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Dynamic parameter estimation to calibrate the activated sludge model for an enhanced biological phosphate removal process

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ABSTRACT

A parameter calibration of activated sludge models (ASMs) was performed to predict effluent chemical oxygen demand (COD), total nitrogen (TN), total phosphate (TP) and total suspended solid (TSS) concentrations of the enhanced biological phosphate removal process. Such calibration is an essential process for simulating the behavior of real-world wastewater treatment processes properly. Six different simulations were attempted to develop a reliable calibration method using two different parameter estimation methods for three objective functions. For the parameter estimation method, dynamic parameter estimation (DPE) and static parameter estimation (SPE) were investigated. The objective functions were based on the effluent quality (EQ) index of benchmark simulation and the effluent quality standards (EQS) in Korea. When using the same parameter estimation method, the predicted errors with the EQS-based objective functions could be decreased by approximately 20% over EQ index-based functions for TSS. When using the same objective function, the error with DPE was around 40% less than the error with SPE for TSS and TP. Therefore, applying DPE to the objective function based on the EQS was a proper calibration method of the ASM to predict a reliable effluent for the real process.

Keywords: Dynamic parameter estimation; Model calibration; Sensitivity analysis; Activated sludge model; Enhanced biological phosphate removal process

1. Introduction

The activated sludge models (ASMs) that were developed by International Water Association (IWA) task group are well accepted for simulating the behavior of the biological wastewater treatment process [1–4]. Researchers can select a specific model among ASM1, ASM2, ASM2d, or ASM3 depending on the target process and contaminant components that they are concerning [5].

These models have been used for various objectives such as process design, optimal operation, and effluent prediction, etc [6]. The calibration of ASMs is essential to simulate properly the behavior of real wastewater treatment processes. The calibration procedure is as follows: selection of target process and water quality components, sensitivity analysis of model parameters, parameter estimation, and model validation [7–11].

The sensitivity analysis helps to select the sensitive parameters that should be estimated for optimizing a mathematical model to simulate the real process. Sensi-

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tivity analysis is the first major task to improve the model predictability [12]. Among many approaches suggested from previous works step variation of a single parameter was reported to be the simplest [13]. The sensitivity index is also important for effectively selecting sensitive parameters The effluent quality (EQ) index, which was originally suggested as a performance index of controllers [14], was used as a sensitivity index by many researchers [13,15].

In general, the estimation of sensitive parameters was carried out by cross-matching simulated data with the measured data. Mathematical parameter estimation was also introduced and validated recently. The model parameter values should be updated when the simulation is performed for a long period because the characteristics of the biological reaction may be altered due to the variations of influent characteristics and the operating conditions; however, many models have used the static parameter estimation (SPE) technique due to its simplicity [16]. The SPE technique uses a whole set of data for estimating model parameters and obtains a set of parameters. Recently ASMs are becoming useful for predictive control of the process. For the purpose of process control, the SPE could not provide enough accuracy for prediction. Due to this reduced accuracy, a dynamic parameter estimation (DPE) technique is proposed in this study. The DPE uses data from an initial short period which are updated periodically. Recent development in computing power enables researchers to use the DPE easily.

In this study, the DPE technique was proposed to improve ASM predictability. For this parameter estimation, a new objective function based on the EQS was also proposed. Superiority of the proposed technique and objective function was verified by comparing the SPE technique and the objective function based on the EQ index, respectively.

2. Materials and methods

For the DPE, influent and effluent data from the initial 7 days were used to estimate parameters. Then, the estimated parameters were used to simulate the next following 7 days. This procedure was repeated continuously. For the SPE, only one set of parameter values was estimated using all influent and effluent data for 150 days. These estimated parameter values were used to predict effluent concentration for the whole simulation periods.

Three objective functions were considered in order to develop a reliable result for estimating parameter values. The first set was based on the EQ index that was presented by the IWA Simulation Benchmark to evaluate the performance of various controllers in a WWTP [14]. The other sets were based on the EQS in Korea to reduce



Fig. 1. General calibration procedure of activated sludge models.

the high weights of nitrogen and phosphate components. A detailed explanation is provided later in this paper.

The calibration of the ASM for the target process was performed by the general procedure of: gathering field plant data (Step 1), defining an objective function based on obtained process data for the simulation (Step 2), performing sensitivity analysis of model parameters (Step 3), estimating the selected sensitive parameters with measured influent and effluent data (step 4), and evaluating the simulated effluent using estimated values of the parameters (Step 5).

2.1. Gathering field plant data (Step 1)

The data for model calibration were obtained from the D-city wastewater plant, which has been operated as a process of five-stage step-feed enhanced biological phosphate removal (fsEBPR) for approximately 250 days from July, 2002 to March, 2003 [16]. The schematic diagram of the fsEBPR process is shown in Fig. 2. Each volume of biological reactors and settler is displayed in Table 1, while influent characteristics and operating con-ditions are summarized in Table 2. The daily measured influent data were used for simulation, and the missing data were interpolated by using a time series model [17].

2.2. Defining objective function (Step 2)

The effluent biological oxygen demand (BOD), total suspended solid (TSS), total nitrogen (TN) and total phosphate (TP) concentrations from the fsEBPR process plant were measured. Then, the objective function (OF) was defined to minimize the sum of weighted absolute errors of the effluent components for 150 days and was built as follows:

$$OF = \mininimize \sum_{i=1}^{150} (\beta_{TSS} | TSS_{obs,e} - TSS_{sim,e} |$$

$$+\beta_{BOD} | BOD_{obs,e} - BOD_{sim,e} |$$

$$+\beta_{TN} | TN_{obs,e} - TN_{sim,e} |$$

$$+\beta_{TP} | TP_{obs,e} - TP_{sim,e} |$$

$$(1)$$



Fig. 2. Schematic diagram of fsEBPR process.

 Table 2

 Influent characteristics and operating conditions in fsEBPR the process

	Influent component (mg/L)				Flow rate (m^3/d)				Temperature, °C
	COD	NH ₄ -N	NO ₃ -N	PO ₄ -P	Influent	Internal recycle	Sludge recycle	Sludge waste	
Minimum	60.2	7.6	0.0	1.0	10,573	14,300	7,400	45.5	12.5
Average	233.6	23.9	0.9	2.3	18,453	2,166	14,268	147.3	19.9
Maximum	428.0	31.7	3.0	3.3	26,213	40,647	26,203	216.0	26.7

Table 3

Three sets of each component weight for calculating the objective function

	TSS	BOD	TN	TP	
Case 1	1	1	10 1	25 10	
Case 3	1	1	1	5	

where β_{TSS} , β_{BOD} , and β_{TP} are the weighting factors for TSS, BOD, TN, and TP components, respectively. The subscript obs and sim represent observed and simulated concentration, respectively. The subscript *e* represents the effluent.

The three combinations of weighting factors were considered in order to develop a reliable objective function. The first set was based on the EQ index (Case 1), while the second set was based on the inverse ratio of effluent quality standards (EQS), BOD 10 mg/L, TSS 10 mg/L, TN 20 mg/L and TP 2 mg/L in Korea was (Case 2). Finally, the weighting factor of TN was doubled in order to avoid the possibility that the calibration result can be affected by the effluent TP predominantly because the weight of the phosphate was ten times the weight of the nitrogen in the second set (Case 3). Table 3 illustrates the weight of each component applied to the three sets.

2.3. Sensitivity analysis (Step 3)

Sensitivity analysis was performed using the reactor layout. Influent characteristics of the fsEBPR process were installed in D-city. Mathematical models were constructed by combining ASM3 for considering organic and nitrogen [4] with modified Bio-P model for phosphate [15] and one-dimensional model for solid settling [18]. The method of step variation of single parameter [13], which is one of the simplest sensitivity analyses, was applied to select more sensitive parameters in the mathematical models.

The sensitivity index (SI) was defined as the maximum derivative of the objective function. Each parameter was changed at the range of $\pm 50\%$ of reference parameter values which have been suggested in the literature [5,19].

$$SI(\theta_i) = \max \frac{\partial OF(\theta_i)}{\partial \theta_i}$$
(2)

where θ_i is *i*th parameter. The higher the SI, the more sensitive the parameter.

2.4. Parameter estimation (Step 4)

Both DPE and SPE were performed on three types of objective functions as mentioned earlier. Results for the process effluent, predicted by using the estimated parameter values, were compared. The proper parameters

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were determined based on the convergence of objective functions with genetic algorithm [20]. The applied genetic operators were tournament selection, uniform crossover, flip mutation and elitism. The number of the population was five.

2.5. Model validation (Step 5)

The model validation was carried out using the 100-day data set for SPE and the 7-day data set for DPE. These data were never used during the parameter estimation.

3. Results and discussion

Six different simulations were attempted to develop a reliable calibration method using two different types of parameter estimation methods for three objective functions. Detailed description of the simulation results is given below.

3.1. Sensitivity analysis

The result from the sensitivity analysis is shown in Table 4. The selected sensitive parameters by Case 1 based on EQ were $Y_{H,O2'}$, $Y_{H,NO'}$, $\mu_{max,A'}$, r_h and r_p . The sensitive parameters chosen by Cases 2 and 3 based on the EQS were $Y_{H,O2'}$, $i_{SS,Xi'}$, v_0 , r_h and r_p . The number of parameters which were related to the biological reaction and settling was close to each other. This indicates that the effluent of the fsEBPR process was strongly affected by the settling process.

3.2. Parameter estimation

The values of the selected sensitive parameters were estimated by a genetic algorithm. The results of simulations using the estimated parameter values are displayed in Figs. 3 and 4 and Table 5. The average absolute errors between measured and predicted effluent concentrations for all simulation cases were presented in Table 5. Those results show comparison among results from different methods used. Fig. 3 shows the predicted effluent profiles using the reference parameter values and using the values determined by static parameter estimation (SPE) with three objective functions for BOD, TN, TP and TSS. In the case of BOD, TN and TP, those results predicted by using reference values (reference in Fig. 3) were similar to the predicted results by using three ways of static parameter estimation (SPE in Fig. 3). This means that the static parameter estimation could not significantly improve the predictability of the model. However, it shows that the predicted values from SPE 2 and 3 were more similar to the measured values than those by SPE1 for TSS. This means that the objective function determined by applying weighting factor sets based on effluent quality standard is more reliable.

The predicted effluent concentrations obtained by the dynamic parameter estimation are presented in Fig. 4. As shown in this figure, there was no significant difference in effluent concentration according to the three objective functions for BOD and TN. By using the dynamic parameter estimation for TP, the decreased errors between predicted and measured values was only about 9.0% as compared to the errors derived from the case using reference values. However, it shows that three DPEs can reduce the errors by 71.1% (decreasing from 2.6 mg/L to 0.8 mg/L) of error caused by using the reference values of the parameters. In addition, the decreased errors with DPE 1, 2 and 3 for TSS were 44.2% (4.0 mg/L), 65.0% (5.9 mg/L) and 72.1% (2.5 mg/L) respectively as compared to the derived error (9.0 mg/L) by using the reference values of the parameters.

The predicted effluent concentrations obtained by the dynamic parameter estimation are presented in Fig. 4. As shown in this figure, there was no significant difference in

Table 4

Selected sensitivity parameters for three cases of objective function

	Sensitiv	ity parameter	S		
Case 1	$Y_{\rm H,O2}$	$\Upsilon_{\rm H,NO}$	r_h	r_p	
Case 2	$Y_{\rm H.O2}$	$i_{SS,Xi}$	r_h	r_{p}	
Case 3	$Y_{\rm H,O2}$	i _{SS,Xi}	r_h	r_p	

Table 5

Average absolute errors between measured and predicted effluent concentrations for seven simulation cases and four components

Reference	SPE1	SPE2	SPE3	DPE1	DPE2	DPE3	
4.3	3.5	2.9	3.8	4.0	3.9	4.0	
2.4	2.2	2.2	1.8	2.2	2.2	2.1	
2.6	1.3	1.3	1.3	0.8	0.8	0.8	
9.0	6.4	4.4	4.7	5.0	3.1	2.5	
	Reference 4.3 2.4 2.6 9.0	Reference SPE1 4.3 3.5 2.4 2.2 2.6 1.3 9.0 6.4	ReferenceSPE1SPE24.33.52.92.42.22.22.61.31.39.06.44.4	ReferenceSPE1SPE2SPE34.33.52.93.82.42.22.21.82.61.31.31.39.06.44.44.7	ReferenceSPE1SPE2SPE3DPE14.33.52.93.84.02.42.22.21.82.22.61.31.31.30.89.06.44.44.75.0	ReferenceSPE1SPE2SPE3DPE1DPE24.33.52.93.84.03.92.42.22.21.82.22.22.61.31.31.30.80.89.06.44.44.75.03.1	ReferenceSPE1SPE2SPE3DPE1DPE2DPE34.33.52.93.84.03.94.02.42.22.21.82.22.22.12.61.31.31.30.80.80.89.06.44.44.75.03.12.5



Fig. 3. Comparison between predicted effluent profiles by the reference values of parameters and by estimated values using static parameter estimation with three objective functions.



Fig. 4. Comparison between predicted effluent profiles by the reference values of parameters and by estimated values using dynamic parameter estimation with three objective functions.



Fig. 5. Comparison between predicted effluent profiles by using static parameter estimation and dynamic parameter estimation.

effluent concentration according to the three objective functions for BOD and TN. By using the dynamic parameter estimation for TP, the decreased errors between predicted and measured values was only about 9.0% as compared to the errors derived from the case using reference values. However, it shows that three DPEs can reduce the errors by 71.1% (decreasing from 2.6 mg/L to 0.8 mg/L) of error caused by using the reference values of the parameters. In addition, the decreased errors with DPE 1, 2 and 3 for TSS were 44.2% (4.0 mg/L), 65.0% (5.9 mg/L) and 72.1% (2.5 mg/L) respectively as compared to the derived error (9.0 mg/L) by using the reference values of the parameters.

Fig. 5 shows the comparisons between the predictability with static parameter estimation (SPE2) and dynamic parameter estimation (DPE2). There were no significant differences between the predicted effluent concentrations with SPE2 and DPE2 for TN. The absolute error of BOD with SPE2 was around 2.0 mg/L smaller than that with DPE2; however, the reduced error resulted from SPE2 was only a 32.8% error from the reference. The absolute errors of TP and TSS with DPE2 were smaller than with SPE2 (about 0.5 mg/L and 1.7 mg/L for TP and TSS). Decrease in error that resulted from DPE2 was 71.1% and 65.0% for TP and TSS, respectively.

From the results described above, the DPE method was proved to be better in prediction efficiency than SPE

because the SPE does not reflect the dynamic characteristics of biological reactions. The objective functions have to be amended according to actual concentrations of effluent appropriately.

4. Conclusions

The static parameter estimation using the determined objective functions based on the effluent quality index (SPE1) was not able to reduce the errors between predicted and measured values because a higher weight factor than BOD and TSS was relatively given to TP and TN for calculating the errors. However, the SPE using the objective functions based on EQS (SPE 2 and 3) could decrease the error by approximately 20% from SPE1 for TSS. It shows that the parameter estimation using the objective functions based on the EQS can predict the effluent more reliably.

For the case of using the same objective function, the errors between predicted and measured effluent with dynamic parameter estimation were fewer than the errors with static parameter estimation for TSS and TP. This is very likely because the simulation with static values of parameters could not reflect the variation of the process state.

The dynamic parameter estimation using the objective function based on the EQS was a proper calibration

method for an activated sludge model to predict a reliable effluent for the real process. Nevertheless, it was not possible significantly to decrease the errors of all components simultaneously. Further studies are recommended in areas of modification of the process model.

5. Symbols

*i*_{SS,Xi} — Suspend solids to COD ration for Xs, gSS/gCOD

- Settling parameter associated with the hindered settling component of settling velocity equation, m³/g
- *r_p* Settling parameter associated with the low concentration and slowly settling component of the suspension, m³/g
- v_0 Maximum practical settling velocity, m/d
- $Y_{\rm H,NO}$ Anoxic yield of heterotrophic biomass
- $Y_{\rm H,O2}$ Aerobic yield of heterotrophic biomass

Greek

 β_i — Weight value for *i*-component

- θ_i *i*th parameter of the mathematical model
- $\mu_{max,A}$ Maximum growth rate of autotrophic biomass, L/d

Subscripts

obs,e		Observed effluent concentration, mg/L
sim,e	—	Simulated effluent concentration, mg/L

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