Modification of ASM3 for the determination of biomass adsorption/storage capacity in bulking sludge control

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Abstract The selector activated sludge (SAS) systems are known to prevent excessive growth of filamentous microorganisms responsible for bulking sludge, but these systems were hardly ever modelled. This study aimed to develop a model capable of predicting rapid substrate removal in the SAS systems. For this purpose, the Activated Sludge Model No. 3 (ASM3) was extended with three processes (adsorption, direct growth on the adsorbed substrate under aerobic or anoxic conditions). The modified ASM3 was tested against the results of batch experiments with the biomass originating from two full-scale SAS systems in Germany. The endogenous biomass was mixed with various readily biodegradable substrates (acetate, peptone, glucose and wastewater) and the utilisation of substrate (expresses as COD) and oxygen uptake rates (OURs) were measured during the experiments. In general, model predictions fitted to the experimental data, but a considerable number of kinetic (5) and stoichiometric (2) parameters needed to be adjusted during model calibration. The simulation results revealed that storage was generally a dominating process compared to direct growth in terms of the adsorbed substrate utilisation. The contribution of storage ranged from 65–71% (Plant A) and 69–92% (Plant B).

Keywords Adsorption capacity; batch test; bulking sludge; dynamic simulation; mathematical modelling

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Introduction

The selector activated sludge (SAS) systems have recently been developed to prevent excessive growth of filamentous microorganisms responsible for "bulking sludge". Although the capabilities of SAS systems have been proved in practice, the principal mechanisms occurring in selectors have not been fully understood and knowledge about these mechanisms is still being accumulated. Mathematical modelling is considered as a useful tool for understanding complex interactions that occur in activated sludge systems. A wide range of these systems can be simulated using the common models, called the activated sludge models (ASMs) (Henze *et al.*, 2000). In the review of Martins *et al.* (2004), however, the authors claimed that the SAS systems were hardly ever modelled and their design principles were primarily developed based on empirical observations. If a general ASM-type concept is to be applied for selectors, then one of the principal factors that should be taken into account is rapid substrate removal.

Different models have been proposed in the literature to describe the carbonaceous substrate conversion including storage, e.g. sequential storage and growth (ASM3), parallel storage and growth, dual substrate, dual biomass (Makinia, 2005). Very few of these models incorporate the adsorption process, even though it has been reported that the addition of adsorption is essential for modelling high rate processes (Larrea *et al.*, 2002), can improve simulation results of oxygen uptake rates (Ginestet *et al.*, 2002) and can account for "lacking COD" in the COD balance (Beccari *et al.*, 2002). The aim of this study was to develop a model that could be capable of predicting rapid substrate removal in the SAS systems. For this purpose, the Activated Sludge Model No. 3

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(ASM3) (Gujer *et al.*, 1999) was used as the core of a model. The newly developed model was tested under dynamic conditions against the data from earlier experiments performed for the determination of adsorption/storage capabilities of biomass originating from different activated sludge systems (Phan and Rosenwinkel, 2004).

Model development

Review of approaches to modelling rapid substrate removal

Storage. Several types of organic storage polymers have been reported in the literature. The most common ones are polyhydroxyalkanoates (PHAs) and polysaccharides (Majone *et al.*, 1999). In particular, poly-3-hydroxybutyrate (PHB) and glycogen are usually stored when the system is fed with acetate and glucose, respectively (Karahan-Gul *et al.*, 2002). PHAs can also be generated from several different substrates including glucose (Majone *et al.*, 1999) and ethanol (Beccari *et al.*, 2002). Glycogen is probably only formed when sugars are present in the influent, but it also plays an essential role in the metabolism of PAO and GAO (van Loosdrecht *et al.*, 1997). The role of lipids is unclear, however, since only a few reports are available without explanation of how a distinction was made between stored lipids and cell/membrane lipids (van Loosdrecht *et al.*, 1997). The identification and role of storage compounds other than glycogen and PHA in the activated sludge processes still remains an important topic for future research (Dircks *et al.*, 2001).

A well-known example of the model assuming simultaneous storage and growth on the storage polymers is ASM3 (Gujer *et al.*, 1999), shown schematically in Figure 1(a). This simplest concept incorporating storage phenomena is not valid mechanistically, due to experimental evidence that microorganisms utilize the stored polymers as a carbon and energy source only after depletion of primary substrate, S_S (Karahan-Gul *et al.*, 2003). A more consistent description of substrate conversion could be provided if growth on primary substrate in the feast period is additionally incorporated in the model (Figure 1(b)). This approach was originally proposed by Krishna and van Loosdrecht (1999) and also used later by Winkler *et al.* (2001), Beccari *et al.* (2002) and Karahan-Gul *et al.* (2003). In the latter case, the authors introduced a switching function for the growth rate on

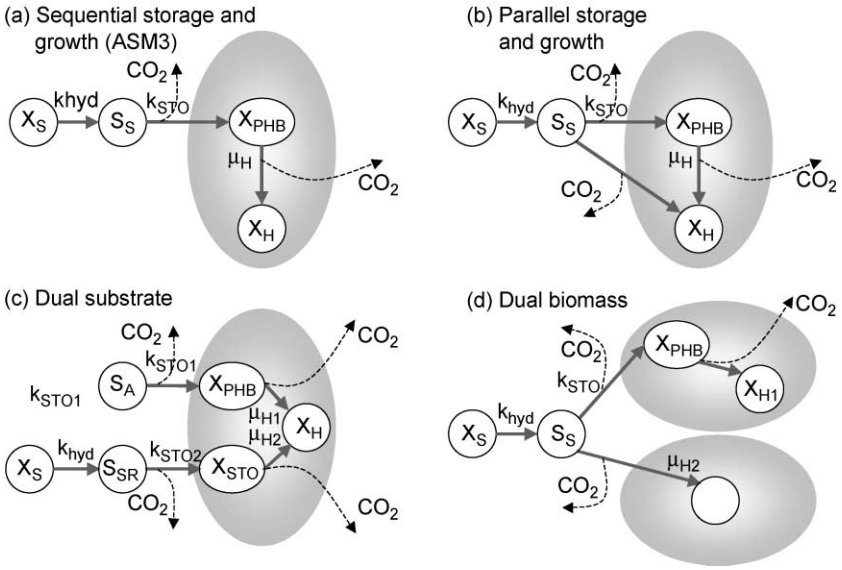

Figure 1 Schematic representation of the substrate flux in various models considering the storage mechanisms: (a) sequential storage and growth, (b) parallel storage and growth, (c) dual substrate, (d) dual biomass

stored polymers in order to prevent this growth before the growth on primary substrate is depleted. Carucci *et al.* (2001) developed a dual substrate model (Figure 1(c)) considering two fractions of readily biodegradable COD: acetate (S_A) and all other readily biodegradable substrates (S_{RB}). Accordingly, two storage compounds were considered: PHB (X_{PHB}) generated only from acetate and a generic storage compound (X_{STO}), which can also include PHB not coming from acetate, generated from S_{SR}. The slowly biodegradable COD (X_S) was assumed to be hydrolysed only to S_{SR}. A single group of heterotrophic biomass (X_H) grows simultaneously on both storage products (X_{PHB} and X_{STO}). In a dual biomass model of Hanada *et al.* (2002), shown in Figure 1(d), the heterotrophic biomass is divided into two fractions: the one with a storage capability (X_{H1}) and another one without a storage capability (X_{H2}). The X_{H1} and X_{H2} fractions grow according to the ASM3 concept and ASM1 concept, respectively.

Adsorption. Adsorption is defined as a simple physical–chemical interaction that can contribute to fast removal of the soluble substrate from the liquid phase, in a similar way to enmeshment (instantaneous physical entrapment) of the particulate substrate (Majone *et al.*, 1999). The adsorption kinetics can be mathematically expressed by the equation of modified Langmuir isotherm (Ekama and Marais, 1979), which relates COD in the liquid phase with COD adsorbed in the sludge flocs by the heterotrophic biomass. This equation was used by Novak *et al.* (1995) for modelling adsorption of two fractions of soluble substrate (S_R and S_S), whereas Beccari *et al.* (2002) modified this equation by using a Monod term $(S_S)/(K_S + S_S)$ instead of the first order expression with respect to S_S. In terms of stoichiometry, some adsorption models (e.g. Novak *et al.*, 1995) are represented by a simple transformation of both soluble substrates (S_S or S_R) to the adsorbed substrate (X_{ADS}) without any energy requirement, whereas the other models (e.g. Beccari *et al.*, 2002) assume a demand for small amount of energy.

Extension of ASM3 including the rapid substrate removal processes

The modified version of ASM3 proposed in this study was extended with three processes including adsorption of soluble substrate and direct growth of heterotrophs on adsorbed substrate under both aerobic and anoxic conditions. The stoichiometry and kinetics of the new processes are presented in Table 1.

The adsorption process was modelled according to the concept proposed by Novak *et al.* (1995). The direct growth was introduced in parallel to storage (Figure 1(b)). Consequently, two separate maximum growth rate constants, $\mu_{H,1}$ and $\mu_{H,2}$, for heterotrophic growth on adsorbed substrate and stored polymers, respectively. The process rate equations of both processes include the same multiple Monod terms to account for limitations of the relevant substrate, nutrients (ammonia), electron acceptors (oxygen/nitrate) and alkalinity. However, a switching function $(K_S)/(K_S + X_{ADS})$ was added to Processes 4 and 5 in ASM3 (aerobic and anoxic growth of heterotrophs) as proposed by Karahan-Gul *et al.* (2003). All of the other processes (i.e. hydrolysis, storage, endogenous respiration, respiration of stored polymers) were modelled using the unchanged ASM3 equations.

Materials and methods

Procedures of lab-scale experiments

In the original study described by Phan and Rosenwinkel (2004), the activated sludge biomass for lab experiments originated from five full-scale municipal wastewater treatment plants (WWTPs) in Germany. For the purpose of this study, the experimental data from only two pre-denitrification systems with aerobic selectors were selected and referred further to as Plant A and Plant B, respectively. Both plants were operated at

Table 1 Stoichiometry and kinetics of the new processes included in the modified version of ASM3

Process	Process stoichiometry					Process rate equation, $ML^{-3}T^{-1}$
	S_O	S_{NO}	S_S	X_{ADS}	X_H	
Adsorption of soluble substrate by heterotrophs	$Y_{ADS}{}^{-1}$		-1	Y_{ADS}		$k_{ADS}\, S_S\, X_H \left(K_{MAX,ADS} - \frac{X_{ADS}}{X_H} \right)$
Aerobic growth of heterotrophs on adsorbed substrate	$\frac{Y_{H,O2}{}^{-1}}{Y_{H,O2}}$			$-\frac{1}{Y_{H,O2}}$	1	$\mu_{H,1} \frac{S_O}{K_{O,H} + S_O} \frac{S_{NH}}{K_{NH,H} + S_{NH}} \frac{S_{ALK}}{K_{ALK,H} + S_{ALK}} \frac{X_{ADS}}{K_{ADS,H} + X_{ADS}} X_H$
Anoxic growth of heterotrophs on adsorbed substrate		$\frac{Y_{H,NO}{}^{-1}}{2.86 Y_{H,NO}}$		$-\frac{1}{Y_{H,NO}}$	1	$\mu_{H,1}\, \eta_G \frac{K_{O,H}}{K_{O,H} + S_O} \frac{S_{NO}}{K_{NO,H} + S_{NO}} \frac{S_{NH}}{K_{NH,H} + S_{NH}} \frac{S_{ALK}}{K_{ALK,H} + S_{ALK}} \frac{X_{ADS}}{K_{ADS,H} + X_{ADS}} X_H$

similar sludge retention times (i.e. 22–23 d), but one of them (Plant B) received a substantial load of industrial wastewater.

Batch tests were carried out under aerobic conditions in an experimental set-up consisting of four parallel batch reactors ($V_{max} = 2.5\,dm^3$ each) equipped with an automatic system for aeration control and measurement of oxygen uptake rates (OURs). Prior to the tests, the biomass was aerated for 16–18 h to reach the endogenous state. The endogenous biomass was mixed with various readily biodegradable substrates including acetate, peptone, glucose and settled wastewater taken from one of the studied plants. The respirometric measurements were conducted for 2.5–3 h and the dissolved oxygen (DO) concentration was constantly maintained at 3–4 $g\,O_2/m^3$. The aeration system was turned off periodically and a decrease in the dissolved oxygen (DO) concentration between 3.8 and 3.0 $g\,O_2/m^3$ was recorded to calculate the corresponding OUR. Prior to the new measurement, the DO concentration in the reactor was risen to 4 $g\,O_2/m^3$. In order to determine the total substrate utilisation, samples of the mixed liquor were withdrawn and filtered. The filtrate was analysed for COD by Dr. Lange LCK 614/514/314/114 methods. The biomass concentration MLSS was measured according to DIN 38414 S 2 at the beginning of each experiment.

Simulator environment and model calibration procedure

Simulations were run using GPS-X ver. 4.0.2 simulation package (Hydromantis, 2002). The new model was implemented using a special spreadsheet utility called Model Developer. The model was calibrated according to an iterative procedure outlined in Figure 2.

Steady-state simulations of the full-scale SAS systems were introduced to obtain the initial biomass composition for the batch tests. During simulations of the experiments with various readily biodegradable substrates (Steps 3 and 4), selected parameters were mathematically optimised using the GPS-X utility called Optimiser (the Simplex method with "sum of squares" as the objective function to minimize).

Results and discussion

Experiments with artificial substrates and real wastewater

The results of model calibration under endogenous conditions and with different readily biodegradable substrates are presented in Figure 3. Table 2 contains a list of modified kinetic and stoichiometric parameters in comparison with the ASM3 defaults and the values proposed by Novak *et al.* (1995) with respect to the adsorption equation shown earlier in Table 1. Three kinetic parameters ($\mu_{H,1}$, k_{STO} and k_{ADS}) were simultaneously optimized based on the measured OURs and soluble COD concentrations using the optimiser utility. Next, the other kinetic parameters, K_{STO} and $K_{MAX,ADS}$, were adjusted to improve predictions of the OUR after the depletion of readily biodegradable (adsorbed) substrates and the COD utilisation rate, respectively. Finally, the stoichiometric parameters (Y_{STO} and Y_{ADS}) were adjusted to improve OUR predictions in the initial

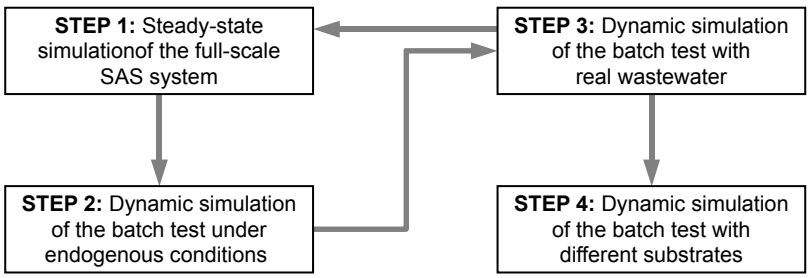

Figure 2 Main steps of the iterative procedure of model calibration

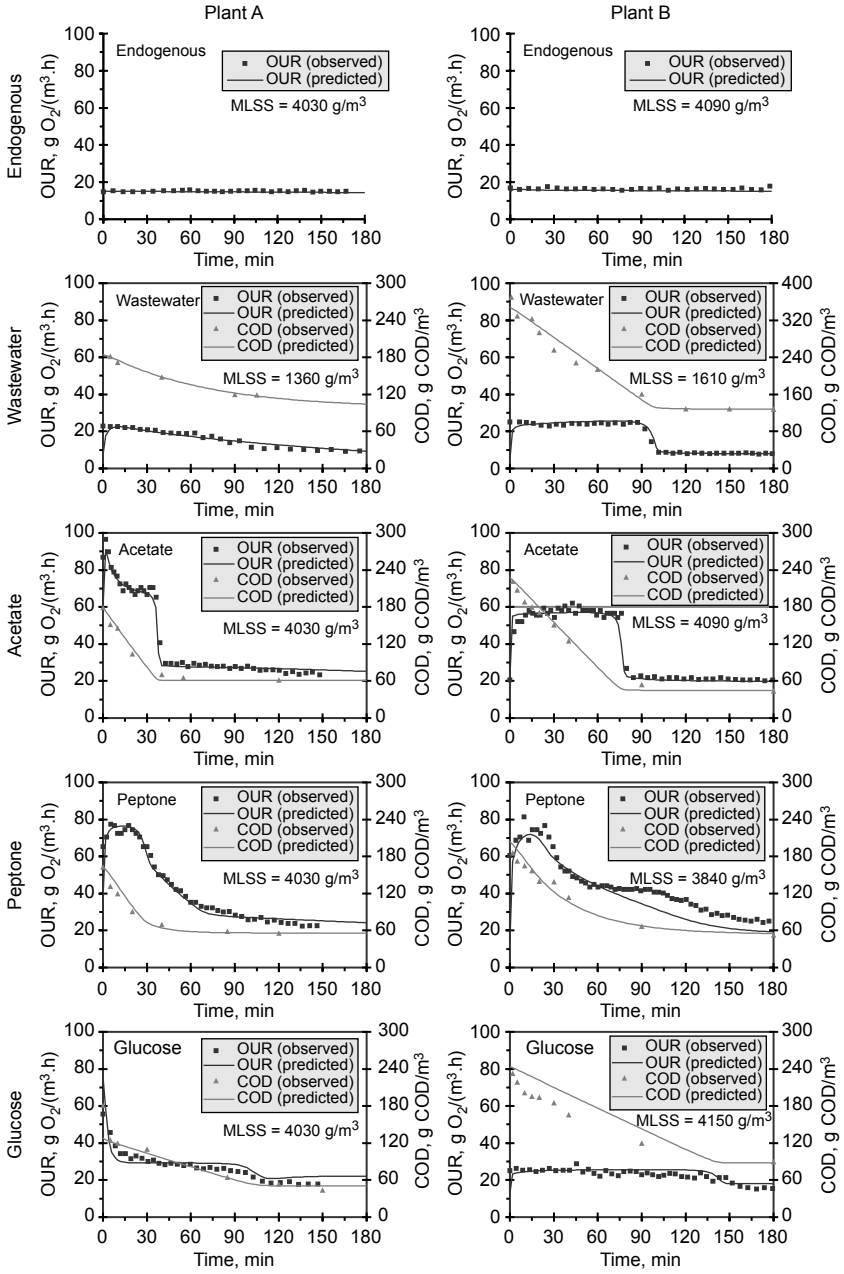

Figure 3 Observed vs. predicted results of measurements in the batch experiments carried out with the biomass from the two studied SAS systems and different sources of readily biodegradable COD

phase of the experiments in the presence of readily biodegradable substrate. The different storage yields, Y_{STO}, for acetate and glucose were adopted based on the literature data (Karahan-Gul *et al.*, 2002). The reported values of Y_{STO} for acetate and glucose were 0.78 and 0.87 g COD_{Xsto}(g COD_{Ss}), respectively.

In general, model predictions fitted to the experimental data (OUR and substrate utilisation) except two cases, i.e. the OUR resulted from the utilisation of stored substrate (the experiment with the "Plant B" biomass and peptone) and a rapid decrease of glucose concentration in the initial phase of the experiment with the "Plant B" biomass (Figure 3).

Table 2 A list of model parameters adjusted during the calibration with various readily biodegradable substrates

Parameter	Unit	Plant A				Plant B			
		WW	ACE	PEP	GLU	WW	ACE	PEP	GLU
$\mu_{H,1}$	d^{-1}	4	4	0.9	2	1.6	2	0.5	0.2
k_{STO}	g COD_{Ss} (g COD_{Xh})$^{-1}$d^{-1}	4	2.1	1.9	0.15	5.2	2.5	4.2	1.1
K_{STO}	g COD_{Xsto} (g COD_{Xh})$^{-1}$	0.1	0.2	0.15	1	3	0.1	1	2
k_{ADS}	m^3 (g COD)$^{-1}$ d^{-1}	0.4	1	0.4	2	1	0.4	0.14	2.8
$K_{MAX,ADS}$	g COD_{Xads} (g COD_{Xh})$^{-1}$	0.15	0.15	0.15	0.15	0.25	0.25	0.25	0.25
$Y_{STO,O2}$	g COD_{Xsto} (g COD_{Ss})$^{-1}$	0.85	0.75	0.85	0.95	0.95	0.7	0.75	0.9
Y_{ADS}	g COD_{Xads} (g COD_{Ss})$^{-1}$	0.97	0.97	0.97	0.97	1	1	1	1

WW – real wastewater; ACE – acetate, PEP – peptone; GLU – glucose

It was not possible to calibrate the model with a single parameter set, but rather a considerable number of kinetic and stoichiometric parameters needed to be adjusted in terms of the substrate used in the experiment. A comparable number of adjusted parameters was reported by Beccari *et al.* (2002) in the study with a similar modified ASM3 and various readily biodegradable substrates (acetate, ethanol, glutamic acid and wastewater.

The simulation results presented in Figure 3 were used to determine the split of COD flows between direct growth and storage. Without considering the experiment with glucose and the "Plant A" biomass, storage was a dominating process of the adsorbed substrate utilisation (Figure 4). The contribution of storage ranged from 65 to 71% for the "Plant A" biomass. For the experiments with the "Plant B" biomass, the highest contribution of storage (92%) was predicted for peptone as a substrate. For the other three substrates, storage accounted for 69–74% of the total COD utilisation. These predictions need to be confirmed in further experiments, in which the concentrations of internal storage compounds will also be determined. It should be noted, however, that the obtained values correspond closely to the findings of Karahan-Gul *et al.* (2003) for the similar batch tests with glucose. The authors reported that 66% of the glucose fed to the system was stored as glycogen, whereas the remaining portion (34%) was used for direct growth. The adjusted storage rate constants, k_{STO}, ranged from 0.15 to 5.2 g COD_{Ss} (g COD_{Xh})$^{-1}$d^{-1} and were lower than the k_{STO} values reported in the literature for simulations with the model presented in Figure 1(b) (parallel storage and growth), i.e. $k_{STO} = 8–14$ g COD_{Ss} (g COD_{Xh})$^{-1}$d^{-1} (Makinia, 2005). The exception was the study of Beccari *et al.* (2002) who used extremely low values of k_{STO} (0.003–0.31 g COD_{Ss} (g COD_{Xh})$^{-1}$d^{-1}) for simulations without considering adsorption in contrast to higher values of k_{STO} (0.06–43 g COD_{Ss} (g COD_{Xh})$^{-1}$d^{-1}) when adsorption was considered in the model.

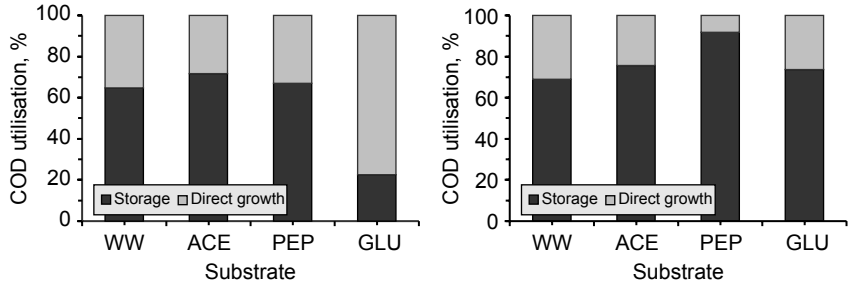

Figure 4 Comparison of predicted relative COD utilisation for parallel storage and direct growth at the two studied plants

Conclusions

Several approaches to modelling the storage phenomena have been reported in the literature. The model concept developed in this study focused on predicting the initial (rapid) phase of substrate removal from the solution and thus the adsorption process was also incorporated in the model. A relationship between the kinetics of adsorption and storage may be a potential factor affecting the growth of different groups of heterotrophic microorganisms including filamentous bacteria. This information may provide a basis for optimisation of the SAS systems to prevent the bulking sludge problem.

The results of this study allowed the evaluation of the biomass adsorption/storage capacity for different substrates under dynamic conditions. However, it was not possible to predict OURs and utilisation rates of the substrates with a single parameter set. The model was calibrated individually for each readily biodegradable compound tested during the previous experimental investigation. This approach resulted in a considerable number of kinetic and stoichiometric coefficients to be adjusted in order to fit the experimental results. Model predictions confirmed the literature data that storage could be a dominating mechanism of the adsorbed substrate utilisation, but the possibility of direct growth on primary substrate should not be neglected. The investigations of full-scale SAS systems are planned to be extended with the measurements of storage polymers, which will give a deeper insight into the differences between the mechanisms of adsorption, storage and direct growth.

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