

## Practical approach to parameter estimation for ASM3+ bio-P module applied to five-stage step-feed EBPR process

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**Abstract** Various parameter optimization approaches to a five-stage step-feed EBPR process modeled using the ASM3+ bio-P module were examined. Five stoichiometric ( $Y_{\text{STO,NO}}$ ,  $Y_{\text{H,O}_2}$ ,  $Y_{\text{H,NO}}$ ,  $Y_{\text{PAO,O}_2}$ ,  $Y_{\text{PO}_4}$ ) and seven kinetic parameters ( $k_{\text{STO}}$ ,  $\eta_{\text{NO}}$ ,  $b_{\text{H}}$ ,  $\mu_{\text{max,PAO}}$ ,  $q_{\text{PHA}}$ ,  $q_{\text{PP}}$ ,  $\mu_{\text{max,A}}$ ) were estimated. The optimization approaches could be classified based on the data sources (batch experiments or CSTR operation data) and the number of target variables used in calculating the objective function. Optimized parameter values obtained by each approach were validated with CSTR operation data that were not used for parameter optimization. The results showed that the parameter optimization only with batch experimental results could not be directly applied to CSTR operation data. ASM3 + bio-P module parameters could be finely optimized only with CSTR operation data when sufficient target variables for objective function calculation were applied. When the number of target variables was increased, prediction performance was significantly improved. Once optimized, the model was able to predict the characteristic features of the five-stage step-feed process; namely, a high PAO yield, fast PAO growth, fast  $X_{\text{PP}}$  storage, slow  $X_{\text{STO}}$  and  $X_{\text{PHA}}$  storage.

**Keywords** Phosphorus accumulating organisms; EBPR; five-stage step-feed process; parameter estimation; sensitivity analysis

### Introduction

The five-stage step-feed enhanced biological phosphorous removal (fsEBPR) process was developed to achieve effective nitrogen and phosphorus removal with minimum external carbon source where wastewater has low C/N and C/P ratios. This process was claimed to reduce sludge production, aeration demands, and external carbon usage (Park *et al.*, 2003). These reductions were possible by employing denitrifying phosphorus accumulating organisms (dPAOs) that accumulate phosphate under anoxic conditions by utilizing nitrate as a final electron acceptor (Barker and Dold, 1996). To simulate this process, ASM3 (Activated Sludge Model No. 3; Henze *et al.*, 1999) was modified by adding a biological phosphorous removal model developed by Rieger *et al.* (2001). Thereafter this modified model was named ASM3 + bio-P. The simulation results were compared with those of ASM2d, and ASM3 + bio-P was recommended as the model of choice (Lee *et al.*, 2005). However, when this work was carried out, one of the most difficult tasks was to obtain proper model parameters. There still has not been enough experience using ASM3 + bio-P to simulate the EBPR process.

In parameter estimation, traditionally researchers have often used data from batch tests (Sollfrank and Gujer, 1990; Bae *et al.*, 1998). In these cases, the batch experiments were usually designed and operated under restricted experimental conditions. Therefore, it was questionable that the parameters determined based on the batch experimental data

would be reliable to predict the behavior of continuous-flow reactors such as the fsEBPR process. The following example supports this suspicion. The maximum specific growth rate of heterotrophs ( $\mu_{\max,H}$ ) was considered as one of the key parameters in batch respirogram analysis. However, the effect of high  $\mu_{\max,H}$  on the effluent quality of CSTR was not significant, because the lowered substrate concentration compensated for this effect (Ko *et al.*, 2004). So, one should be very careful when parameters obtained from batch experiments are used in simulating continuous-flow reactors. During model calibration, especially for bio-P models, in-process measurements can be much more informative than effluent concentrations for calibration of model parameters (Gernaey *et al.*, 2002). Indeed, van Veldhuizen *et al.* (1999) observed large deviations between the measured and simulated nitrate and phosphate concentration profiles for different in-process locations in model calibration, although the model fit to effluent concentrations seemed reasonable. Thus, in-process measurements contribute substantially to proper calibration of plant model gains.

In this paper, five cases of parameter estimation are compared in the context of the application of ASM3 + bio-P to the fsEBPR process. The five different approaches included traditional parameter estimation techniques based mainly on batch experimental data and on continuous-flow reactor data. Also, the effect of the number of target variables used to calculate objective functions was tested. From the results of those approaches, the best set of parameters was selected and their validity was tested. Finally these parameters were confirmed against a field-scale fsEBPR process. The purpose of this paper is to highlight the most reliable parameter estimation technique and the validation of those selected parameters in a full-scale plant.

## Methods

### Parameter estimation approaches

For ASM3 + bio-P model, five stoichiometric parameters ( $Y_{\text{STO,NO}}$ ,  $Y_{\text{H,O}_2}$ ,  $Y_{\text{H,NO}}$ ,  $Y_{\text{PAO,O}_2}$ ,  $Y_{\text{PO}_4}$ ) and seven kinetic parameters ( $k_{\text{STO}}$ ,  $\eta_{\text{NO}}$ ,  $b_{\text{H}}$ ,  $\mu_{\max,\text{PAO}}$ ,  $q_{\text{PHA}}$ ,  $q_{\text{PP}}$ ,  $\mu_{\max,\text{A}}$ ) have been identified as sensitive by previous researchers (Lee *et al.*, 2005). Among these parameters,  $Y_{\text{PO}_4}$  and  $\eta_{\text{NO,PAO}}$  were calculated with batch experimental data when these were available. Other sensitive parameters were adjusted and determined by fitting batch or continuous operating data with ASM3 + bio-P model, whereas all other non-sensitive model parameters were fixed with default values suggested by Rieger *et al.* (2001). Tables 1 and 2 show a comparison of parameter optimization approaches that are classified as the following. One-dimensional settling model by Takacs *et al.* (1991) was used for the modeling of the second clarifier.

- (1) Case #1 (batch data available) This case was developed considering only PAOs, which might be the most important micro-organisms in the fsEBPR process. In addition, the batch test was designed to identify phosphate release and accumulation.  $Y_{\text{PO}_4}$  and  $\eta_{\text{NO,PAO}}$  were directly calculated from the batch experimental results. Four other sensitive parameters related to the PAO reactions were determined by data fitting using the batch data. The rest of the sensitive parameters were adopted from the default values.
- (2) Case #2 (batch data available) In this case, the most sensitive parameters were determined using the batch data.  $Y_{\text{PO}_4}$  and  $\eta_{\text{NO,PAO}}$  were directly calculated from batch data. Eleven sensitive parameters were determined by data fitting using the batch data, except that the  $\mu_{\max,\text{A}}$  value was obtained from the default value because nitrification was inhibited.
- (3) Case #3 (batch and continuous data available) In this case, data from batch and continuous reactors were used to determine the sensitive parameters.  $Y_{\text{PO}_4}$  and  $\eta_{\text{NO,PAO}}$

**Table 1** Summary of cases of parameter estimation approaches using batch reactor data

	Case #1	Case #2
Parameter estimation	Calculated with batch data	$Y_{PO_4}, \eta_{NO,PAO}$
	Determined by data fitting with batch data	$Y_{STO,NO}, Y_{H,O_2}, Y_{H,NO}, Y_{PAO,O_2}, K_{STO}, \eta_{NO}, b_H, \mu_{max,PAO}, q_{PHA}, q_{PP}$
	Used default values	$\mu_{max,A}$ and all insensitive ones
	Data sets for validation	Batch results at initial COD of 55 and 105 mg/L and continuous reactor operation data during 46–87 days

Target variables for the objective function were the batch results of COD,  $PO_4^{3-}$ -P and  $NO_3^-$ -N concentration. Parameter estimation by data fitting was done using batch results at initial COD of 75 mg/L

were calculated from the batch test results. The remaining parameters were determined by data fitting using the data from 35 days of continuous-flow reactor operation. The estimated parameters were validated with 41 days of operational data from the same continuous-flow reactor but over a different operating period.

- (4) Case #4 (continuous data available) All the sensitive parameters were determined by data fitting using only the continuous-flow reactor.
- (5) Case #5 (continuous data available) In this case, only the objective function and the number of target variables were somewhat different from those of Case #4.

### Objective functions

The objective of optimization for determining parameters was to minimize the sum of the relative squared error of COD,  $PO_4^{3-}$ -P,  $NH_4^+$ -N, and  $NO_3^-$ -N concentrations shown in Equation (1). The algorithm was the Nelder–Mead simplex method. Simulations for most of these parameter estimations were conducted using the Optimizer module in GPS-X (Hydromantis Inc.). Case #5 had 24 target variables, which were too many for the GPS-X Optimizer. In this case, the output from GPS-X was analyzed in Excel with an aim to find a parameter set that minimized the weighted sum of squared normalized error

**Table 2** Summary of cases of parameter estimation approaches using continuous reactor

	Case #3	Case #4	Case #5
Parameter estimation	Calculated with batch data	$Y_{PO_4}, \eta_{NO,PAO}$	None
	Determined by data fitting with continuous data	$Y_{STO,NO}, Y_{H,O_2}, Y_{H,NO}, Y_{PAO,O_2}, K_{STO}, \eta_{NO}, b_H, \mu_{max,A}, \mu_{max,PAO}, q_{PHA}, q_{PP}$	All sensitive ones
	Used default values	All insensitive ones except $\eta_{NO,PAO}$	All insensitive ones
	Target variables for the objective function	$PO_4^{3-}$ -P, $NH_4^+$ -N and $NO_3^-$ -N in anaerobic, anoxic1 reactor and effluent, SCOD in anaerobic reactor (total number = 10)	COD, $PO_4^{3-}$ -P, $NH_4^+$ -N and $NO_3^-$ -N in each reactor and effluent (total number = 24)

Optimization data set was obtained from CSTR operation results during 10–45 days. Validation data set was obtained from CSTR operation results during 46–87 days

(WSSNE) shown in Equation (2). The process model was optimized by applying the Jacobi method (the direct method of Gauss–Jordan) (Press *et al.*, 1992).

$$P_{\text{mat}}^{\min} J(P_{\text{mat}}) = \sum_{t=0}^{t_f} \sum_{i=1}^n \left[ \frac{(C_{i,t,\text{measured}} - C_{i,t,\text{predicted}})}{C_{i,t,\text{measured}}} \right]^2 \quad (1)$$

$$P_{\text{mat}}^{\min} J(P_{\text{mat}}) = wf_1 \cdot wf_2 \cdot \sum_{t=0}^{t_f} \sum_{i=1}^n \left[ \frac{(C_{i,t,\text{measured}} - C_{i,t,\text{predicted}})}{C_{i,t,\text{measured}}} \right]^2 \quad (2)$$

$C_{i,t}$  = concentration of  $i$ th components at time  $t$  in effluent and each reactor

$i$  = SCOD,  $S_{\text{NH}}$ ,  $S_{\text{NO}}$ , and  $S_{\text{P}}$

$wf_1$  = weight factor for effluent (5 for effluent, 1 for reactors)

$wf_2$  = weight factor for nutrient component (2 for  $S_{\text{NH}}$ ,  $S_{\text{NO}}$  and  $S_{\text{P}}$ )

#### Five-stage step-feed EBPR process

This process consists of five tanks in a series as shown in Figure 1. The major function of each reactor is described as the following:

- Pre-anoxic tank for denitrifying nitrate in the recycled sludge, where 10% of influent was fed
- Anaerobic tank for phosphate release and PHA storage, where 60% of influent was fed
- Anoxic1 for denitrifying nitrate from the nitrate recycle flow with internally stored carbon and simultaneous phosphate uptake
- Anoxic2 tank for denitrifying residual nitrate, where 30% of influent was fed
- Aerobic tank for nitrification and phosphate uptake

The total working volume of the lab-scale reactor was 39.4 L, and the volume ratio of each tank was 1:2:1:4:7, respectively. The sludge recycle flow rate and the nitrate recycle flow rate were 0.3Q and 2Q, respectively, where Q represented influent flow rate, as shown in Figure 1. The nominal SRT and temperature were maintained at 15 days and 20 °C, respectively. The activated sludge samples from this plant were collected for the batch reactor experiments.

#### Batch experiments to confirm PAOs

To obtain the stoichiometric and kinetic parameters, two sets of batch experiments were performed. The activated sludge samples for these experiments were collected from the aeration tank after running the lab-scale fsEBPR reactor for 80 days. Figure 2 shows the experimental conditions of the batch tests. Experimental Set #1 was designed to identify phosphate accumulation under the anoxic condition by utilizing nitrate as a final electron acceptor. Experimental Set #2 was performed as a control without an anoxic period. The initial  $\text{PO}_4^{3-}\text{-P}$  and  $\text{NO}_3^- \text{-N}$  concentrations, at the beginning of the anaerobic and anoxic periods, were adjusted to 25 and 50 mg/L by adding  $\text{H}_3\text{PO}_4$  and  $\text{KNO}_3$ , respectively.

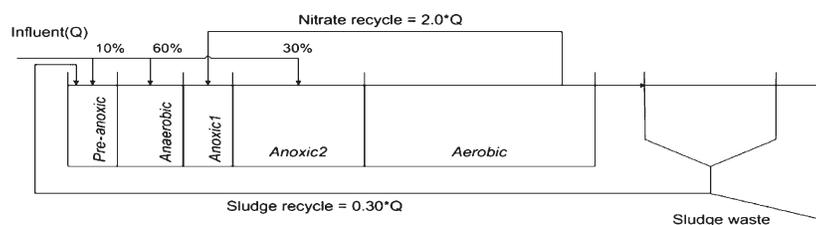
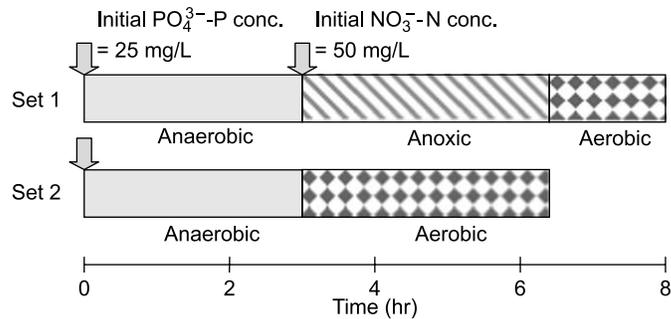


Figure 1 Schematic diagram of five-stage step-feed EBPR process



**Figure 2** Operating conditions of batch experiments

Each set had four different runs using various initial SCOD concentrations such as 40, 55, 75, and 105 mg/L, respectively. These concentrations were adjusted by adding ethanol. Because the supernatant of the sludge contained 40 mg COD/L of inert organic, the resulting biodegradable SCOD concentration was 0, 15, 35 and 65 mg/L, respectively. The initial VSS concentration was  $2000 \pm 200$  mg/L. The temperature and pH were maintained at  $20 \pm 2^\circ\text{C}$  and  $7.5 \pm 0.1$ , respectively. ATU (allyl tio-urea) was added to inhibit nitrification and prevent competition for oxygen between autotrophic micro-organisms and PAOs.

#### Confirmation of validation of selected parameters at a full-scale plant

Operational data from a full-scale plant, Daegue, South Korea, were used to confirm the validation of the parameter sets obtained in the above Case #5 parameter estimation approaches. Data were collected at a sewage treatment plant having nine serial reactors with a total working volume of  $1,036 \text{ m}^3$  and treating 60,000 p.e. of sewage. Table 3 shows the operating conditions and hydraulic retention time of each reactor. This plant was initially constructed as an  $\text{A}^2\text{O}$  process and modified to an fSEBPR process later; therefore, the volume ratio of the reactors was different from that of a laboratory-scale reactor.

## Results and discussion

#### Parameter estimation using batch reactor data

The parameters were optimized using data from batch experiments that had an initial COD concentration of 75 mg/L and an initial VSS concentration of  $2000 \pm 200$  mg/L.  $Y_{\text{PO}_4}$  and  $\eta_{\text{NO}_3, \text{PAO}}$  were calculated based on the experimental results. They were similar to, or the same as, the model default values of 0.35 and 0.60 (Rieger *et al.*, 2001), respectively.

$$Y_{\text{PO}_4} = \frac{\text{Mass of P released during anaerobic period}}{\text{Mass of COD removed during anaerobic period}} = \frac{4.80 \text{ gP/L}}{12.7 \text{ gCOD/L}} = 0.38 \text{ gP/gCOD}$$

$$\eta_{\text{NO}_3, \text{PAO}} = \frac{\text{Max. P uptake rate in anoxic period}}{\text{Max. P uptake rate in aerobic period}} = \frac{9.79 \text{ mgP/L}\cdot\text{hr}}{16.2 \text{ mgP/L}\cdot\text{hr}} = 0.60$$

#### Parameter estimation using continuous-flow reactor data

The parameters determined by each optimization approach were quite different from the model defaults (Table 4). The parameters that show more than a 20% difference from the defaults and that were optimized by Case #2 were  $Y_{\text{PAO}, \text{O}_2}$ ,  $K_{\text{STO}}$ ,  $b_{\text{H}}$ ,  $q_{\text{PHA}}$ ,  $q_{\text{PP}}$ , and  $\mu_{\text{max}, \text{PAO}}$ . It should be emphasized that all of these parameters, except  $b_{\text{H}}$ , also exhibited

**Table 3** Operating conditions and hydraulic retention time of Jisan sewage treatment plant

Sludge recycle	Internal recycle	Temp. (°C)	SRT (day)	F/M ratio(-)	Hydraulic retention time (hr)					
					Total	Preatoxic	Anaerobic	Anoxic1	Anoxic2	Aerobic
0.4–1.5Q	1.5–2.5Q	12–26	15–25	0.07–0.15	11.25	1.25	1.25	1.25	2.5	5.0

high-percentage differences according to the approach used. This phenomenon could represent characteristics of the fsEBPR process such as high PAO yield, fast PAO growth, fast  $X_{PP}$  storage, and slow  $X_{STO}$  and  $X_{PHA}$  storage.

#### Validation of parameters determined based on batch experimental data

The results were then validated using the batch experimental data that had initial COD concentration of 55 and 105 mg /L. Figure 3 shows the measured COD,  $NO_3^-$ -N, and  $PO_4^{3-}$ -P concentrations (initial COD concentration of 105 mg/L) together with the simulation results using the optimized parameters from Cases #1 and #2. The parameters optimized in Case #1 could not show reliable results. The COD removal prediction in the anoxic period of Set #1 was faster, and the  $PO_4^{3-}$ -P uptake in the aerobic period of Set #2 was slower, than observed (Figure 3). This result means that the optimization of only PAO-related parameters, Case #1, was not the proper approach to explain the batch experimental results because of substrate competition for nitrate between heterotrops and dPAOs in the reactor, even though experiments were designed to identify phosphate release and accumulation. By contrast, the parameters obtained in Case #2 were able to predict the batch results more accurately, but did underestimate the  $PO_4^{3-}$ -P variation in the CSTR (Figure 4). Based on these results it was concluded that the parameters optimized with batch results could not be directly applied to this CSTR, and it was reasoned that that was caused in part because the batch experiments were operated under restricted conditions quite different from those of the CSTR.

#### Validation of parameters determined based on data from continuous-flow reactor

The parameters obtained in Case #3 could successfully predict  $PO_4^{3-}$ -P variation in the anaerobic reactor, but differences in the experimental data and in model prediction were observed in the effluent (Figure 4). WSSNE was significantly decreased when compared to the Case #2 results (Table 4). This showed that the parameter optimization performance could be considerably increased by using both batch and CSTR operational results. The difference between Case #3 and Case #4 was the selection method of the  $Y_{PO_4}$  value. In Case #3,  $Y_{PO_4}$  was experimentally estimated, but it was mathematically optimized in Case #4. The value of  $Y_{PO_4}$  in Case #4 was estimated to be 0.43 and resulted in improved WSSNE after validation. This should not imply that Case #4 is a better approach, but rather indicates that Case #3 was not fully optimized. However, the reliability of parameter optimization with CSTR operational data was confirmed. This further indicated the need for a larger-scale optimization with a larger number of target variables, such as Case #5 (Figure 5). Case #5 had the largest numbers of target variables, such as COD,  $PO_4^{3-}$ -P,  $NH_4^+$ -N, and  $NO_3^-$ -N concentration, in each reactor and effluent. The validation of Case #5 presented the lowest WSSNE of 298. This is especially low when it is considered that an  $NH_4^+$ -N difference of 0.1 in each reactor and in the effluent results in a WSSNE of 80 after applying a weighting factor and the full simulation days. It was concluded that parameter optimization with CSTR operational data could produce reliable results when enough target variables were applied.

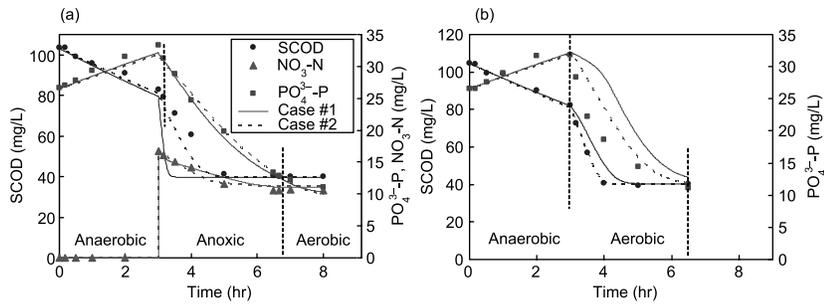
#### Confirmation of validity of selected parameters at a field-scale plant

The Case #5 approach was applied to field plant for validation. The parameter values were optimized with 100 days of pilot plant data. The effluent T-N and T-P concentrations were successfully predicted (Figure 6). The temperature and sludge recycle flow rates varied significantly during the simulation period, but these impacts were predicted with the optimized model.

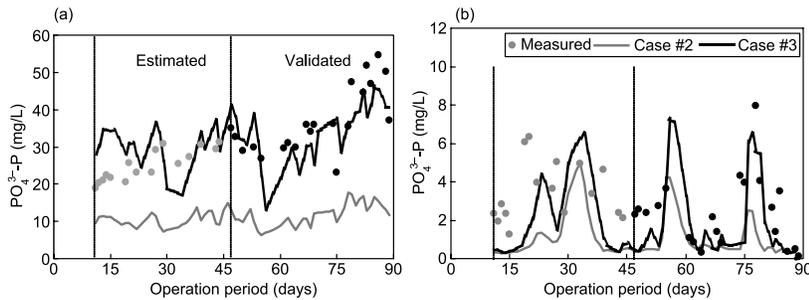
**Table 4** Summary of sensitive parameters determined based on batch or continuous operation data

	Estimated parameter values																
	Default			Case #1			Case #2			Case #3			Case #4			Case #5	
	Value	%Diff.*	Value	%Diff.*	Value	%Diff.*	Value	%Diff.*	Value	%Diff.*	Value	%Diff.*	Value	%Diff.*	Value	%Diff.*	
$Y_{STO,NO}$	0.70	***	0.73	4.3	0.40	-42.9	0.71	1.4	0.71	1.4	0.71	1.4	0.71	1.4	0.71	1.4	
$Y_{H_2O_2}$	0.80	***	0.98	22.5	0.96	20.0	0.85	6.2	0.85	6.2	0.85	6.2	0.91	13.8	0.91	13.8	
$Y_{H_2NO}$	0.65	***	0.77	18.5	0.28	-56.9	0.26	-60.0	0.26	-60.0	0.26	-60.0	0.52	-20.0	0.52	-20.0	
$Y_{PAO_2}$	0.60	65.0	0.86	43.3	0.82	36.7	0.94	56.7	0.94	56.7	0.94	56.7	0.83	38.3	0.83	38.3	
$Y_{PO_4}$	0.35	8.6	0.38	8.6	0.38	8.6	0.43	22.9	0.43	22.9	0.43	22.9	0.34	-2.9	0.34	-2.9	
$\eta_{NO,PAO}$	0.60	0.0	0.60	0.0	0.60	0.0	***	***	***	***	***	***	***	***	***	***	
$K_{STO}$	12.50	***	16.55	32.4	16.39	31.1	15.17	21.4	15.17	21.4	15.17	21.4	16.83	34.6	16.83	34.6	
$\eta_{NO}$	0.80	***	0.44	-45.0	0.84	5.0	0.91	13.8	0.91	13.8	0.91	13.8	0.93	16.3	0.93	16.3	
$b_H$	0.30	***	0.30	0.0	0.18	-40.0	0.28	-6.7	0.28	-6.7	0.28	-6.7	0.22	-26.7	0.22	-26.7	
$\mu_{max,A}$	1.80	***	***	***	3.00	66.7	2.67	48.3	2.67	48.3	2.67	48.3	1.66	-7.8	1.66	-7.8	
$q_{PHA}$	6.00	-72.6	1.28	-78.7	2.32	-61.3	2.22	-63.0	2.22	-63.0	2.22	-63.0	3.32	-44.7	3.32	-44.7	
$q_{PP}$	1.50	111.9	3.41	127.3	4.67	211.3	3.67	144.7	3.67	144.7	3.67	144.7	3.03	102.0	3.03	102.0	
$\mu_{max,PAO}$	1.00	40.5	2.00	100.0	1.64	64.0	2.81	181.0	2.81	181.0	2.81	181.0	2.31	131.0	2.31	131.0	
WSSNE**			3,186		513		408		298								

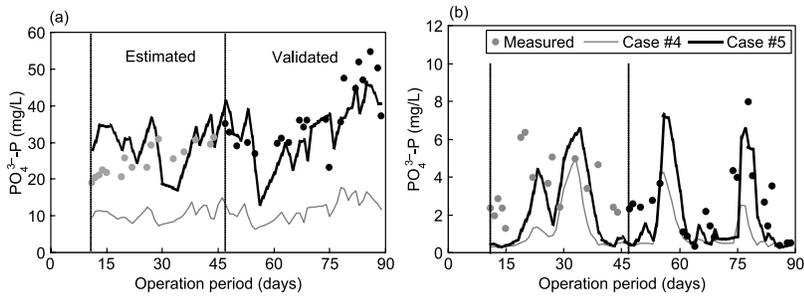
\*: % difference compared with default value; \*\*: When applied to 46–87 days of CSTR operation data; \*\*\*default values used *italic*; parameters with more than 20% difference from default values



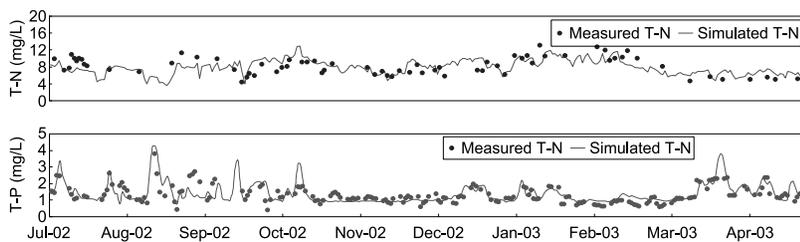
**Figure 3** Validation of optimized parameters with batch results; initial COD of 105 mg/L. (a) Set #1 (anaerobic/anoxic/aerobic); (b) Set #2 (anaerobic/aerobic)



**Figure 4** Prediction of  $\text{PO}_4^{3-}\text{-P}$  concentration with optimized parameters by each approach using the batch test; (a) in the anaerobic reactor; and (b) in the effluent



**Figure 5** Prediction of  $\text{PO}_4^{3-}\text{-P}$  concentration with optimized parameters by each approach used the continuous-flow reactor data; (a) in the anaerobic reactor; and (b) in the effluent



**Figure 6** Measured and simulated effluent T-P and T-N concentrations at sewage treatment plant

## Conclusions

From the comparison of five parameter optimization approaches for the ASM3 + bio-P module, the following conclusions were drawn. Optimizing only the PAO-related parameters was not sufficient to explain the batch experimental results, even though the batch experiments were designed to identify phosphate release and accumulation. Phosphate release and uptake is closely related to biodegradable COD in the anaerobic phase and stored PHA in the anoxic/aerobic phase; therefore, other heterotrophic processes have an impact on phosphate removal. Consequently, other non-PAO parameters should be estimated simultaneously.

The parameters that were optimized only with batch experimental results could not be directly applied to the CSTR. For this, parameters should be validated with CSTR operational data.

The parameters of the ASM3 + bio-P module model could be optimized with CSTR operational data alone when sufficient target variables were applied. The number of target variables was 24 in Case #5, but fewer were used in the other approaches. Case #5 resulted in the best effluent quality prediction performance.

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