8th International IFAC Symposium on
Dynamics and Control of Process Systems
Preprints Vol.1, June 6-8, 2007, Cancún, Mexico

DEVELOPMENT OF A 4-MEASURABLE STATES ACTIVATED SLUDGE PROCESS MODEL DEDUCED FROM THE ASM1

Michela Mulas, Stefania Tronci, Roberto Baratti

Università degli Studi di Cagliari, Dipartimento di Ingegneria Chimica e Materiali, Cagliari, Italy

Abstract: The Activated Sludge Model No.1 (ASM1) allows the prediction of organic matter degradation, nitrification and denitrification in the activated sludge bioreactors using thirteen states variables. This paper deals with modal reduction procedure applied to the ASM1, that followed by physical considerations about the process allows the development of a 4-state variables model which is still able to describe the nonlinear behavior of bioreactors in the Activated Sludge Process (ASP). Furthermore, coupling the reduced bioreactor model with a simplified model for the secondary settler (as the Takács model), the overall ASP behavior is deduced.

Keywords: ASM1, Modal reduction, Identifiability, Parameter estimation

1. INTRODUCTION

Wastewater treatment plants improvement represent a mandatory task to preserve water resources and to assure the regulation regarding water quality preservation. In this sense, the application of advanced control systems represents an economic alternative to achieve this requirement. Moreover, since hardware instrumentation is still expensive, with undesirable time-delays, or unavailable, the development of reliable simplified models and soft sensors is a prerequisite to continuous monitoring the effluent quality.

In a biological wastewater treatment plant, the activated sludge process (ASP) represents the main unit where the biodegradation of the carbon and nitrogen compounds takes place. The state-of-the-art model for the bioreactor is the Activated Sludge Model No.1 (Henze *et al.*, 1987) that could be coupled with a simplified, one dimensional, model of the secondary settler, Takács model (Takács *et al.*, 1991), to describe the behavior of an ASP. The ASM1 describes the nonlinear dynamics of the bioreactor using thirteen state variables and nineteen parameters. Moreover, it refers to state variables that not always can be acquired in a wastewater treatment plant; also in such a sense the model is limited for on-line process monitoring purposes. For instance, measurable components such as COD can be obtained only as composite variable. For these reasons in literature a wide number of reduced-order models for the ASP is present, as for instance: (Jeppsson and Olsson, 1993), (Steffens *et al.*, 1997), (Gómez-Quintero *et al.*, 2000), (Chachuat *et al.*, 2003), (Smets *et al.*, 2003), (Spérandio and Queinnec, 2004).

In this paper, we will propose a simplified model, with state variables directly related with the typical measurements used in an ASP, to obtain a fast and reliable instrument to represent the process itself or with an estimator. The model complexity is reduced in the following way: starting from a systematic definition of the process dynamics and classifying the state variables on a time basis, the model order is preventively reduced. Afterwards,

the acquired knowledge about the process is used to further reduce the model. The validation of the obtained simpler model is then carried out by means of the frequency response analysis, using as input variables the influent flow rate and/or load, for different linearization points. In this context, Bode and singular value plots are useful tools to corroborate the dynamic consistency of the reduced- with respect to the full-model (ASM1) as a function of frequency, considering the SISO or MIMO configurations, respectively.

2. MODEL REDUCTION PROCEDURE

The procedure used to obtain the proposed model starts with the classification of the state variables on time basis. The major problem with this approach is to discriminate the different modes present in the system. This can be achieved by considering the solution of the linear approximation of the nonlinear process, where the different time scales are measured by the system eigenvalues. Obviously, the analysis of the linearized system is valid around the conditions where the Jacobian matrix, $\mathbf{A}$, is calculated; hence in this case the linearization of the mass balance of the ASM1 has been accomplished by considering different data sets and operating points. In such a way the information obtainable from the different Jacobian matrixes can be considered representative for a wide range of operating conditions.

The eigenvalues of the linearized system indicate the existence of different time scales in the process, hence the second important aspect of this procedure concerns with the association of the model modes to the model states. The assessment of relationships between states and dynamics of the system is developed through the homotopy analysis. This method requires starting with a system with a defined relationship between eigenvalues and states: the diagonal elements of the Jacobian matrix ($\mathbf{A}_D$). In such a way each diagonal element (i.e., each eigenvalue) is directly related to the state. Then the system is transformed using the homotopy parameter $r \in [0, 1]$, by means of a continuation method (Robertson and Cameron, 1997), into the actual system while tracing the eigenvalues:

$$\mathbf{H}(r) = (1 - r)\mathbf{A}_D + r\mathbf{A}. \qquad (1)$$

From the homotopy matrix, the state variables could be classified in:

- Fast states: with time constants of seconds.
- Medium states: with time constants of minutes.
- Slow states: with time constants of hours.

Furthermore, considering the region of interest, states with dynamics at either extreme (fast or slow) can be discharged from model equations and a systematic approach can be used to reduce the ASM1 complexity. Modal reduction techniques, such as modal truncation and residualization (Skogestad and Postlethwaite, 1998), provide the mathematical basis for reduction on time-scale separation. The lower order model obtained with the systematic approach could be further reduced by means of physical considerations: in fact, the knowledge and experience acquired by the modeler can be used to define a simpler model.

In the following the reduction procedure is applied to the ASM1.

3. REDUCED MODEL DEVELOPMENT

As a case study, we consider the full-scale wastewater treatment plant reported in (Mulas, 2006). The ASP has a classic configuration: the bioreactor consists of an anoxic (denitrification) followed by an aerobic (nitrification) zone. To maintain the microbiological population, the sludge from the settler is recirculated into the anoxic basin, while the sludge concentration is kept constant by means of sludge withdrawn from the settler. The process representation is obtained with Matlab/Simulink (R14).

The inputs to the model are selected in order to represent the variations in wastewater flow rate and concentrations by using the functions proposed by Isaacs and Thornberg (1998) for urban wastewater treatment plants. Furthermore, this representation is fulfilled by considering the situation of an equalization basin, which could be present or not in the plant. The dynamical model for this unit describes the dilution of wastewater components, assuming that no biological reactions occur.

Flow rate	=	6152	$[m^3/d]$
COD	=	221	$[gCOD/m^3]$
TSS	=	46	$[gSS/m^3]$
S_{NO}	=	0.22	$[gN/m^3]$
TKN	=	22	$[gN/m^3]$
f_{NH}	=	0.36	–

Table 1. Influent average conditions for the considered plant.

Having first defined the input data for the system (by multiplying the average influent data in Table 1 for the mentioned periodic functions, we obtain a typical evolution under dry weather condition), different data sets and operating points need to be considered to face different operating modes in order to investigate the state-space model representation by means of the homotopy matrix in Equation 1.

Component → Process ↓	1 S_I	2 S_S	3 X_S	4 S_O	5 S_{NO}	6 S_{NH}	Reaction (r)
1. Het.growth (aero)		$-\frac{1}{Y_H}$		$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$	$\theta_1 \frac{S_S}{K_S+S_S}\frac{S_O}{S_O+K_{OH}}$
2. Het.growth (anox)		$-\frac{1}{Y_H}$			$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$	$\theta_1 \frac{S_S}{K_S+S_S}\frac{K_{OH}}{S_O+K_{OH}}\frac{S_{NO}}{S_{NO}+K_{NO}}\eta_g$
3. Autot.growth				$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$	$\theta_2 \frac{S_{NH}}{S_{NH}+K_{NH}}\frac{S_O}{S_O+K_{OA}}$
4. Decay			1				θ_3
5. Ammonification						1	θ_4
6. Hydrolysis		1	-1				$\theta_5 \frac{X_S}{\theta_6+X_S}(\frac{S_O}{S_O+K_{OH}}$ $+\eta_h \frac{K_{OH}}{S_O+K_{OH}}\frac{S_{NO}}{S_{NO}+K_{NO}})$

Table 2. Reduced model with 6 state variables.

It is worth noting that, even if anoxic and aerated zones are being represented with the same ASM1, those present different dissolved oxygen concentration that influences the state variable dynamics by mean of the switching function. In both cases, the state variables can be classified as fast, medium and slow and considering as region of interest the one with the eigenvalues comprised between 250 and 90 d^{-1}, we noticed that the system does not behave in the same way in the two zones. Strictly considering the homotopy analysis, we would have obtained different models for the biological reactor zones. This means that some more assumptions should be made in order to obtain a more suitable model.

As a first attempt, we came out with a model involving only six state variables:

$$\mathbf{x}^{6s} = [S_I,\, S_S,\, X_S,\, S_O,\, S_{NO},\, S_{NH}]^T \qquad (2)$$

As mentioned, the remaining ASM1 state variables can be truncated, in order to preserve the steady state behavior of the original system without losing the physical interaction between the state variables, or residualized, i.e. the derivatives of those states variables are approached to zero leading to a system involving differential and algebraic equations. The later approach involves inevitably longer computational CPU time indeed without improving the reduced model behavior; for this reason the state variables not included in $\mathbf{x}^{6s}$ have been truncated and we will refer to this model as *Model6s* which is summarized in a Petersen matrix form shown in Table 2. The model involves ten kinetic and stoichiometric parameters that keep the same meaning as in the ASM1:

$$\begin{aligned}\mathbf{p} =&[Y_H,\, Y_A,\, i_{XB},\, K_S,\, K_{OH},\, K_{NO},\\ &K_{NH},\, K_{OA},\, \eta_g,\, \eta_h]^T\end{aligned} \qquad (3)$$

and the following *new* parameters:

$$\begin{aligned}\theta_1 &= \mu_H X_{BH}^{Trunc}\\ \theta_2 &= \mu_A X_{BA}^{Trunc}\\ \theta_3 &= (1-f_P)(b_H X_{BH}^{Trunc} + b_A X_{BA}^{Trunc})\\ \theta_4 &= k_a S_{ND}^{Trunc} X_{BH}^{Trunc}\\ \theta_5 &= k_h X_{BH}^{Trunc}\\ \theta_6 &= K_X X_{BH}^{Trunc}\end{aligned} \qquad (4)$$

The values of θ_i $(i = 1, 6)$ parameters depend on the truncated state variables evaluated at the nominal process conditions (as evidenced by the superscript $Trunc$) and used as tuned parameters. These variables exhibit the slowest dynamics of the system; hence their variations can be considered negligible with respect to the other states. This means that all the terms in 4 can be considered constant and retain the same value in anoxic and aerated conditions, except for θ_4, which depends on S_{ND}^{Trunc}, that has different constant concentration depending on the zone.
We can go a step further noticing that being S_I, S_S and X_S not directly measurable, *Model6s* is not suitable for online utilization. For this reason, following the idea of Jeppsson and Olsson (1993) and further used by Chachuat *et al.* (2003), we lump together the organic components to represent a single state variable, the "reduced" COD: $R_{COD} = S_I + S_S + X_S$. This is assumed to be directly measurable and representative of the COD in the activated sludge process. From Equations 5, another important simplification follows. We notice that lumping the organic component in *Model6s* means that the hydrolysis process r_6 is not considered anymore in the simpler *Model4s* as shown in Equations 6.

$$\begin{aligned}\frac{dS_I}{dt} &= D(S_I^{in} - S_I^{Out})\\ \frac{dS_S}{dt} &= D(S_S^{in} - S_S^{Out}) - \frac{1}{Y_H}(r_1 + r_2) + r_6\\ \frac{dX_S}{dt} &= D(X_S^{in} - X_S^{Out}) + r_4 - r_6\end{aligned} \qquad (5)$$

Component → Process ↓	1 R_{COD}	2 S_O	3 S_{NO}	4 S_{NH}	Reaction (r)
1. R_{COD} growth(aero)	$-\frac{1}{Y_H}$	$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$	$\theta_1 \frac{R_{COD}}{K_r^{Aero}+R_{COD}} \frac{S_O}{S_O+K_{OH}}$
2. R_{COD} growth(anox)	$-\frac{1}{Y_H}$		$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$	$\theta_1 \frac{R_{COD}}{K_r^{Anox}+R_{COD}} \frac{K_{OH}}{S_O+K_{OH}} \frac{S_{NO}}{S_{NO}+K_{NO}} \eta_g$
3. R_{COD} growth(due to N)		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$	$\theta_2 \frac{S_{NH}}{S_{NH}+K_{NH}} \frac{S_O}{S_O+K_{OA}}$
4. Decay	1				θ_3
5. Ammonification				1	θ_4

Table 3. Reduced model with 4 measurable state variables.

$$\begin{aligned}\frac{dR_{COD}}{dt} =& D(R_{COD}^{in} - R_{COD}^{in}) \\ & - \frac{1}{Y_H}(r_1 + r_2) + r_3\end{aligned} \tag{6}$$

Reaction rates r_1 and r_2 in Equation 6, are reported in Table 3; where a new parameter has been introduced: $K_r = K_S \frac{S_I+S_S+X_S}{S_S}$. K_r is a function of the organic compounds in the system and it seems a too hard approximation consider it constant during anoxic or aerobic oxygenation conditions. For this reason, the following assumption is made:

$$\begin{aligned}K_r^{Aero} &= K_r \frac{S_O}{K_{OH}+S_O} \\ K_r^{Anox} &= K_r \frac{K_{OH}}{K_{OH}+S_O}\end{aligned} \tag{7}$$

In this way, even if the K_r is kept constant the reaction rates behave differently depending on the oxygen conditions. Whereas, θ_1, θ_2, θ_3, θ_4 keep the same meaning as in Equation 4.
Summarizing, *Model4s* involves:

- 4 state variables:
  $\mathbf{x}^{4s} = [R_{COD}, S_O, S_{NO}, S_{NH}]^T$;
- 8 kinetic and stoichiometric coefficients from the ASM1
  $\mathbf{p} = [Y_H, Y_A, i_{XB}, K_{OH}, K_{NO}, K_{NH}, K_{OA}, \eta_g]^T$
- 5 new parameters:
  $\mathbf{n} = [\theta_1, \theta_2, \theta_3, \theta_4, K_r]^T$

Before being able to use this model for any practical purpose it first need to be calibrated. An appropriate objective function is constructed, quantifying the deviation of the model from the data and the minimization of this function is obtained by optimal selection of the parameter vector. It is important to underline that the $\mathbf{p}$ vector is maintained at its default value as proposed in the ASM1, while the calibration procedure is only performed with respect to $\mathbf{n}$. It means that the proposed model also leads to the reduction of the adjustable parameters, significantly decreasing the effort for its calibration.

The task at this point is to assess the practical identifiability of the reduced model, that is performed by analyzing the Fisher Information Matrix (FIM). The FIM expresses the information content in the experimental data:

$$FIM = \sum_{i=1}^{N} (\frac{\partial \mathbf{y}}{\partial \mathbf{p}}(t_i))^T \mathbf{Q_i} (\frac{\partial \mathbf{y}}{\partial \mathbf{p}}(t_i)) \tag{8}$$

The terms $\frac{\partial \mathbf{y}}{\partial \mathbf{p}}$ are the output sensitivity functions and quantify the dependence of the model predictions on the parameter values. They are central to the evaluation of practical identifiability as they are a major component of the FIM, and hence also of the parameter estimation covariance matrix. An easy way to investigate it could be plot the sensitivity equations, however stronger evidence of proportionality between sensitivities can be obtained by calculation of the rank of the Fisher information matrix. In our case, FIM is a full rank matrix considering both aerobic and anoxic zone models, meaning that nonlinear dependency exists and that the resulting model is fully identifiable.

As mentioned, in order to test the dynamic behavior of the obtained models two situations are considered: with and without equalization basin before the activated sludge process considering, in both cases, periodic influent loads.

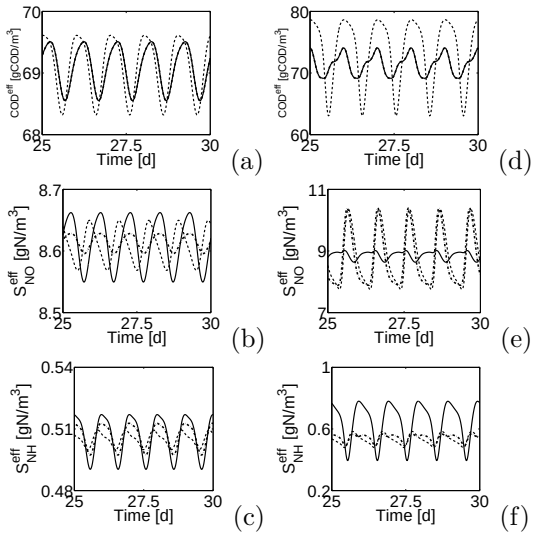

Fig. 1. Test motion with periodic *"equalized"* (left column) and *"non-equalized"* (right column) data. Models with 6 state variables (dot) and with 4 state variables (dot-dashed) are compared with the ASM1 (solid)

The models have been running for 30 simulation days using the weighting functions for both load and flow and plotting only the last 5 days, corresponding to stable regimes, to evaluate the test

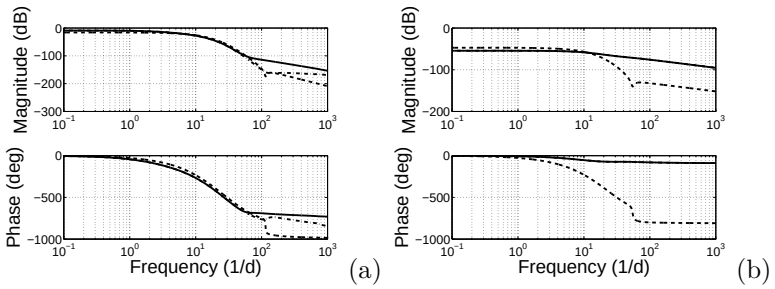

Fig. 2. Frequency responses to a sinusoidal influent COD for models with 6 state variables (dot-dashed) and with 4 state variables (dashed) are compared with the ASM1 (solid).

motions in these conditions. In Figure 1, we report the behavior of the main effluent concentrations in the wastewater treatment plant obtained with ASM1, *Model6s* and *Model4s*. It should be noted that when six states are considered the agreement is better than when only four are taken into account. This is quite obvious if we consider the assumptions made. Anyway, the results obtained with *Model4s* are promising, both because the mismatch between the two reduced models is not so large if one considers that *Model4s* has four states and only five adjustable parameters, and because it presents several advantages with respect to *Model6s*. First of all, *Model4s* is based on directly measurable state variables; in fact, the influent R_{COD} is assumed to be the influent COD measured from the wastewater treatment plant and the same holds for the nitrogen compounds and for the dissolved oxygen (which is assumed equal to zero in the influent flow). Follows that there is not need of an influent model and that with respect to the ASM1 and to the *Model6s* as well, there is not need of suspended solids measurements. In fact, the secondary settler model is a very simple model (always based on the Takács model) that with only a percentage of the R_{COD} considered particulate can represent the TSS concentration in the effluent and in the recycle line. Eventually, the CPU simulation time is also considerably reduced with respect to *Model6s* also.

4. FREQUENCY ANALYSIS

In the previous section, *Model6s* is considered as the starting point for *Model4s* development and the test motion analysis suggests a more detailed analysis in order to validate this assumption. This can be done by means of a frequency analysis that allows a representation of system's response to sinusoidal inputs at varying frequency that can be graphically analyzed using either *Bode plots* or *Singular value plots*. The considered frequency range is: $\omega \in [1e-1\ , 1e+3]\ (1/d)$, this means to consider a time range of 10 days to around 1.4 min.

In the first case, we look at the response to a singular sinusoidal input; for simplicity, only effluent COD is plotted in Figure 2, being the most representative of the system behavior. The gain plot displays the ratio of the output amplitude to the input one in *decibels* (dB) and the phase displays the time shift of the output in degrees. From Figure 2a, we note that at low frequency the gain of *Model4s* (dashed) is slightly different from that of *Model6s* (dot-dashed) and ASM1 (solid). This difference decreases when the frequency increases until circa 55 $(1/d)$, while for higher frequency the asymptote of the reduced models is quite different from that of the ASM1. The same considerations hold for the phase plot: a different phase lag behavior for *Model4s* is evident when it is compared to the other models. In Figure 2b influent flow rate variations are also considered (representing the absence of the equalization basin) and we note that *Model6s* presents the same gain of ASM1 in the whole frequency interval, while the simplest model shows a mismatch that increases at high frequency values. Conversely, the phase lag agreement between *Model4s* and ASM1 is good for frequency values lower than 1 $(1/d)$. Considering that the input frequency in a real plant is circa 1 $(1/d)$, we can conclude that the behavior of *Model4s* is satisfactory when the COD and flow rate are varied.

For the sake of completeness, frequency response for every influent concentration should be investigated for MIMO systems. This can be made with a singular value plot, which provides a means to generalize this information. Furthermore, by means of this plot effects of influent flow rate variations can be also explored in conjunction of the other input variations; we can consider in a more comprehensive way the presence or not of an equalization basin before the activated sludge process. In Figure 3a, the singular value plot for the effluent COD is considered when the equalized situation is occurring. We observe that the evidences noted in Figure 1a are justified by the singular value analysis; in fact we can note the different behavior of *Model4s* with respect to ASM1 and *Model6s*. The mismatch decreases when the frequency ranges in a small neighborhood of 1e1, but

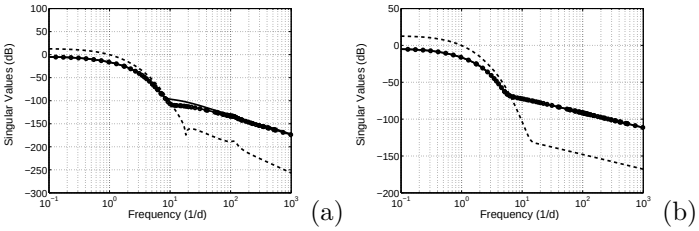

Fig. 3. Sigma plots non-varying (a) and varying (b) influent flow rate for models with 6 state variables (dot-dashed) and with 4 state variables (dashed) are compared with the ASM1 (solid).

then the difference between the simplest model and the others increases significantly. The same considerations hold by analyzing Figure 3b, which is in agreement with the results plotted in Figure 1.

5. CONCLUSIONS

In this work we considered the bioreactor model in an activated sludge process, and starting from the ASM1, we obtained a simpler model with only four state variables which is able to reconstruct the main effluent pollutant concentrations from a wastewater treatment plant. The simplest model, obtained by a modal reduction followed by physical consideration, is able to qualitatively and quantitatively, especially when an equalization basin is present, capture the main feature of the system dynamics and shows several advantages. In fact, it consists of only four state variables, five adjustable parameters, and describes the dynamics of variables, which can be directly measured in the plants.

REFERENCES

Chachuat, B., N. Roche and M. A. Latifi (2003). Reduction of the ASM1 model for optimal control of small-size activated sludge treatment plants. *Rev. Sci. Eau* **16**, 837–858. (In French).

Gómez-Quintero, C., I. Queinnec and J. P. Babary (2000). A reduced nonlinear model of an activated sludge process. In: *Int. Symp. on Advanced Control on Chemical Processes*. pp. 1037–1042. Pisa, Italy.

Henze, M., C. P. Leslie Grady, W. Gujer, G. V. R. Maris and T. Matsuo (1987). Activated sludge process model No. 1. Technical report. IAWQ Scientific and Technical Report 1.

Isaacs, S. and D. Thornberg (1998). A comparison between model and rule based control of a periodic activated sludge process. *Water Sci. Technol.* **37**(12), 343–351.

Jeppsson, U. and G. Olsson (1993). Reduced order models for on-line parameter identification of the activated sludge process. *Water Sci. Technol.* **28**(11/12), 173–183.

Mulas, M. (2006). Modelling and control of activated sludge processes. PhD thesis. Università di Cagliari.

Robertson, G. A. and I. T. Cameron (1997). Analysis of dynamic process models for structural analysis insight and model reduction - part 1. structural identification measures. *Comput. Chem. Eng.* **21**(5), 455–473.

Skogestad, S. and I. Postlethwaite (1998). *Multivariable feedback control*. John Wiley and Sons.

Smets, I. Y., V. J. Haegebaert, R. Carrette and J. F. Van Impe (2003). Linearization of the activated sludge model ASM1 for fast and reliable prediction. *Water Res.* **37**(8), 1831–1851.

Spérandio, M. and I. Queinnec (2004). Online estimation of wastewater nitrifiable nitrogen, nitrification and denitrification rates, using ORP and DO dynamics. *Water Sci. Technol.* **49**(1), 31–39.

Steffens, M. A., P. A. Lant and R. B. Newell (1997). A systematic approach for reducing complex biological wastewater treatment model. *Water Res.* **31**(3), 590–606.

Takács, I., G. G. Patry and D. Nolasco (1991). A dynamic model of the clarification-thickening process. *Water Res.* **25**(10), 1263–1271.

NOMENCLATURE

r	Continuation parameter
$\mathbf{A}$	Linearized system matrix
COD	Chemical Oxygen Demand
Q	Volumetric Flowrate
TKN	Total Kjeldahl Nitrogen
TSS	Total Suspended Solids
f_{NH}	Ammonia/TKN ratio
	ASM1 State Variables
S_I	Soluble inert organic matter
X_I	Particulate inert organic matter
S_S	Readily biodegradable substrate
X_S	Slowly biodegradable substrate
X_{BH}	Active heterotrophic biomass
X_{BA}	Active autotrophic biomass
X_P	Particulate products from biomass decay
S_O	Oxygen
S_{NO}	Nitrate and nitrite nitrogen
S_{NH}	Free and ionized ammonia nitrogen
S_{ND}	Soluble biodegradable organic nitrogen
X_{ND}	Particulate biodegradable organic nitrogen