally too late to achieve well-timed adaptive process control accommodating influent fluctuation and other disturbances, especially for advanced wastewater treatment requiring more precise and timely controls. To overcome these problems, software sensors were developed to estimate hard-to-measure process variables from other on-line measurable process variables [2,3].

Neural networks have been proved to be able to model non-linear systems [4] and successfully applied for modeling various non-linear processes [5,6]. Recently, the use of neural networks is also gaining popularity in modeling biological wastewater treatment processes [7–9]. Neural networks can map a set of input patterns onto a corresponding set of output patterns after learning a series of past process data from a given system. Moreover, a neural network model has distinctive ability of learning non-linear functional relationships without requirement of the structural knowledge of process to be modeled. There have been several successful developments of software sensor based on neural network approach [10,11].

In this work, the on-line software sensor for nutrients was developed using the neural network approach with auto-regressive and exogenous inputs (ARX) representations. The proposed method, which can provide an accurate prediction of hard-to-measure process variables, was applied to a bench-scale
sequencing batch reactor (SBR) for the advanced wastewater treatment.

2. Materials and methods

2.1. Sequencing batch reactor

The data used in this work were collected from a bench-scale SBR system as shown in Fig. 1. A fill-and-draw SBR system with a 4 l working volume was operated in an 8 h cyclic mode and each cycle consists of 2 h anaerobic (including 10 min filling), 4 h 30 min aerobic, 1 h 30 min settling and drawing phases. The temperature of the reactor was controlled at 20 ± 1°C using a water circulation system. Clarified supernatant of 2 l was withdrawn from the reactor at the end of settling stage and fresh (synthetic) wastewater of 2 L was pumped into the reactor during the filling stage. Solid retention time (SRT) was maintained at about 12 days by wasting mixed liquor suspended solids (MLSS) at the end of aerobic stage. Loading amounts of COD (as CH₃COOH), NH₄⁺-N and PO₄³⁻-P per cycle in a standard condition were 600, 40 and 15 mg/l, respectively. The controls of duration/sequence of phases and on/off of peristaltic pumps, mixer, air supply were automatically achieved by an in-house developed data acquisition and control (DAC) system. The DAC system consisted of computer, interface cards, meters, transmitters and solid-state relays (SSR). Electrodes of pH (Ingold), Oxidation-Reduction Potential (Cole-Parmer) and Dissolved Oxygen (Ingold) were installed and connected to individual meter. The status of reactor and the value of electrode signal were displayed in a computer monitor, and stored in the data file. Profiles of on-line sensor values in a typical SBR cycle are shown in Fig. 2.

During the operation of SBR for the development of neural network model, one of nutrients (COD, NH₄⁺ or PO₄³⁻) in feed solution was changed to create 18 data sets while others were kept at the standard influent concentration:

- COD (as CH₃COOH): 500, 700, 800, 900, 1000 mg/l
- NH₄⁺-N: 0, 10, 20, 30, 50, 60, 70, 80 mg/l
- PO₄³⁻-P: 0, 5, 10, 20, 25, 30 mg/l

Disturbance was delivered to the reactor only for one cycle in order to keep the SBR process under the standard operation condition. A broad range of experimental conditions was employed to develop a model, which can cover the entire range of possible conditions in actual processes. Therefore, including six normal operation sets with the standard influent loadings, a total 24 data sets were employed to develop an on-line software sensor. The on-line pH, ORP and DO signals were stored in the data file every 1 min during the experiments. However, only the first 390 sampling time instants were used to develop the model since biological reactions in the settling and drawing phases (corresponding to those of the last 90 time instants) were assumed as negligible. Moreover, the sensor signals were unreliable due to the absence of mixing. The performance of the SBR system was also monitored by off-line analyses of PO₄³⁻, NO₃⁻, NH₄⁺ and TOC concentrations every 30 min. All chemical analyses were performed according to standard methods [12].

2.2. Multiway principal component analysis (MPCA)

In a typical batch run $j = 1, \ldots, J$ variables are measured at each of $k = 1, 2, \ldots, K$ time intervals throughout the batch. Similar data will exist on a number of batches $i = 1, 2, \ldots, I$. All the data can be summarized in a matrix $X(i \times J \times K)$ representing the historical database. MPCA is equivalent to unfolding the three-dimensional data matrix $X$ into a large two-dimensional matrix $\bar{X}$, and then performing a regular PCA [13]. In case of monitoring batch processes, it is important to determine differences between batches and to project new batches on the model. Therefore, in this work, $\bar{X}$ was unfolded in such a way as to put each of its vertical slices ($I$ side by side to the right, starting with the one corresponding to the first time interval. The result-
ing two-dimensional matrix has size \((I \times JK)\). This unfolding allows for analyzing the variability among the batches in \(X\) by summarizing the information in the data with respect to both variables and their time variation. Then MPCA decomposes the data into a series of principal components consisting of score vectors \((t_r)\) and loadings \((p_r)\), plus residuals \((E)\):

\[
X = \sum_{r=1}^{R} t_r p_r + E
\]

(1)

The loading vectors \((p_r)\) define the reduced dimension space \((R)\) and the directions of maximum variability. Each element of the score vectors \((t_r)\) corresponds to a single batch and depicts the overall variability of this batch with respect to the other batches in the data base throughout the whole batch duration. Usually, a few principal components can express most of the variability in the data and is as small as possible in a least squares sense. The NIPALS (nonlinear iterative partial least squares) algorithm can be used for sequential computation of the dominant principal components [14].

2.3. Artificial neural networks

A variety of artificial neural network architectures and training algorithms has been proposed and used to model non-linear systems. However, there has been no guideline for choosing network architectures for the optimal representation of a given problem. A feed-forward back-propagation neural network (FBNN) was employed for our purpose, which has been successfully applied in modeling wide range of non-linear systems, especially chemical/biological engineering processes. Typical FBNN structure consists of one input layer, one (or multiple) hidden layers and one output layer. Each layer could have a number of nodes (processing elements), which are connected linearly by weights to the nodes in the neighboring layers. The training process adjusts weights to minimize the error between the measured output and the output produced by the network. Through this adjustment, the neural network learns the input–output behaviors of the system. In this work, a generalized delta-rule with momentum and adaptive learning rate was used for the training process implemented in MATLAB, which is a common scientific programming language.

Prior to neural network training, the data sets were scaled by using the zero-mean normalization method. The first layer, \(x_{1}^{j}\), consists of the input values of the model and then, the inputs, \(x_{l-1}^{j}\), from the previous layer are combined by a linear combination to produce outputs, \(O_{l}^{j}\):

\[
O_{l}^{j} = \sum_{i} w_{ji} x_{l-1}^{i} + \theta_{j}
\]

(2)

where \(w_{ji}\) is the weight value connecting the \(i\)th element in the previous layer and the \(j\)th element in the \(l\)th layer, and \(\theta_{j}\) is the bias term. The outputs from the nodes are obtained from a transformation of the outputs \(O_{l}^{j}\) as shown in the equation below:

\[
y_{l}^{j} = f(O_{l}^{j})
\]

(3)

where \(y_{l}^{j}\) is the activity or state of the \(j\)th node in the \(l\)th layer, and \(f\) is the activation function. The hyperbolic tangent function gave the best performance compared to other activation functions in the learning process and was chosen as the activation function in this work.

2.4. Autoregressive with exogenous input

The auto regressive with exogenous inputs(ARX) structure employs delayed inputs and outputs in order to determine a prediction of the output at one (or more) sample interval(s) in the future. It is of the form:

\[
\hat{y}(t) = f(x(t), x(t - 1), \ldots, x(t - N))
\]

(4)

where \(\hat{y}(t)\) represents the model prediction, \(x(t), x(t - 1), \ldots, x(t - N)\) represent the vector of current and past inputs, outputs and additive prefiltered noise and \(f(\cdot)\) is some function of \(x(t)\). In this case, the function is a back-propagation neural network with one or more hidden layer of nonlinear transfer function [15].

Fig. 3. Score plot of all batch data. The dotted line is 95% confidence limit. The numbers indicate the batch number.
3. Results and discussion

3.1. Pretreatment of SBR data sets

It has been reported that the on-line sensor values are somehow related with dynamic characteristics of the nutrient concentrations (NH$_4^+$, PO$_4^{3-}$ and NO$_3^-$) in SBRs [16,17]. The derivatives of pH, ORP and DO profiles can accurately detect the ends of phosphate release, ammonia conversion and phosphate uptake, and be a useful information source. Therefore, the derivatives of pH, ORP and DO were calculated from the on-line sensor profiles and included into the database. Since the differencing operation magnifies the noise it is necessary to smooth the data beforehand. This can be done by Savitzky–Golay smoothing which is a moving window method fitting a polynome by least squares [18].

3.2. Analysis of historical process data

MPCA was used for analysis of the whole process data set of 24 batches. The key idea of MPCA is to compress the normal batch data and extract the important information by projecting the data onto a low-dimensional space that summarizes both the variables and their time trajectories. By examining the process data in the reduced projection spaces defined by a small number of latent variables, it is often possible to extract very useful information to interpret the behavior of the SBR process. Four principal components, which explained approximately 83.9% of the total variability were determined by cross validation [19]. Fig. 3 shows a score plot of the collected data in the space of the resulting principal components. The score plot can give a picture that well represents the process behavior. As can be seen from Fig. 3, most of the operating batch points are contained within the confidence limits. The training data sets were selected as 18 batch operations among those inside the confidence limit. However, three batch operations (batch numbers 5, 6 and 21) are outside the confidence limits. These batch operations were not included in the training data sets of the neural network model and used as those of the validation data sets to examine the extrapolation ability of the developed software sensor model.

3.3. Neural network software sensor

The proposed software sensor model was based on neural network approach along with auto-regressive with exogenous (ARX) inputs. First of all, when a typical FBNN was trained with the collected data, it was very difficult to obtain acceptable modeling performance. It was assumed that the network could not learn correct process behavior due to abrupt physical environment changes caused by aeration. To solve this problem, separate neural networks were developed for anaerobic and aerobic phases, respectively. Each network was intended to capture
specific aspects of the corresponding phases. The target on-line monitoring interval was assigned to 5 min. For the inputs of FBNNs, the response variables (nutrient concentrations) at time \((k-1)\) were used alongside the previous five measurements from time \((k-1)\) to \((k-5)\) and their corresponding derivatives of pH, ORP and DO. The hyperbolic tangent function gave the best performance compared to other activation functions in the training process and was chosen as the activation function. The FBNN structure with two hidden layers consisting of 10 and 5 nodes for each hidden layer was satisfactory to monitoring the nutrient dynamics for both anaerobic and aerobic phases of SBR system, which was optimized by trial and error during the training process (Fig. 4).

Table 1
RMSE of the training and validation data sets

<table>
<thead>
<tr>
<th>Models</th>
<th>RMSE(_{\text{training}}) (18 training batches)</th>
<th>RMSE(_{\text{validation}}) (3 normal batches)</th>
<th>RMSE(_{\text{validation}}) (3 abnormal batches)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anaerobic</td>
<td>1.687</td>
<td>1.873</td>
<td>3.229</td>
</tr>
<tr>
<td>Aerobic</td>
<td>0.809</td>
<td>1.310</td>
<td>3.511</td>
</tr>
</tbody>
</table>

Figs. 5 and 6 represent the validation results of the proposed neural network model. For normal batch operations (Fig. 5) corresponding to three data points inside the confidence limit determined by MPCA (Fig. 3), excellent monitoring capability could be obtained from the developed software sensor model. However, the software sensor showed poor predicting ability for other validating data sets consisting of abnormal batch operations detected from MPCA analysis (Fig. 6). Since the neural network was trained with training data sets that only spanned the normal operating range, the results were not satisfactory for the batch operations beyond the training data sets, which exemplifies the weakness of the neural network in making extrapolation. However, this problem could be overcome in actual process monitoring with the aid of MPCA, because MPCA could effectively detect the outlier situations in on-line manner. Table 1 summarizes the root mean square errors (RMSE) values of the training and validation data sets. The RMSE performance index was defined as:

\[ \text{RMSE} = \sqrt{\frac{\sum(y - \hat{y})^2}{n}} \quad (5) \]

where \(y\) is the measured values, \(\hat{y}\) the corresponding predicted values and \(n\) is the number of samples. It could be noted that the validation error of the abnormal batch operations were much higher than the training error for both the anaerobic and aerobic model, whereas the validation error of the normal batch operations were comparable to the training error.

4. Conclusion

Devices for the on-line measurement of nutrient concentrations (\(\text{NH}_4^+, \text{NO}_3^-\) and \(\text{PO}_4^{3-}\)) in wastewater treatment are now available but these devices are still expensive, require high maintenance, and are not quite reliable. In this work, a software sensor was developed to estimate the nutrient dynamics of the SBR operation using more reliable on-line measurements of pH, ORP and DO as input data. The software sensor, based on the neural network model, can be effectively applied to SBR processes in order to cope with influent variations that are typical of municipal wastewater and the phase duration of SBR operation can be optimized and adjusted in real time.

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