



Modification of the kinetics for modeling substrate storage and biomass growth mechanism in activated sludge system under aerobic condition

Ji Fan^{a,b}, Peter A. Vanrolleghem^b, Shuguang Lu^{a,*}, Zhaofu Qiu^a

^a State Environmental Protection Key Laboratory of Environmental Risk Assessment and Control on Chemical Process, Shanghai key Laboratory of Functional Material Chemistry, East China University of Science and Technology, No.130, Mei Long Road, Shanghai 200237, China

^b modelEAU, Département de génie civil et de génie des eaux, Université Laval, Quebec, QC G1V0A6, Canada

HIGHLIGHTS

- ▶ During feast phase the SSSG process includes storage and growth using X_{STO} or substrate processes.
- ▶ There is no Monod inhibition function for the consumption of X_{STO} .
- ▶ The X_{STO} concentration before pulse addition of acetate can affect OUR profile.

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ABSTRACT

Based on the activated sludge model no.3 (ASM3), a new kinetic expression describing substrate removal and biomass growth mechanism occurring in activated sludge system under aerobic condition was established. The new model proposed that under feast condition, one part of substrate was utilized directly for biomass growth and the other part was stored as internal storage products and simultaneously the storage products were used for biomass growth. The model was successfully calibrated on oxygen uptake rate (OUR) data and off-line soluble chemical oxygen demand (COD) dynamic variations obtained from batch experiments with biomass from a full-scale wastewater treatment plant (WWTP). OUR predictions with the calibrated model could reasonably describe the OUR profile after pulse addition of acetate, i.e., the OUR transiently reached a very high level, and then increased gradually to a maximum level until the initial substrate was taken up for storage and biomass growth. This new model also, for the first time, highlighted the significant effect of the biomass storage products concentration before pulse addition of acetate on OUR profile.

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1. Introduction

White-box modeling is widely applied in activated sludge systems for the simulation of wastewater treatment processes thanks to the comprehensive understanding of the reactions catalyzed by the microorganisms involved under various operational conditions (Gernaey et al., 2004). Since the publications of Activated Sludge Model No. 3 (ASM3) (Gujer et al., 1999; Henze et al., 2000), more and more researchers developed or modified the mechanism of substrate metabolism based upon it, trying to explore a better picture of the substrate degradation process by biomass in activated sludge system, i.e., the simultaneous substrate storage and growth (SSSG) process during the feast phase (Krishna and van Loosdrecht, 1999; Beun et al., 2000; Winkler

et al., 2001; Beccari et al., 2002; Karahan-Gül et al., 2003, 2006; Sin et al., 2005; Makinia et al., 2006; Su and Yu, 2006; Ni and Yu, 2008a, 2008b), which is different from what is included in ASM3, i.e., substrate was stored initially before being used for growth (Gujer et al., 1999).

The major driving force behind this modeling was the increased understanding of the simultaneous substrate storage and direct biomass growth mechanism that allowed to interpret the experimental oxygen uptake rate (OUR) profiles, whereas the ASM3 failed to simulate properly for the following three parts, i.e., (a) the discontinuity in the biomass growth rate observed during feast and famine phases; (b) the prediction of higher levels of internal storage polymers than measured which allowed to fit the oxygen consumption during the feast and famine phases (Krishna and van Loosdrecht, 1999), and (c) the higher OUR in the feast phase and the lower OUR in the famine phase when using the single growth process definition (Karahana-Gül et al., 2003). This fact led to the formulation of the SSSG model in order to better interpret the above

* Corresponding author. Tel./fax: +86 21 64250709.
E-mail address: lvshuguang@ecust.edu.cn (S. Lu).

phenomenon. In addition, based on the fact that most wastewater treatment plants (WWTPs) with nutrient removal purpose are typically operated at long sludge retention time (SRT) resulting in biomass with a rather low average growth rate ($\sim 1/\text{SRT}$), it leads to the conclusion that the apparent maximum substrate uptake rate (q_{MAX}) of biomass could be higher than the amount needed for the average biomass growth rate, since one part of substrate is initially stored and the other part directly degraded. Sin et al. (2005) proposed a clear relationship among the parameters associated with the SSSG process, making the model calibration focus on the estimation of two parameters, i.e., the fraction of substrate used for storage f_{STO} and q_{MAX} . However, this parameter relationship indirectly inhibits biomass growth on storage products (X_{STO}) under feast condition resulting in the inability to simulate the peak of the observed OUR profiles. Other approaches, i.e., Krishna and van Loosdrecht, 1999; Beun et al., 2000; Winkler et al., 2001; etc. did not recognize this relationship, which causes practical identifiability problems that resulted in unrealistic and nonmechanistic parameter estimates when using batch OUR data, the traditional way in model calibration, while their models could give better descriptions of OUR profiles under feast condition.

Therefore, this research aims to further improve the modeling of the mechanisms of SSSG process occurring in activated sludge system under aerobic condition. To this aim, a new model is developed, which is particularly focused on the relationship among the parameters associated with SSSG process and the kinetic description of the degradation of X_{STO} under feast condition. The established model is calibrated and validated using experimental results of batch OUR tests fed with acetate. In addition, its comparison with Sin et al. (2005) model was also carried out to explore the mechanism of substrate metabolism by biomass.

2. Materials and methods

2.1. Experimental set-up

The batch experiments were performed using a hybrid respirometer with static gas/non-continuous flowing liquid (Spanjers et al., 1996; Spanjers and Olsson, 1992; Spanjers, 1993; Vanrolleghem and Spanjers, 1994). The respirometer consists of a 2.0 L open aerated vessel and a 0.5 L closed non-aeration respiration chamber equipped with a dissolved oxygen (DO) probe and a pump. Sludge is non-continuously pumped every several minutes between the aeration vessel and the respiration chamber. Liquid in these two reactors are mixed with an electric stirrer and a magnetic stirrer, respectively. During the experiments, the pH was fixed at 7.5 ± 0.3 using a pH controller, the temperature of the sludge in both tanks was kept at 20 ± 0.1 °C and allylthiourea (ATU, 30 mg/L) was added to avoid nitrification. Two different OUR tests were conducted for model

calibration and validation. Experiment 1 was performed with one pulse addition of acetate (40 mg/L) at the beginning of the experiment. Experiment 2 was performed with two pulse additions of equal amounts of acetate (40 mg/L) where the second acetate pulse was added after 160 min of the exhaustion of the first acetate pulse.

For the batch experiments, the sludge was taken from a secondary sedimentation tank of a local municipal WWTP with sequencing batch process (Quebec, Canada) which performed chemical oxygen demand (COD) removal, nitrification and denitrification. It was filtered to remove small particles and hair to prevent pump blocking, diluted with tap water to an appropriate concentration and aerated for a whole night to reach the endogenous state. Then, the sludge was washed with clean water (filtrate from tap water using 0.45 μm PVDF membrane filters) to remove the background COD. Finally, sodium acetate and ammonia were added into the system.

Soluble COD (SCOD) and ammonium (S_{NH}) were determined every several minutes during the batch experiment. SCOD was assessed using 0.45 μm membrane filters (PVDF). Other analyses were performed following Standard Methods (APHA, 1999).

2.2. Simulation strategy

Since the proposed model may include ill-defined parameters that can not be measured with a high degree of accuracy in the field or in the laboratory and these ill-defined parameters will severely limit the accuracy of simulation and increase the difficulty of assessing the applicability and utility of the model to a practical situation, therefore the multi-parametric sensitivity analysis was applied to distinguish the sensitive parameters by assigning a degree of uncertainty to each parameter (Hornberger and Spear, 1981; Chang and Delleur, 1992; Choi et al., 1998). These identified parameters associated with OUR were q_{MAX} , $\mu_{\text{MAX,STO}}$, f_{STO} , $Y_{\text{H,S}}$, $Y_{\text{H,STO}}$, K_{STO} and Y_{STO} , and associated with SCOD dynamic variations were q_{MAX} , f_{STO} , $Y_{\text{H,S}}$, Y_{STO} and K_{S} , while the other model parameters, such as f_{i} , K_{O} , b_{H} and b_{STO} have no significant effect on the OUR or the SCOD dynamic variations since there are no statistically difference for these four parameters after simulations with random assigned values within the design range. The definition of these parameters can be referred to Table 1.

Modeling the batch system, simulation and parameter estimation were performed using MATLAB 7.0. The differential equations were solved with the Runge–Kutta–Fehlberg algorithm (ode45).

3. Model kinetics

The proposed model for describing the biological reactions in activated sludge system reflects an appropriate modification of ASM3 with a consideration of direct growth on substrate. Compared to ASM3, the new model has another one new process,

Table 1
Kinetic and stoichiometric coefficients for the optimal calibration of experimental data with sodium acetate.

Parameter	Definition	Values	Source
Y_{STO}	Yield coefficient for storage, $\text{gCOD}_{X_{\text{STO}}}/\text{gCOD}_{S_{\text{S}}}$	0.8	This study
$Y_{\text{H,S}}$	Yield coefficient for growth on S_{S} , $\text{gCOD}_{X_{\text{H}}}/\text{gCOD}_{S_{\text{S}}}$	0.6	This study
$Y_{\text{H,STO}}$	Yield coefficient for growth on X_{STO} , $\text{gCOD}_{X_{\text{H}}}/\text{gCOD}_{X_{\text{STO}}}$	0.68	This study
q_{MAX}	maximum substrate uptake rate, per day	1.2	This study
f_{i}	Fraction of X_{i} in decay, $\text{gCOD}_{X_{\text{i}}}/\text{gCOD}_{X_{\text{BM}}}$	0.2	Henze et al., 2000
f_{STO}	Fraction of substrate used for storage, $\text{gCOD}_{X_{\text{STO}}}/\text{gCOD}_{S_{\text{S}}}$	0.6	This study
K_{STO}	Storage products affinity constant, $\text{gCOD}_{X_{\text{STO}}}/\text{m}^3$	0.024	This study
$\mu_{\text{MAX,STO}}$	Maximum growth rate on X_{STO} , per day	2	This study
K_{S}	Substrate affinity constant, $\text{gCOD}_{S_{\text{S}}}/\text{m}^3$	0.7	This study
K_{O}	DO affinity constant, gO_2/m^3	0.2	Henze et al., 2000
b_{H}	Biomass endogenous decay rate coefficient, per day	0.2	Henze et al., 2000
b_{STO}	Endogenous decay rate coefficient of X_{STO} , per day	0.2	Henze et al., 2000

namely direct growth on substrate under aerobic condition. Only the related kinetics and stoichiometric processes of the extended ASM3 model are presented in Table 2 as a matrix format to highlight the interactions among the model components and processes, while other processes are as the same as ASM3. Nitrifiers are not mentioned in this matrix due to the addition of ATU.

3.1. Kinetic processes under feast phase

Under feast condition, substrate is ample enough that the heterotrophic organisms can uptake more substrate than needed for the maximum growth itself. The difference is diverted to the formation of storage polymers. Experimental observations show that the ratio of substrate utilized for storage (f_{STO}) can be considered as constant (Beun et al., 2000, 2002; Dircks et al., 2001). Therefore, from a mathematical point of view, it is hypothesized that the ratio of storage products to substrate uptake is constant around a certain value (e.g., 0.67 mgCOD/mgCOD; van Loosdrecht and Heijnen, 2002). The kinetic expression of the substrate storage rate (r_{STO}) is given in Eq. (1), while the rate of direct aerobic growth on substrate ($r_{growth,S}$) is defined in Eq. (2), which are similar to these part of Sin et al. (2005) model.

$$r_{STO} = f_{STO} \times q_{MAX} \times Y_{STO} \times \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \times \frac{S_S}{K_S + S_S} X_H \quad (1)$$

$$r_{growth,S} = (1 - f_{STO}) \times q_{MAX} \times Y_{H,S} \times \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \times \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \times \frac{S_S}{K_S + S_S} X_H \quad (2)$$

where f_{STO} is the ratio of storage product to substrate taken up; q_{MAX} represents the maximum substrate uptake rate; $Y_{H,S}$ represents the yield of heterotrophic biomass. The other notations used are taken from the ASM3 terminologies. Eqs. (1) and (2) also show the internal relationships between the parameters (i.e., q_{MAX} , f_{STO} , $Y_{H,S}$ and Y_{STO}) and heterotrophic maximum growth rate or storage rate constant, respectively. The deductions of these relationships between substrate used for storage and growth are consistent with the actual situations in full-scale WWTPs which most WWTPs are typically operated at high SRT to achieve complete biological nutrient removal, therefore, the q_{MAX} is higher than the amount needed for the average biomass growth rate, i.e., part of substrate diverted to formation of the storage polymers (Sin et al., 2005).

However, it does not mean that during the feast phase biomass can not consume X_{STO} for growth simultaneously, which is different from what was proposed in other literatures (Krishna and van Loosdrecht, 1999; Sin et al., 2005; etc.). In their studies the growth rate of biomass on X_{STO} was assumed to occur under strictly famine conditions. In our study, there is no Monod inhibition function for external substrate, i.e., the switch function $K_S/(K_S + S_S)$, in the kinetic description of the aerobic growth rate on storage products

($r_{growth,STO}$) (see Eq. (3)) controlling the consumption of internal storage products X_{STO} during the feast phase as the experiments in this study fully support this mechanism.

$$r_{growth,STO} = \mu_{MAX,STO} \times \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \times \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \times \frac{X_{STO}/X_H}{K_{STO} + X_{STO}/X_H} X_H \quad (3)$$

Where $\mu_{MAX,STO}$ is the maximum growth rate of biomass.

3.2. Kinetic processes under famine phase

Under famine condition, readily soluble biodegradable substrates have been exhausted and internal storage products X_{STO} are the main energy source (Eq. (3)).

4. Results

4.1. OUR for monitoring simultaneous storage and growth process

Respirometric measurements obtained after pulse addition of a certain amount of sodium acetate to endogenously respiring activated sludge are shown in Fig. 1 (Experiment 1) and 2 (Experiment 2). The DO measurements are also shown in both figures. The variation of the DO concentration can directly explain the rate of oxygen utilization by biomass. Titrimetric measurements represented by the pH values are also shown in the same figures. The substrate uptake can be recognized in the titrimetric measurements as sodium acetate is a strong base/weak acid which means that acetate consumption results in an alkalinity increase (Gernaey et al., 2002).

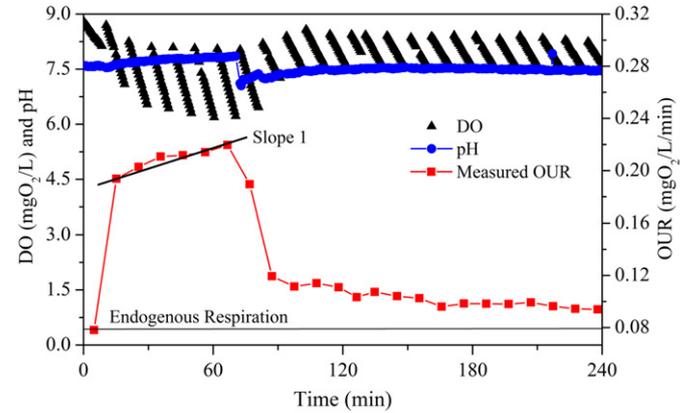


Fig. 1. Experiment 1: OUR along with DO and pH measurements after pulse addition of sodium acetate to endogenously respiring biomass.

Table 2

The proposed model matrix (simultaneous storage and growth): simplified stoichiometric and component matrix.

Processes	S_O gO ₂	S_S gCOD	S_{NH} gN	X_I gCOD	X_H gCOD	X_{STO} gCOD	Kinetics
Storage of S_S	$-1 + Y_{STO}$	-1	i_{N,S_S}			Y_{STO}	Eq. (1)
Growth on S_S	$1 - 1/Y_{H,S}$	$-1/Y_{H,S}$	$-i_{N,BM} + i_{N,S_S}/Y_{H,S}$		1		Eq. (2)
Growth on X_{STO}	$1 - 1/Y_{H,STO}$		$-i_{N,BM}$		1	$-1/Y_{H,STO}$	Eq. (3)
Endogenous respiration of X_H	$-1 + f_1$		$i_{N,BM} - f_1 \cdot i_{N,X_I}$	f_1	-1		$b_H \cdot M_O \cdot X_H$
Endogenous respiration of X_{STO}	-1					-1	$b_{STO} \cdot M_O \cdot X_{STO}$

Note:

- Nitrifiers are not contained in this matrix due to the addition of ATU;
- Other parts not shown in this model matrix are as the same as the original ASM3.
- $M_O = S_{O_2}/(K_{O_2} + S_{O_2})$.

As can be seen in Fig. 1 (Experiment 1), the area under the entire OUR curve and above the endogenous OUR level (0.08 mgO₂/L/min) represents the amount of oxygen utilized for the consumption of substrate fed to the batch. Under feast condition, the OUR first reaches a very high level (0.19 mgO₂/L/min) through a transient, and then increases gradually to a maximum level (0.22 mgO₂/L/min, see slope 1 in Fig. 1), the biomass activity continues at this maximum level until all external substrate is taken up for storage and growth. These phenomena were first observed by Krishna and van Loosdrecht (1999). During the famine phase, the OUR declines from the maximum level to a level (0.09 mgO₂/L/min) just above the endogenous OUR level. From then on, biomass grows on internal storage products which accumulated in the previous phase.

Fig. 2 shows the Experiment 2 with two pulse additions of equal amounts of sodium acetate into the same activated sludge system where the second acetate pulse is added 160 min after the first acetate pulse is consumed. During this interval, the internal storage X_{STO} is possibly exhausted as evidenced by the comparison of endogenous OUR and the end-tested OUR. Both OUR curves in Fig. 2 show the same trend as the one in Fig. 1 with the OUR reaching a high level (0.2 mgO₂/L/min for the first OUR, 0.25 mgO₂/L/min for the second OUR), increasing gradually to a maximum level (0.22 mgO₂/L/min for the first OUR, 0.26 mgO₂/L/min for the second OUR), and then continuing at this maximum level until all external substrate is taken up for storage and growth (see slopes 1 and 4 in Fig. 2). It can also be seen clearly that the peak of the second OUR curve during the feast phase are a little higher than that under the first feast condition.

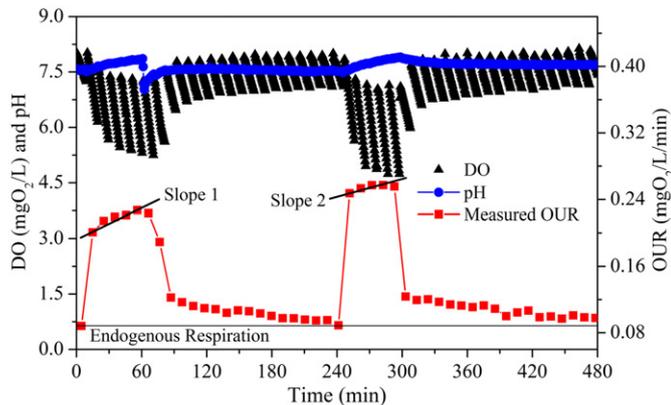


Fig. 2. Experiment 2: OUR along with DO and pH measurements with twice pulse additions of sodium acetate to endogenously respiring biomass.

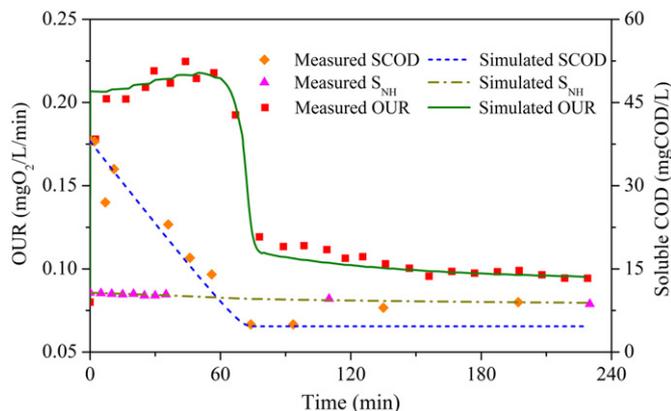


Fig. 3. Model calibration for the experimental data: OUR, SCOD and S_{NH} ; the R for best model fits of OUR, SCOD and S_{NH} are 0.992, 0.98 and 0.201, respectively.

4.2. SCOD and ammonia measurements campaign along with the OUR test

SCOD and ammonia (S_{NH}) measurements along with the OUR test are shown in Fig. 3. During Experiment 1, the soluble readily biodegradable substrate is taken up rapidly to a very low value in around 70 min. Here, the reason for the residual SCOD in the lowest point could be due to the background COD. The SCOD curve can therefore be used to calibrate the parameter K_S as the substrate uptake is the main metabolism under feast condition.

5. Discussion

5.1. Model calibration and parameter identification

Model calibration is a process adjusting model parameter values to make the simulated results consistent with the measured data. From a practical parameter estimation point of view, the calibration strategy tends to change as few constants as possible to simplify the calibration process and to consider the limited variability of some parameters (Xu and Hultman, 1996). According to this guideline and considering the parameter sensitivity analysis in this study, eight parameters (q_{MAX} , f_{STO} , $Y_{H,S}$, $Y_{H,STO}$, $\mu_{MAX,STO}$, K_{STO} and K_S) are adjusted based on the dependence of the parameters on OUR measurements and SCOD dynamic variations. Other parameter values are directly from data in literatures due to their non-sensitivity. The parameter estimation results are summarized in Table 1 while the best fits of the model to the experimental data are shown in Fig. 3. The simulated results showed that the model fits were quite acceptable since the correlation coefficients (R) for OUR, SCOD and S_{NH} were 0.992, 0.980 and 0.971, respectively (Fig. 3).

For the calibration of the new model, ascertaining the initial concentration of the heterotrophs, $X_H(0)$, is critical. A good method proposed by Sin et al. (2005) is based on the baseline endogenous OUR level prior to substrate addition (Eq. (4)):

$$OUR_{end}(0) = -(1-f_I) \times b_H \times X_H(0) \quad (4)$$

In our approach, the calibration strategy of trial and error method is used to estimate the parameters. f_I is fixed at 0.2 mgCOD/mgCOD, as mentioned in ASM3 (see Table 1). The parameter b_H is initially given the default value from ASM3 to obtain an initial $X_H(0)$ value based on Eq. (4). These parameters ($X_H(0)$ and b_H) are double-calculated from the simulation of whole OUR profiles in Figs. 1–3. The endogenous decay rate of storage products, b_{STO} , is taken the same value as b_H , which is similar to the approach adopted in ASM3.

5.2. Determination of simultaneous storage and growth kinetics

The transient OUR phenomenon observed immediately after addition of substrate (Vanrolleghem et al., 1998, 2004), followed by a gradual increase to a maximum level which continues or not at the maximum level until all external substrate is taken up for storage and growth, made modelers realize that it was necessary to modify ASM3 to include direct growth on primary substrate as a significant biological mechanism (Krishna and van Loosdrecht, 1999; Beun et al., 2000; Karahan-Gül et al., 2003, 2006; Sin et al., 2005; Karahan-Gül et al., 2006; Ni and Yu, 2008a, 2008b). However, their models did not identify the internal relationships among the parameters associated with substrate storage and direct growth processes as described by Sin et al. (2005), or can not simulate the OUR phenomena obtained from the tests by Krishna and van Loosdrecht (1999) and our study because the function $K_S/(K_S + S_S)$ inhibits the degradation of X_{STO} . According to above, it can be deduced that during the feast phase the microbial

metabolism should be described by three simultaneous processes, i.e., substrate storage, direct biomass growth on substrates and growth on internal storage.

Hence, according to the above discussion, it seems that removing the inhibition function $K_S/(K_S+S_S)$ from the kinetic expression of growth on X_{STO} can realize the three simultaneous processes, as illustrated by the simulation results in Fig. 4. This figure shows the comparison of the simulation results of models with and without inhibition function $K_S/(K_S+S_S)$. When calibrating the model with the OUR data, the curve of the model with inhibition function just fits the OUR profile under famine condition, while the model without inhibition function can not only fit the OUR data under feast phase, but also fit the data under the famine condition. The R and the sum of squared errors (SSE) for the model with and without inhibition function were 0.849, 0.023 and 0.893, 0.013, respectively.

5.3. Discussions for the different OUR phenomena

Throughout the literature investigation, it can be found that there are two different kinds of OUR phenomena occurring in the batch experiments after pulse addition of a certain amount of substrate. One is that the OUR goes transiently to a high level after adding the substrate, and then increases gradually to a maximum level and

continues at the maximum level until all external substrate is taken up for storage and growth (Figs. 1–4). This OUR curve phenomenon was observed in this study as well as other studies (Vanrolleghem et al., 1998; Krishna and van Loosdrecht, 1999; Karahan-Gül et al., 2003; Sin et al., 2005). The other more common OUR phenomenon shows that first it transiently goes to a maximum level, continues at this maximum level, and then decreases gradually to a lower level until all the external substrate is exhausted.

However, these two phenomena have been attributed to one factor in this study, i.e., the initial concentration of X_{STO} in the biomass before adding substrate. It means that when the initial X_{STO} is low at the beginning, the OUR resulting from biomass growth on X_{STO} (OUR $_{X_{STO}}$) can be neglected, and the total OUR mostly results from the oxygen consumption for biomass storage and direct growth on substrate (OUR $_{S_S}$). As the net X_{STO} (X_{STO} formation minus X_{STO} degradation) increases, OUR $_{X_{STO}}$ increases too. If the increase rate of OUR $_{X_{STO}}$ (slope 4 in Fig. 5A) is faster than the OUR $_{S_S}$ decrease rate (slope 2 plus slope 3 in Fig. 5A), then the first OUR phenomenon will be seen (Fig. 5A), otherwise the other phenomenon will be observed (Fig. 6B). When the initial X_{STO} concentration is high enough in the beginning, the rate of X_{STO} formation equals or is lower than the rate of X_{STO} consumption, and the total OUR (OUR $_{S_S}$ +OUR $_{X_{STO}}$) at the beginning reaches a maximum immediately as described in the second phenomenon (Fig. 6B).

The above explanation can also be supported by another OUR phenomenon observed in this study (see Fig. 6) and other investigations (Sin et al., 2005) when the experiments were conducted with two pulse additions of equal amounts of sodium acetate. The difference between these two OUR experiments is that in the experiments of Sin et al. (2005) the second OUR peak reaches a maximum value through a transient and then decreases gradually till the feast phase end, while in this study the second OUR peak reaches a high level through a transient and from then increases to the maximum under feast condition (Fig. 6). The reason is probably due to the time left between the last substrate pulse after the initial substrate addition was exhausted, i.e., 160 min in this study and 20 min in their experiments. In other words, the longer famine phase leads to a lower amount of X_{STO} left before the second addition. It can also be seen in Fig. 6 that the maximum value of the first OUR profile is lower than that of the second OUR. The different X_{STO} concentrations before pulse addition of the substrate can also be used to explain this phenomenon (see D1 in Fig. 6). As can be seen in Fig. 7, when the initial X_{STO} concentration increases, the OUR profiles increase too. Another possible reason for this

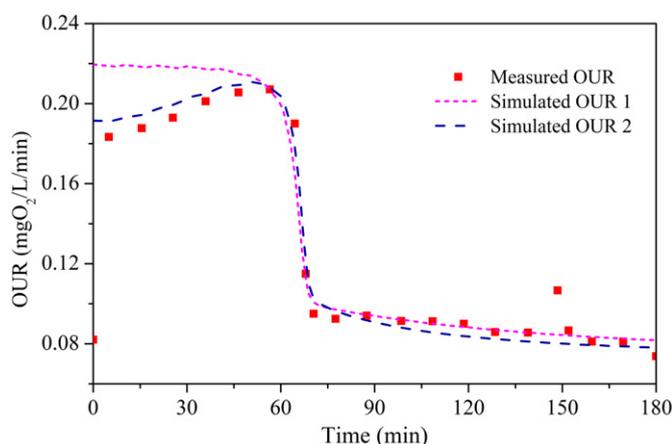


Fig. 4. Comparison of two biomass growth on X_{STO} mechanisms: OUR 1 is the kinetic expression with substrate inhibition function ($K_S/(S_S+K_S)$) (R and SSE are 0.849 and 0.023, respectively) and OUR 2 without substrate inhibition function (R and SSE are 0.893 and 0.013, respectively).

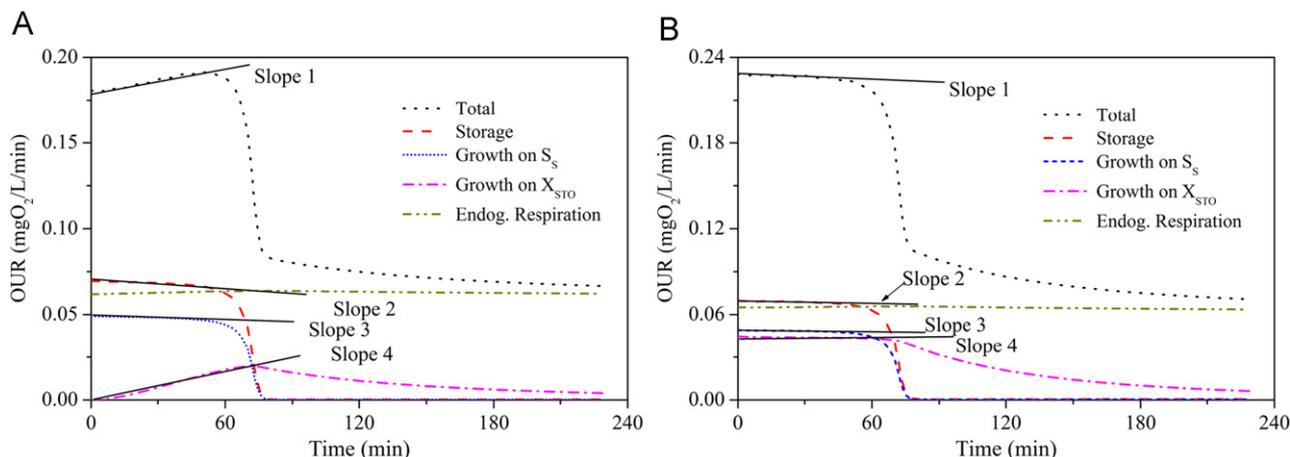


Fig. 5. Simulation of two different OUR profiles: A. The OUR reaches transiently to a high level, and then increases gradually to a maximum level until all the external substrate is taken up; B. The OUR first reaches transiently to a maximum level, and then decreases gradually to a little low level until all the external substrate is exhausted.

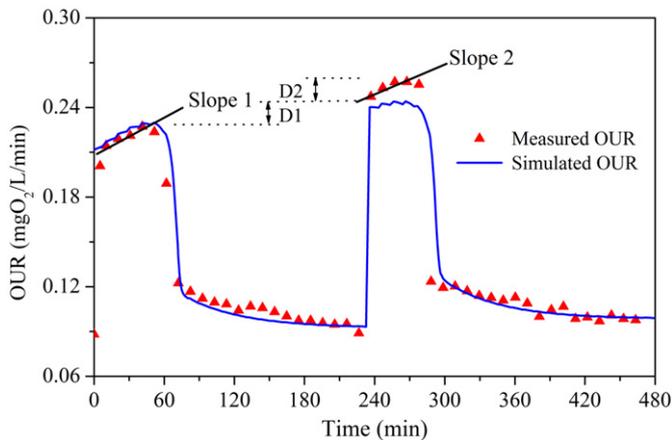


Fig. 6. Model fits to the experiment with two pulse additions of equal amounts of sodium acetate where the second acetate pulse is added after 160 min.

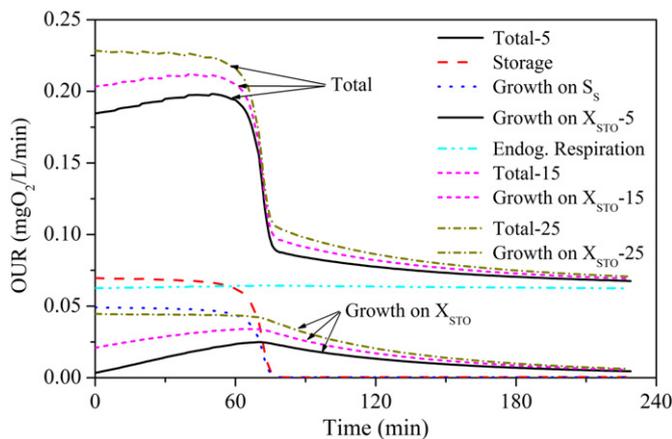


Fig. 7. Simulated OUR profiles with different initial X_{STO} concentration: $X_{STO}=5$ mgCOD/L; $X_{STO}=15$ mgCOD/L; $X_{STO}=25$ mgCOD/L. Only OURs for storage, direct growth on S_s and endogenous respiration processes with initial $X_{STO}=5$ mgCOD/L are kept in this Figure as these OURs with different initial X_{STO} are nearly overlapped.

discrepancy (see D2 in Fig. 6) is the improved activity of biomass to sustain a higher growth rate after the first pulse of acetate (Sin et al., 2005; Lavallee et al., 2005; Vanrolleghem et al., 1998; van Loosdrecht and Heijnen, 2002).

6. Conclusions

In this study, a new extension of ASM3 with the consideration of simultaneous substrate storage and biomass direct growth under aerobic condition was successfully established. Under feast condition, a new carbon source metabolic pathway was proposed, stating that the internal storage products X_{STO} can be degraded along with the substrate uptake without inhibiting X_{STO} consumption until the initial substrate is almost used up. Consequently, a new kinetic expression for growth on X_{STO} was developed to describe the degradation of storage products.

The model was successfully calibrated with OUR data obtained from batch experiments. The predictions of the calibrated model were also confirmed by a series of off-line SCOD and ammonia concentration measurements in Experiment 1 and another OUR experiment in Experiment 2. This novel extension of ASM3 is able to handle the main limitation of ASM3, i.e., ASM3 fails to simulate the kind of observed OUR profile in which OUR transiently reaches

a high level, then increases gradually to a maximum level, and continues at this maximum level until all external substrate is taken up. The new model also indicates that the initial X_{STO} concentration present before pulse addition of substrate can significantly affect the OUR profiles. However, since most of the WWTPs are also operated under anoxic condition, it is necessary to extend the proposed model to describe simultaneous substrate storage and biomass direct growth under anoxic condition and conduct further model evaluation with real wastewater in full-scale WWTPs under aerobic and anoxic conditions before the proposed model can be expected to guide wastewater treatment plant operation.

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