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## Numerical Modelling COD, N and P Removal in a Full-scale WWTP of China

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**Abstract:** ASM3-bio-P model is based on ASM3 with an additional module for phosphorus removal using modified processes from ASM2d. The model includes removal of organic, nitrogen and phosphorus. This study uses ASM3-bio-P model to set up a computer simulation system to model an actual A/A/O process in a municipal wastewater plant. Method of quickest descent is applied to calibrate model parameters. This enables us to model and predict effluent quality of municipal wastewater treatment plant in the indices of COD, TN, TP. The results show good correspondence between measured and simulated values. The feasibility of applying ASM3-bio-P model to simulate a WWTP in China is validated and an optimization method on solving calibration of model parameters is also proposed.

**Key words:** Municipal wastewater, biochemical treatment process, ASM3-Bio-P model, numerical modelling, quickest descent method, WWTP

### INTRODUCTION

Activated sludge process is one of the most applied municipal wastewater treatment methods. Since the publication of the activated sludge model No.1 (ASM1) by International Water Association (IWA) in 1987 (Henze *et al.*, 1987), the model has been improved. And ASM3 (Gujer *et al.*, 1999) based on new mechanism was introduced in 1999. ASMs provide a platform for the development of activated sludge theory. EAWAG thesis group adopted some ASM2d's views (Henze *et al.*, 1995, 1999) and added phosphorus removal module to ASM3, making it possible to model phosphorus removal (Gernaey *et al.*, 2004). ASM3-bio-P model was calibrated and validated in municipal wastewater plant of Switzerland (Rieger *et al.*, 2001).

Returning and aerating of A/A/O process is so complex that exact description of returning and aerating is needed for simulation system. Since A/A/O process can remove nitrogen and phosphorus, modelling nitrogen removal and phosphorus removal is also needed (Van-Veldhuizen *et al.*, 1999; Brdjanovic *et al.*, 2000; Van Loosdrecht and Henze, 1999). IWA gives each ASM model a set of values for parameters so as to calibrate program easily. However, these parameters are from old ASMs' empirical datum and productivity tests. They must be validated when water qualities and treatment conditions are different between each country.

### MATHEMATICAL SYMBOL CONVENTION FOR THE MODEL

ASM3-bio-P model is based on mass balance; its basic form can be formulated as follows:

$$\text{Accumulation} = \text{influent-effluent} \pm \text{reaction} \quad (1)$$

Because influent and effluent is determined by physical laws of process system, the problem is how to deal with the return speed for the reaction system with a settling separation unit. The return speed of soluble components S can be expressed simply as product of return rate R and concentration S:

$$\text{Influent rate}_s = RS \quad (2)$$

Material balance for particulate components must include waste sludge and loss of settling tank's effluent. If the IWA's assumption-there is no sludge loss in secondary clarifier, waste sludge is discharged in return line and all particulate components settle together-is still to be used, clarifier's return rate of particulate components can be expressed as follows:

$$\text{Influent rate}_x = (1 + R)QX^n - \frac{\sum_{k=1}^n \sum_h V^k X_h^k}{\text{SRT}} \frac{X_j^n}{\sum_h X_h^n} \quad (3)$$

Where Q is influent flow rate for a system with n reactors and SRT is Sludge Retention Time.

Definite mathematical expression of correspondingly complex influent rate has been obtained from the above definition. Reacting amount is the next item that needs to be identified. Reacting amount determined by activated sludge activity is a main problem that needs to be solved for activated sludge model. The model covers three matrixes: composition matrix (L), stoichiometric matrix (V) and rate expression matrix (P).  $L_{kj}$  in composition matrix

indicates component *j* relative to conservative *k*. Composition coefficients that can not be measured directly by COD in stoichiometric matrix can be obtained from the conservation equation.

$$L_k V = 0 \tag{4}$$

Hence integrated stoichiometric matrix can be obtained. Composition concentration variations caused by biochemical reaction is available.

$$\text{Reaction} = VP \tag{5}$$

Concentration variation *C* of component *j* in tank *i* is illustrated in Eq. (6).

$$\frac{dC_j^i}{dt} = \frac{dC_{in,j}^i}{dt} - \frac{dC_{e,j}^i}{dt} + V_j P \tag{6}$$

Where  $C_j^i$  is concentration of component *j* in tank *i*,  $C_{in,j}^i$  is influent concentration of component *j* in tank *i*,  $C_{e,j}^i$  is effluent concentration of component *j* in tank *i*,  $V_j$  is stoichiometric matrix of component *j* and *P* is the biological reaction rate expression matrix. The Eq. (6) is actually an expression of mass balance.

### NUMERICAL MODEL IN A/A/O WASTEWATER TREATMENT PROCESS

Lay-out of a wastewater treatment plan with A/A/O biochemical treatment process is presented in Fig. 1.

From Eq. (2), (3) and (6), numerical model of the plant can be obtained (superscripts just denote the number of tank, *kla* is oxygen transmission rate, *DO* is concentration of dissolved oxygen).

- Differential equation that describes each soluble component *j* in anaerobic tank is

$$\frac{dS_j^1}{dt} = \frac{dQ}{dt} \cdot (S_j^0 + RS_j^3) - \frac{dQ}{dt} \cdot (1+R)S_j^1 + V_j P \tag{7}$$

- Differential equation that describes particulate component *j* in the tank is

$$\frac{dX_j^1}{dt} = \frac{dQ}{dt} \cdot [X_j^0 + (1+R)X_j^3] - \frac{\sum_{k=1}^3 \sum_h V^k X_h^k}{SRT} \frac{X_j^3}{\sum_h X_h^3} - \frac{dQ}{dt} \cdot (1+R)X_j^1 + V_j P \tag{8}$$

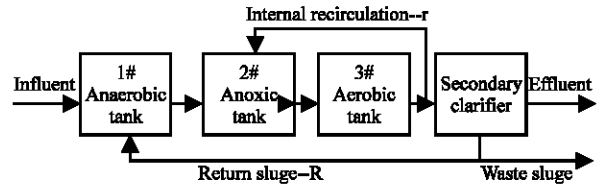


Fig. 1: Lay-out of the wastewater treatment plan with A/A/O biochemical treatment process

- There is no oxygen exchange in gas-liquid interface in the tank. Therefore it is liquid influent that brings dissolved oxygen, whose differential equation is

$$\frac{dS_o^1}{dt} = \frac{dQ}{dt} \cdot (S_o^0 + RS_o^3) - \frac{dQ}{dt} \cdot (1+R)S_o^1 + V_o P \tag{9}$$

- Since there is oxygen exchange in gas-liquid interface in anoxic tank, differential equations can be expressed as follows.

#### Soluble components:

$$\frac{dS_j^2}{dt} = \frac{dQ}{dt} \cdot [(1+R)S_j^1 + rS_j^3] - \frac{dQ}{dt} \cdot (1+R+r)S_j^2 + V_j P \tag{10}$$

#### Particulate components:

$$\frac{dX_j^2}{dt} = \frac{dQ}{dt} \cdot [(1+R)X_j^1 + rX_j^3] - \frac{dQ}{dt} \cdot (1+R+r)X_j^2 + V_j P \tag{11}$$

#### Dissolved oxygen:

$$\frac{dS_o^2}{dt} = \frac{dQ}{dt} \cdot [(1+R)S_o^1 + rS_o^3] + kla^2 \cdot (S_o - S_o^2) - \frac{dQ}{dt} \cdot (1+R+r)S_o^2 + V_o P \tag{12}$$

- Soluble components and particulate components in aerobic tank are given by:

$$\frac{dY_j^3}{dt} = \frac{dQ}{dt} \cdot (1+R+r)Y_j^2 - \frac{dQ}{dt} \cdot (1+R+r)Y_j^3 + V_j P \tag{13}$$

- Because there is an aerating system, the dissolved oxygen in aerobic tank can be expressed as:

$$\frac{dS_o^3}{dt} = \frac{dQ}{dt} \cdot (1+R+r)S_o^2 + kla^3 \cdot (S_o - S_o^3) - \frac{dQ}{dt} \cdot (1+R+r)S_o^3 + V_o P \tag{14}$$

The plant's recent influent flow rate is 300 Km<sup>3</sup> d<sup>-1</sup> and peak flow rate is 16250 m<sup>3</sup> h<sup>-1</sup>, of which 60% is trade sewage. Mean concentration of COD is 370 mg L<sup>-1</sup> and hydraulic retention time in biochemical tank is 12.36 h (of which 1 h is in anaerobic tank, 3.83 h is in anoxic tank and 7.5 h is in aerobic tank). The sludge age is 19.2 d, the return sludge flow rate is 200% of influent flow rate and mixed liquor flow rate is 115% of influent flow rate.

**CALIBRATION OF MODEL PARAMETERS AND NUMERICAL SIMULATION**

Both strictness in mathematics and accuracy in parameters are the keys to simulation system's success. Though the strictness in mathematics of model is fully tested, all parameters must be calibrated because of the differences in treatment object, treatment process and physical condition.

Firstly, a testing system with steady running condition needs to be set up. It's running temperature, PH, influent components and microbial community is stable. Seventeen components are included in simulation objects, but only COD, BOD, TN, TP, TSS is provided by municipal wastewater plants. Therefore it is necessary to change COD, BOD, TN, TP into model compositions. By testing (Yang, 2004), influent components in this research are calculated according to: S<sub>i</sub> = 0.07COD; S<sub>s</sub> = 0.29COD; X<sub>i</sub> = 0.22COD; X<sub>s</sub> = 0.32COD; X<sub>H</sub> = 0.1COD; S<sub>NH</sub> = C<sub>TN</sub> - 0.02X<sub>s</sub> - 0.005X<sub>i</sub> - 0.001S<sub>s</sub> - 0.002S<sub>r</sub> - 0.005X<sub>H</sub>; S<sub>PO4</sub> = C<sub>TP</sub> - 0.001X<sub>s</sub> - 0.005X<sub>i</sub>. Effluent quality indices can be calculated from effluent components according to: COD = S<sub>s</sub> + S<sub>i</sub> + X<sub>s</sub> + X<sub>i</sub>; NH<sub>4</sub><sup>+</sup>-N = S<sub>NH</sub>; NO<sub>3</sub><sup>-</sup>-N = S<sub>NO</sub>; TN = S<sub>NO</sub> + S<sub>NH</sub>; TP = 1.1S<sub>PO4</sub>. Secondly, steady influent condition is selected to get steady effluent data. Computing speed may become a great constraint because of complexity of models. So Runge-Kutta of changing step is used to solve the problem. For the differences between computer simulation system and physical model, numerical model are modified as follows.

**Anaerobic tank:**

$$\frac{dS_o^1}{dt} = t^1 \cdot \left( \frac{1}{1+R} S_o^0 + \frac{R}{1+R} DO_{anoxic} + DO_{anaerobic} - S_o^1 \right) + V_o P \tag{15}$$

$$\frac{dS_j^1}{dt} = t^1 \cdot \left( \frac{1}{1+R} S_j^0 + \frac{R}{1+R} S_j^3 - S_j^1 \right) + V_j P \tag{16}$$

$$\frac{dX_j^1}{dt} = t^1 \cdot \left( \frac{1}{1+R} X_j^0 + X_j^3 \right) - t^1 X_j^1 - \frac{1}{1+R} \cdot \frac{\sum_h [t^1 X_h^1 (1+R) + t^2 X_h^2 (1+R+r) + t^3 X_h^3 (1+R+r)]}{SRT} \tag{17}$$

$$\frac{X_j^3}{\sum_h X_h^3} + V_j P$$

**Anoxic tank:**

$$\frac{dS_o^2}{dt} = t^2 \cdot \left[ \frac{1+R}{1+R+r} S_o^1 + \frac{r}{1+R+r} S_o^3 \right] + V_o P \tag{18}$$

$$\left[ +kla^2 (DO_{anoxic} - S_o^2) - S_o^2 \right]$$

$$\frac{dS_j^2}{dt} = t^2 \cdot \left( \frac{1+R}{1+R+r} S_j^1 + \frac{r}{1+R+r} S_j^3 - S_j^2 \right) + V_j P \tag{19}$$

$$\frac{dX_j^2}{dt} = t^2 \cdot \left( \frac{1+R}{1+R+r} X_j^1 + \frac{r}{1+R+r} X_j^3 - X_j^2 \right) + V_j P \tag{20}$$

**Aerobic tank:**

$$\frac{dS_o^3}{dt} = t^3 \cdot [S_o^2 + kla^3 \cdot (DO_{aerobic} - S_o^3) - S_o^3] + V_o P \tag{21}$$

$$\frac{dS_j^3}{dt} = t^3 \cdot (S_j^2 - S_j^3) + V_j P \tag{22}$$

$$\frac{dX_j^3}{dt} = t^3 \cdot (X_j^2 - X_j^3) + V_j P \tag{23}$$

Because of the differences between numerical simulation and real result, parameters should be adjusted by quickest descent method of approximate squared error. F is identified as:

$$F = E[e^T e] = E(Z_t - Z_a)^T (Z_t - Z_a) \tag{24}$$

where Z<sub>a</sub> stands for computing effluent and Z<sub>t</sub> is real effluent data.

**Approximate squared error:**

$$\hat{F} = (Z_t - Z_a)^T (Z_t - Z_a) = e^T e \tag{25}$$

Table 1: Model parameters' calibration

Parameter	Description	Initial value	Calibration value
$\epsilon_{NO}$	Anoxic reduction factor	0.6	0.7
$K_{O_2}$	Saturation constant for $S_{O_2}$	0.2	0.18
$K_{S_{STO}}$	Aerobic storage rate constant	1	1.5
$\mu_H$	Max. aerobic growth rate of $X_H$	2	1.5
$b_{H,O_2}$	Aerobic endogenous respiration rate of $X_H$	0.18	0.15
$b_{H,NO}$	Anoxic endogenous respiration rate of $X_H$	0.1	0.12
$b_{S_{STO},O_2}$	Aerobic endogenous respiration rate of $X_{S_{STO}}$	0.22	0.25
$b_{S_{STO},NO}$	Anoxic endogenous respiration rate of $X_{S_{STO}}$	0.08	0.09
$\mu_A$	Max. growth rate of $X_A$	1.2	1.2
$b_{PHA}$	Respiration rate for $X_{PHA}$	0.22	0.25
$Y_{S_{STO},O_2}$	Aerobic yield of stored products per SS	0.9	0.95
$Y_{S_{STO},NO}$	Anoxic yield of stored products per SS	0.78	0.75
$Y_{H,O_2}$	Aerobic yield growth $X_H$ on $X_{S_{STO}}$	0.68	0.75
$Y_{H,NO}$	Anoxic yield growth $X_H$ on $X_{S_{STO}}$	0.54	0.6
$Y_A$	Yield growth $X_A$ on $S_{NO}$	0.24	0.28
$f_{XI}$	Production of $X_I$ in endogenous respiration.		
	biomass respiration	0.2	0.28

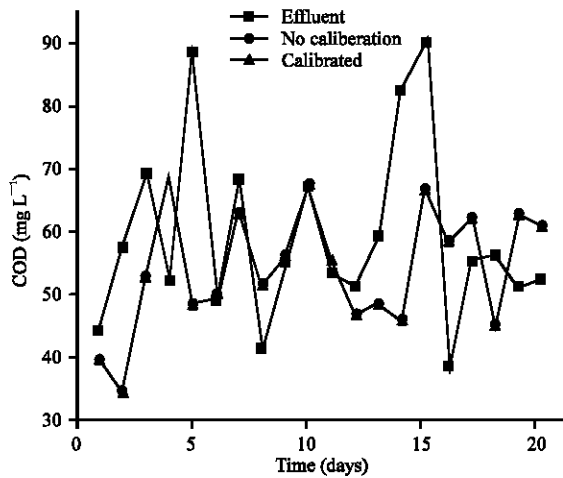


Fig. 2: Calibrated variations of COD

$g(k)$  is defined as function  $g$ 's  $k$  times effluent, then:

$$\hat{F}(k) = e^T(k)e(k) \tag{26}$$

If  $n$  is a parameter that needs to be adjusted, quickest descent method of approximate squared error can be expressed as:

$$n(k+1) = n(k) - \alpha \frac{\partial \hat{F}(k)}{\partial n(k)} \tag{27}$$

Where,  $\alpha$  means studying speed, which is 0.8 in this modelling in order to meet computation need. By adjusting the parameters, simulation result corresponds with real result. The parameters adjusted are shown as follows in Table 1. Using the mentioned parameters above, the results for numerical simulation in Fig. 2-4 can be obtained. Simulation effluent error can be controlled in an acceptable range by calibrating the parameters.

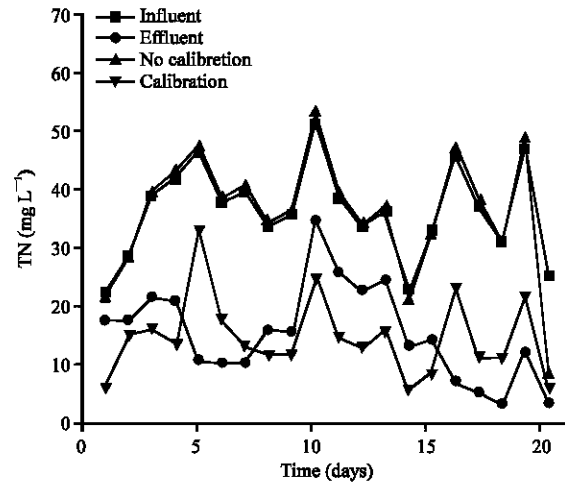


Fig. 3: Calibrated variation of TN

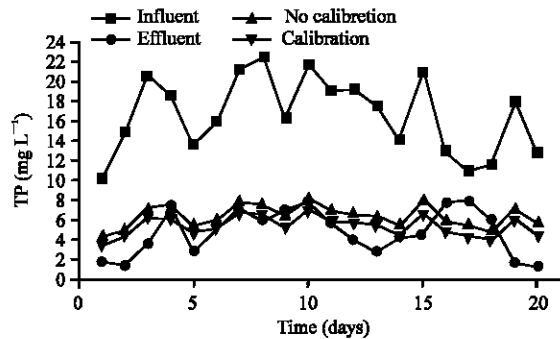


Fig. 4: The scheme for simulation of wastewater-biological treatment processes

### CONCLUSION

ASM3-bio-P model on the basis of ASM3 is quite mature for simulating COD and can approach real effluent very well. The model can also predict the trend well for simulating nitrogen and phosphor. Because of the differences in the wastewater quality and treatment condition between each country, there is no satisfying result using the parameters recommended by IWA. This problem is successfully solved in this article that parameters are calibrated by the quickest descent method.

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