Parameter estimation of ASM3+Bio-P Module for step-feed EBPR process by batch tests and CSTR operation data

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Abstract

Various parameter optimization approaches of ASM3+Bio-P Module were examined for five-stage step-feed EBPR process. Optimization approaches could be classified to the data sources from batch experiments or CSTR operation data and the number of target variables for calculating objective function. Optimized parameters values by each approach were validated with CSTR operation data which were not used for parameter optimization step. Results showed that the parameters 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 enough target variables for objective function calculation were applied. When increased the number of target variables, prediction performance was significantly improved. Optimized parameters values could present the characteristic of five-stage step-feed process; high PAO yield, fast PAO growth, fast X_{PP} storage and slow X_{STO} and X_{PHA} storage.

Keywords：dPAO, EBPR, five-stage step-feed process, parameter estimation, sensitivity analysis

INTRODUCTION

A five-stage step-feed EBPR process was developed to get the effective nitrogen and phosphorus removal from wastewater which had low C/N and C/P ratio with minimum external carbon. These were made possible by employing denitrifying phosphorus accumulating organisms (dPAOs) which could accumulate phosphate under anoxic condition by utilizing nitrate as a final electron acceptor (Barker and Dold, 1996; Kuba *et al.*, 1993). ASM2d (Henze *et al.*, 1999) and ASM3 (Gujer *et al.*, 1999) with EAWAG Bio-P Module (Rieger *et al.*, 2001) were compared for their applicability to this process, and ASM3+Bio-P Module was proved to be a proper model (Lee *et al.*, 2004). Many researchers have often used batch test data for the parameter estimation (Ekama *et al.*, 1986; Sollfrank and Gujer, 1991; Ko *et al.*, 2001). In these cases, the batch experiments were usually designed and operated under restricted experimental conditions. Therefore, it was difficult to convince that the estimated parameters found from the batch experimental results would be valid to predict the behavior of continuous flow reactors; commonly expressed as CSTR (Completely Stirred Tanks Reactor).

The purpose of this paper was to find a proper approach for parameter estimation with minimum calibration efforts for the application of ASM3+Bio-P Module to five-stage step-feed EBPR process. Five different approaches were examined which could be classified to the data sources from batch experiments or CSTR operation data and the number of target variables for calculating objective function. Optimized parameters values by each approach were validated with CSTR operation data which were not used for parameter optimization step. Consequently, the most proper approach was selected and validated using operation data of the field scale five-stage step-feed EBPR process.

METHODS

Five-stage step-feed EBPR process & Batch experiments

Total working volume of the lab-scale reactor was 39.4 L. The volume ratio of pre-anoxic, anaerobic, anoxic1, anoxic2, and aerobic was 1:2:1:4:7 approximately. The sludge recycle flow and the nitrate recycle flow were 0.3Q and 2Q, respectively as showed in Fig. 1. SRT and temperature was maintained as 15 days and 20℃, respectively.

Two sets of batch experiments were performed using sludge from the CSTR after 80 days of operation. Fig. 2 shows the operating conditions of the batch experiments. Experimental set #1 was designed to identify the phosphate accumulation under anoxic condition by utilizing nitrate as a final electron acceptor. Experimental set #2 was done as control experiments. Initial PO_4^{3-}-P and NO_3^--N concentration at anaerobic and anoxic period were adjusted as 25 and 50 mg/L by the addition of H_3PO_4 and KNO_3, respectively. Each set had four different runs according to various initial SCOD concentrations such as 40, 55, 75, and 105 mg/L which were adjusted by addition of ethanol. Because the supernatant of mixture contained 40 mg COD/L of inert organic, the biodegradable SCOD was 0, 15, 35 and 65 mg/L. Initial VSS was 2000±200 mg/L. Temperature and pH was adjusted as 20±2 °C and 7.5±0.1, respectively.

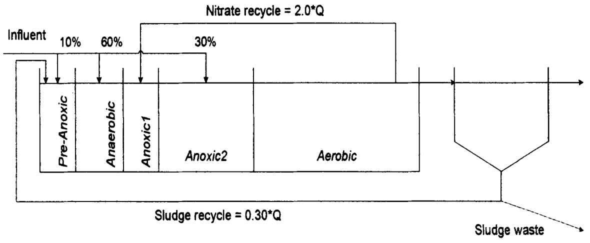


Fig. 1. Schematic diagram of five-stage step-feed EBPR process.

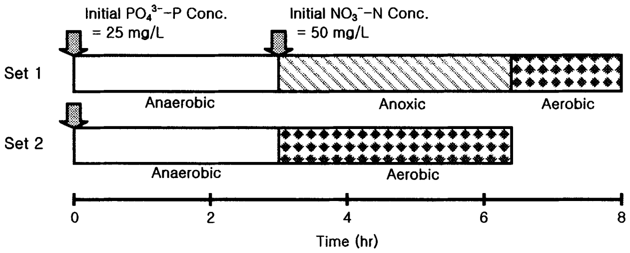


Fig. 2. Operating conditions of batch experiments.

Parameter estimation approaches

Sensitive ASM3+Bio-P Module parameters were selected according to the previous work which aimed at same process (Lee *et al.*, 2004); five stoichiometric; $Y_{STO,NO}$, $Y_{H,O2}$, $Y_{H,NO}$, $Y_{PAO,O2}$, Y_{PO4} and seven kinetic parameters; k_{STO}, η_{NO}, b_H, $\mu_{max,PAO}$, q_{PHA}, q_{PP}, $\mu_{max,A}$. Only these sensitive parameters were optimized experimentally or mathematically, while others were fixed as model defaults suggested by Rieger *et al.* (2001).

1) *For the case of using only batch experimental results:* Two approaches of Opti.B1 and Opti.B2 were proposed. In both cases, Y_{PO4} and $\eta_{NO,PAO}$ were directly calculated from batch experimental results. For Opti.B1, only four parameters related with PAO reactions were optimized mathematically, whereas rest of them were adopted from the default values. For Opti.B2, eleven sensitive parameters except $\mu_{max,A}$ were optimized mathematically. However, $\mu_{max,A}$ could not be optimized experimentally nor mathematically, because nitrification was inhibited, therefore it was assumed as default.
2) *For the case of using both batch and CSTR operation data:* This approach was expressed as Opti.B+C. As it was done for the cases of using only batch experimental results, Y_{PO4} and $\eta_{NO,PAO}$ were calculated with batch results. Other sensitive parameters were mathematically optimized with CSTR operation data during 10-45 days. Data 1-10 days were ignored, because operation was unstable. Estimated parameters were validated with the operation data during 46-87 days.
3) *For the case of using only CSTR operation data:* In these cases, all sensitive parameters were mathematically optimized only with CSTR operation data. The parameter estimation was conducted using two different approaches such as Opti.C1 and Opti.C2 that were different in objective function and the number of target variables.

Objective functions

The objective function was to minimize the sum of relative squared error on TSS, COD, PO_4^{3-}-P, NH_4^+-N and NO_3^--N. Most of parameter estimation was conducted using Optimizer in GPS-X (Hydromantis Inc.) except Opti.C2, because it had 24 target variables while Optimizer in GPS-X can handle the maximum 10 target variables at a time. The objective function of Opti.C2 was to find parameter set minimizing WSSNE (Weighted Sum of Squared Normalized Error).

Validation of parameter estimation approach using data from field-scale plant

The operation data of field plant were used for the validation of parameter estimation approach. Data were collected at J. sewage treatment plant consists of nine serial reactors with total working volume of 1,036m^3 that treats 80,000 p.e. of sewage.

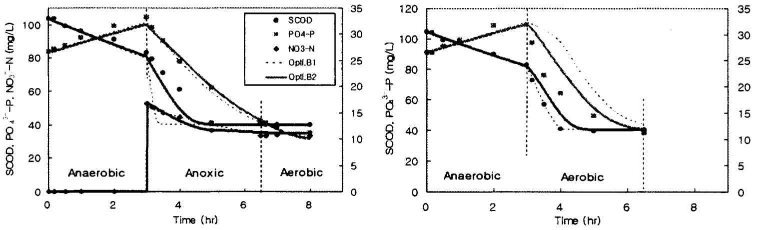
RESULTS AND DISCUSSTION

Parameter estimation and validation with batch results

Sensitive parameters were optimized with batch experimental results at initial COD of 75 mg/L and validated with those at initial COD of 55 and 105 mg /L in this cases. Fig. 3 shows the measured COD, NO_3^--N and PO_4^{3-}-P concentrations at initial COD of 105 mg/L together with simulation results using optimized parameters by Opti.B1 and Opti.B2. Y_{PO4} and $\eta_{NO,PAO}$ were calculated based on the experimental results as 0.38P/gCOD and 0.60. Model prediction showed too fast COD removal at anoxic period of set #1 and too slow PO_4^{3-}-P uptake at aerobic period of set #2 compared with measured data (Fig. 3). It meant that the optimization of only PAO related parameters, Opti.B1, was not the proper approach to explain the bath experimental results, even though experiments were designed to identify phosphate release and accumulation. The simulation using parameters optimized with Opti.B2 could explain the batch results more accurately. However, it underestimated the PO_4^{3-}-P variation in CSTR as shown in Fig. 4. Based on the prediction results which Opti.B2 shown, it could be said as that the parameters optimized with batch results could not be directly applied to CSTR, because the batch experiments were operated under restricted conditions which were quite different from CSTR.

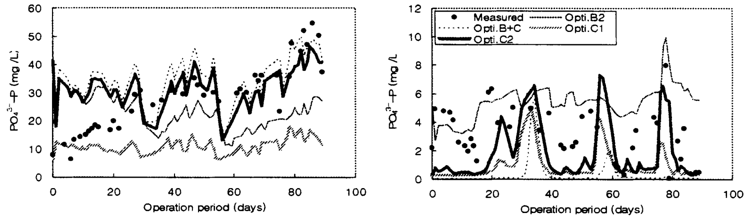
Parameter optimization and validation with CSTR operation data

The parameters optimized by Opti.B+C could successfully predict PO_4^{3-}-P variation in anaerobic reactor, while inconsistency between the experimental data and model prediction was observed in PO_4^{3-}-P variation of effluent (Fig. 4). WSSNE was significantly decreased from 3,186 to 513 compared to Opti.B2 (Tab. 1). It meant that parameter optimization performance could be considerably increased by using both of batch and CSTR operation results. The difference between Opti.B+C and Opti.C1 was the selection method of Y_{PO4} value. At Opti.B+C, Y_{PO4} was experimentally estimated while mathematically optimized at Opti.C1. The value of Y_{PO4} in Opti.C1 was over-estimated to 0.43, but resulted in improved WSSNE at validation. It did not mean that Opti.C1 was better approach than Opti.B+C, but implied Opti.B+C approach was not fully optimized. However, the reliability of parameters optimization only with CSTR operation data was confirmed, and need for strict optimization was arisen, such as Opti.C2. Opti.C2 had the largest numbers of target variables such as COD, PO_4^{3-}-P, NH_4^+-N & NO_3^--N in each reactor and effluent. Validation of Opti.C2 presented the lowest WSSNE of 298. It was concluded as that parameters optimization only with CSTR operation data could produce reliable results when enough target variables were applied.



(a) (b)

Fig. 3. Validation of optimized parameters with batch results; Initial COD of 105 mg/L. (a) Set #1, (b) Set #2



(a) (b)

Fig. 4. Prediction of PO_4^{3-}-P concentration with optimized parameters by each approach (a) in anaerobic reactor and (b) in effluent.

Tab. 1. Optimized values of sensitive parameters by each approach.

	Default	Opti.B1		Opti.B2		Opti.B+C		Opti.C1		Opti.C2	
		Value	%Diff.*	Value	%Diff.*	Value	%Diff.*	Value	%Diff.*	Value	%Diff.*
$Y_{STO,NO}$	0.70	0.70	0.0	0.73	4.3	*0.40*	*-42.9*	0.71	1.4	0.71	1.4
$Y_{H,O2}$	0.80	0.80	0.0	*0.98*	*22.5*	0.96	20.0	0.85	6.2	0.91	13.8
$Y_{H,NO}$	0.65	0.65	0.0	0.77	18.5	*0.28*	*-56.9*	*0.26*	*-60.0*	0.52	-20.0
$Y_{PAO,O2}$	0.60	*0.99*	*65.0*	*0.86*	*43.3*	*0.82*	*36.7*	*0.94*	*56.7*	*0.83*	*38.3*
Y_{PO4}	0.35	0.38	8.6	0.38	8.6	0.38	8.6	*0.43*	*22.9*	0.34	-2.9
K_{STO}	12.50	12.50	0.0	*16.55*	*32.4*	*16.39*	*31.1*	*15.17*	*21.4*	*16.83*	*34.6*
η_{NO}	0.80	0.80	0.0	*0.44*	*-45.0*	0.84	5.0	0.91	13.8	0.93	16.3
b_H	0.30	0.30	0.0	0.30	0.0	*0.18*	*-40.0*	0.28	-6.7	*0.22*	*-26.7*
$\mu_{max,A}$	1.80	1.80	0.0	1.80	0.0	*3.00*	*66.7*	*2.67*	*48.3*	1.66	-7.8
q_{PHA}	6.00	*1.65*	*-72.6*	*1.28*	*-78.7*	*2.32*	*-61.3*	*2.22*	*-63.0*	*3.32*	*-44.7*
q_{PP}	1.50	*3.18*	*111.9*	*3.41*	*127.3*	*4.67*	*211.3*	*3.67*	*144.7*	*3.03*	*102.0*
$\mu_{max,PAO}$	1.00	*1.41*	*40.5*	*2.00*	*100.0*	*1.64*	*64.0*	*2.81*	*181.0*	*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,
italic : parameter has over than 20% of difference

Discussion on optimized parameters values

Parameters determined by each optimization approach were quite different from model defaults as shown in Tab. 1. Parameters which shown more than 20% of difference between defaults and optimized by Opti.C2 were $Y_{PAO,O2}$, K_{STO}, b_H, q_{PHA}, q_{PP} and $\mu_{max,PAO}$. It should be emphasized that all of them except b_H, also exhibited high differences at any other approach. This phenomenon could present the characteristic of five-stage step-feed EBPR process such as high PAO yield, fast PAO growth, fast X_{PP} storage and slow X_{STO} and X_{PHA} storage.

Validation of parameter estimation approach using data from field-scale plant

Opti.C2 approach was applied to J. sewage treatment plant in T. city for the validation. Parameters values were optimized with 100 days of pilot plant operation data and employed without additional tuning. The effluent T-N and T-P concentrations were successfully predicted as shown in Fig. 5. Temperature and sludge recycle flowrate was changed in high degree during simulation period, and their effects were excellently explained.

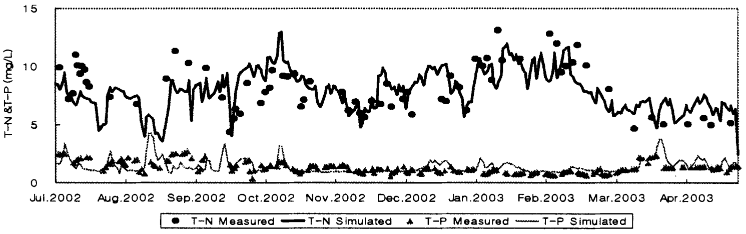


Fig. 5. Measured and simulated effluent T-P and T-N concentrations at J. sewage treatment plant.

CONCLUSIONS

From the comparison of five parameters optimization approaches for ASM3+Bio-P Module, it could be concluded that:

- Optimizing only PAO related parameters was not sufficient to analyze batch experimental results. Phosphate release and uptake is closely related with biodegradable COD in anaerobic phase and stored PHA in anoxic/aerobic phase, therefore other heterotrophic processes take serious effect on phosphate removal. Consequently, other sensitive parameters of heterotrophic processes should be estimated simultaneously.
- Parameters which were optimized only with batch experimental results could not directly be applied to CSTR. For this, parameters should be validated with CSTR operation data.
- Parameters of ASM3+Bio-P Module could be finely optimized only with CSTR operation data when enough target variables were applied. Number of target variables was 24 at Opti.C2, while same or less than 10 at other approaches. It resulted in best effluent quality prediction performance and reliable parameters values.
- Optimized parameters values by Opti.C2 could present the characteristic of five-stage step-feed process; high PAO yield, fast PAO growth, fast X_{PP} storage and slow X_{STO} and X_{PHA} storage.

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REFERENCES

Barker P. S. and Dold P. L. (1996). Denitrification behavior in biological phosphorus removal activated sludge system-review paper. *Wat. Res.*, **30**(4), 769-780.

Copp J. B. and Dold P. L.(1998). Comparing sludge production under aerobic and anoxic conditions. *Wat. Sci. Tech.*, **38**(1), 285-294.

Gujer W., Henze M., Mino T., Matsuo T. and van Loosdrecht M. C. M. (1999). Activated Sludge Model No.3. *Wat. Sci. Tech.*, **39**(1), 183-193.

Gujer W., Henze M., Mino T., Matsuo T., Wentzel M. C., Marais G. v. R. (1995). Activated Sludge Model No.2: Biological phosphorus removal. *Wat. Sci. Tech.*, **31**(2), 1-11.

Henze M., Gujer W., Mino T., Matsuo T., Wentzel M. C., Marais G. v. R. and van Loosdrecht M. C. M. (1999). Activated Sludge Model No. 2d. ASM2d. *Wat. Sci. Tech.*, **39**(1), 165-182.

Hydromantis (2001). GPS-X Tutorial Guide, Hydromantis Inc. Canada.

Ko J. H., Woo H. J., Copp J. B., Kim, S. H. and Kim C. W. (2002). Evaluation of several respirometry-based activated sludge toxicity control strategies. *Wat. Sci. Tech.*, **45**(4-5), 143-150.

Kuba T., Smolders G. J. F., van Loosdrecht M. C. M. and Heijnen J. J. (1993). Biological phosphorus removal from wastewater by anaerobic-anoxic sequencing batch reactor. *Water Sci. Tech.* **27**, 241-252.

Lee S. H., Ko J. H., Park J. B., Im J. H., Poo K. M., Woo H. J. and Kim C. W. (2004). Validation and field application of ASM2d and ASM3+Bio-P Module for the five-stage step-feed EBPR process. Submitted to Marrakech 2004, IWA Biennial Conference 19-24 Sep. 2004, Marrakech, Morocco.

Park J. B., Han W. L., Lee S. Y., Lee J. O, Choi E. S., Park D. H. and Park Y. K. (2003). The microbial community analysis of 5-stage biological nutrient removal process with step-feed system *J. Microbial. Biotechnol.*, **12**(6), 929~935.

Rieger L., Koch G., Kuhni M., Gujer W. and Siegrist H. (2001). The EAWAG bio-P module for Activated Sludge Model No. 3. *Wat. Res.*, **35**, 3887-3903.