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PARAMETRIC SENSITIVITY AND EVALUATION OF A DYNAMIC MODEL FOR SINGLE-STAGE WASTEWATER TREATMENT PLANT

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Abstract

Simulation models of the activated sludge process are believed to be a useful tool for research, process optimisation and troubleshooting at full-scale treatment plants, teaching and design assistance. However, the application of the models in most treatment plants is limited due to a lack of advanced input parameter values required by the models. Although the numbers of typical conversion factors and stoichiometric constants are presented in the literature, the range of some parameters is too wide considering the parametric sensitivity of the dynamic model. On the other hand, it is well known that the values of some parameters depend on the nature of a specific wastewater treatment plant.

The present paper is concerned with a dynamic model of the activated sludge process taking place in the single stage wastewater treatment plant with parametric sensitivity and evaluation. Model calibration was successfully experimentally confirmed for the steady-state operational conditions.

Introduction

Activated sludge is a complex dynamic process and simulation of such system must necessarily account for a large number of reactions between a large number of components. Successful process modeling requires good knowledge of process variables such as the most influential kinetic and stoichiometric parameters and the resulting biomass composition. Model parameters and state estimation associated with modern control studies based on the available noisy process measurements.

Dedicated to the memory of Prof. Dr. Jože Šiftar.

The parameters of biological models usually vary with environmental conditions and need to be frequently updated through on- and off-line algorithms [1]. An alternative parameter approach is via laboratory analysis. These procedures of the IAWPRC Activated Sludge Model I [2] are presented in Ekama *et* al. [3,4]. However, an important aspect of instrumentation theory is that measurements are never deterministic variables, since they always involve random noise as well as experimental random errors [5]. On the other hand, many authors discuss various nonlinear numerical estimation methods (Bayesian estimation method – [6]; Maximum Likelihood methods – [7]). Kabouris and Georgakakos [1] presented a continuous process model formulation in state-space form. The model is discretized to allow for different time-steps in numerical integration and measurements acquisition. They presented the measurement model, including the relationship between measured quantities and model state variables, followed by development of the Linearized Maximum Likelihood (LML) algorithm.

In this study attempts were made to present the dynamic model for activated sludge process taking place in a pilot single-stage wastewater treatment plant. Efforts were made to simplify the parameter evaluation procedure. The calibration of the dynamic model was successfully experimentally confirmed.

Experimental

The laboratory at Vodovod-Kanalizacija Ltd., Ljubljana, monitors daily the activated sludge process of a pilot single-stage wastewater treatment plant with reactor volume, V_1 = 1.585 m^3, and settler volume, V_2 = 0.709 m^3 (Figure 1). For the purpose of this work, some additional analyses were made. The concentrations of autotrophic nitrifying biomass, X_A, heterotrophic biomass, X_H, activated sludge concentration, inlet and outlet ammonium, A, dissolved oxygen, S_O, and the concentration of inlet and outlet substrate (in g COD m^{-3}), S_{COD}, were determined by standard methods (Standard Methods for Water and Wastewater, 19th Edition, AWWA, Washington d.c., 1995): SIST ISO 6060, SM 4500-NH3C, SM 2540 D, SM 2540 E. The average measured values with deviations for the period from 4 to 20 July 1998 are presented in Table 1.

Table 1. The average measured values of process parameters for period from 4 to 20 July 1998 (source: *JP Vodovod Kanalizacija Ltd., Ljubljana).*

Q_0 (inlet flow)	$0.263 \pm 0.001 m^3 h^{-1}$
S_O	3.6 ± 1.0 gO_2 m^{-3}
$S_{COD,0}$ (inlet)	416 ± 50 g *COD* m^{-3}
A_0 (inlet)	16.1 ± 6.0 g$N\text{-}NH_4^+$ m^{-3}
$S_{COD,2} = S_{COD,1}$ (outlet)	42 ± 10 g *COD* m^{-3}
$A_2 = A_1$ (outlet)	0.5 ± 0.2 g$N\text{-}NH_4^+$ m^{-3}
$X_{H,1}$	3104 g m^{-3}
$X_{A,1}$	96 g m^{-3}
Activated sludge concentration	4920 ± 400 g m^{-3}
Biomass fraction	65 %

* 1 – reactor, 2 - settler

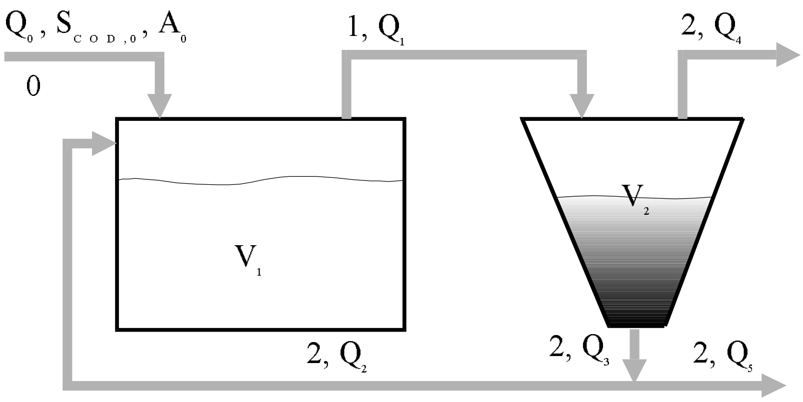

Figure 1. Sketch of the single-stage wastewater treatment plant.

Simulation Model

Considering the mass balances of substrate, ammonium, autotrophic and heterotrophic biomass for the single-stage wastewater treatment plant (Figure 1), the following set of linear differential equations is obtained, separately for the reactor and the settler [1,2,8]:

♦ *reactor*

$$V_1 \frac{dS_{COD,1}}{dt} = Q_0 S_{COD,0} + Q_2 S_{COD,2} - Q_1 S_{COD,1} - \frac{R_H V_1}{Y_H} \tag{1}$$

$$V_1 \frac{dX_{H,1}}{dt} = Q_2 X_{H,2} - Q_1 X_{H,1} + R_H V_1 - b_H X_{H,1} V_1 \tag{2}$$

$$V_1 \frac{dA_1}{dt} = Q_0 A_0 + Q_2 A_2 - Q_1 A_1 - \frac{R_A V_1}{Y_A} - i_X R_H V_1 - i_X R_A V_1 \tag{3}$$

$$V_1 \frac{dX_{A,1}}{dt} = Q_2 X_{A,2} - Q_1 X_{A,1} + R_A V_1 - b_A X_{A,1} V_1 \tag{4}$$

♦ *settler*

$$V_2 \frac{dS_{COD,2}}{dt} = Q_1 S_{COD,1} - Q_3 S_{COD,2} - Q_4 S_{COD,2} \tag{5}$$

$$V_2 \frac{dX_{H,2}}{dt} = Q_1 X_{H,1} - Q_3 X_{H,2} \tag{6}$$

$$V_2 \frac{dA_2}{dt} = Q_1 A_1 - Q_3 A_2 - Q_4 A_2 \tag{7}$$

$$V_2 \frac{dX_{A,2}}{dt} = Q_1 X_{A,1} - Q_3 A_{A,2} \tag{8}$$

Aerobic growth of heterotrophs and autotrophs:

$$R_H = \mu_{max,H} \left(\frac{S_{COD,1}}{S_{COD,1} + K_S} \right) \left(\frac{S_O}{S_O + K_{O,H}} \right) X_{H,1} \tag{9}$$

$$R_A = \mu_{max,A} \left(\frac{A_1}{A_1 + K_A} \right) \left(\frac{S_O}{S_O + K_{O,A}} \right) X_{A,1} \tag{10}$$

Flow rates, as shown in Figure 1, can be described:

$$Q_1 = Q_0 + Q_2 \tag{11}$$

$$Q_2 = Q_0 - \frac{Q_0 \left[(S_{COD,0} - S_{COD,1}) Y_H + (A_0 - A_1) Y_A \right]}{(X_{H,1} + X_{A,1})} + \frac{b_H X_{H,1} V_1}{(X_{H,1} + X_{A,1})} + \frac{b_A X_{A,1} V_1}{(X_{H,1} + X_{A,1})} \tag{12}$$

$$Q_5 = \frac{Q_0 \left[(S_{COD,0} - S_{COD,1}) Y_H + (A_0 - A_1) Y_A \right]}{2(X_{H,1} + X_{A,1})} - \frac{b_H X_{H,1} V_1 + b_A X_{A,1} V_1}{2(X_{H,1} + X_{A,1})} = \frac{Q_0 - Q_2}{2} \tag{13}$$

$$Q_3 = Q_2 + Q_5 \tag{14}$$

$$Q_4 = Q_1 - Q_3 \tag{15}$$

The flow equations for recycle, Q_2 (eq 12), and sludge wastage, Q_5 (eq 13), are obtained considering the basic flow relation (eq 11) and the mass balances for heterotrophic and autotrophic biomass. In addition, the following conditions are applied:

$$X_{H,2} = 2X_{H,1} \text{ and } X_{A,2} = 2X_{A,1}, \tag{16}$$

In the described algorithm all flows ($Q_{1\text{-}5}$, (m^3h^{-1})) are time dependent.

Table 2. Definition and typical values for the kinetic and stoichiometric coefficients, used in our model (Hence *et al.*, 1994).

Temperature	20 ^{0}C	10 ^{0}C	Units
$\mu_{max,H}$ = *Maximum growth rate (heterotrophic org.)*	*6.0*	*3.0*	*day^{-1}*
$\mu_{max,A}$ = *Maximum growth rate (autotrophic org.)*	*1.0*	*0.35*	*day^{-1}*
b_H = *Heterotrophic decay rate*	*0.4-0.2*		*day^{-1}*
b_A = *Decay rate for nitrifiers*	*0.15-0.05*		*day^{-1}*
K_S = *Substrate half saturation*	*4 – 20*		*g COD m^{-3}*
K_A = *Ammonia half saturation*	*1*		*g N m^{-3}*
$K_{O,H}$ = *Oxygen half saturation (heterotrophic org.)*	*0.2*		*gO_2 m^{-3}*
$K_{O,A}$ = *Oxygen half saturation (autotrophic org.)*	*0.5*		*gO_2 m^{-3}*
Y_H = *Heterotrophic yield coefficient*	*0.63*		*gCOD(gCOD^{-1})*
Y_A = *Autotrophic yield coefficient*	*0.24*		*gCOD(gN^{-1})*
i_X = *N content of biomass*	*0.07*		*gN (gCOD)$^{-1}$*

The model can now be solved by an appropriate numerical method, using the literature data on the kinetic and stoichiometric parameters (Table 2). However, in order to get acceptable agreement between the measured (Table 1) and predicted sludge process, numerical estimation of some parameters is necessary. To simplify this procedure, considering that the experiments were performed at steady-state conditions, the dynamic model was rebuilt for the case of steady-state operation. In this way, the set of differential equations (1-8) becomes a set of ordinary equations and the equations for flow rates (11-15) become time independent. On the basis of the experimental values of sludge process variables (Table 1) and by using some of the parameters from literature

(Y_H, Y_A, $K_{O,H}$, $K_{O,A}$, K_A) the estimation of other parameters ($\mu_{max,H}$, $\mu_{max,A}$, b_H, b_A, i_X) can be obtained by steady-state model calibration, using an appropriate numerical method. However, it was found again that the parametric sensitivity of the simplified model is still very high and we are unable to simply calibrate the parameters with ordinary numerical methods, built in a powerful mathematical package (Mathematica 3.0). The following iterative procedures was eventually found as most effective and successful method for model calibration:

a) Some parameters (Y_H, Y_A, $K_{O,H}$, $K_{O,A}$, K_A) were adopted from literature (Table 2).
b) The assumed value for K_S can be found in the literature (Table 2) as the initial value for calibration. The study of parametric sensitivity of the dynamic model has shown that the influence of K_S (*in range 4-60 gCOD* m^{-3}) on system stability is negligible in our case. On the other hand, the linear dependence of K_S on evaluation of the maximum growth rate of heterotrophic organisms can be obtained (Eq. 18: $\mu_{max,H}[K_S=4\ gCOD\ m^{-3}] = 0.0146\ h^{-1}$; $\mu_{max,H}[K_S=60\ gCOD\ m^{-3}] = 0.0324\ h^{-1}$).
c) The assumed value for i_X can be found in the literature (*0.07 gN* $(gCOD)^{-1}$, Table 2) as the initial value for calibration.
d) The assumed value for b_A can also be found in the literature (*0.0063-0.002* h^{-1}, Table 2) as the initial value for calibration (*0.002* h^{-1}).
e) The value for heterotrophic decay rate, b_H, is calculated from the following equation (Eq. 17):

$$b_H = b_A + \left(\frac{Q_0 (S_{COD,0} - S_{COD,1}) Y_H}{V_1 \cdot X_{H,1}} \right) - \left(\frac{Q_0 (A_0 - A_1) Y_A}{V_1 \cdot X_{A,1}} \right), \tag{17}$$

which can be obtained by equalizing equations 1 and 2 arranged for steady-state, considering a simple flow relation (Eq. 11), substrate concentration equality ($S_{COD,1}$=$S_{COD,2}$), and condition $X_{H,2}=2X_{H,1}$ (Eq. 16).

f) The value for maximum growth rate of heterotrophic organisms, $\mu_{max,H}$, can now be calculated from the equation (Eq. 18):

$$\mu_{\max,H} = \left(\frac{Q_0\left(S_{COD,0} - S_{COD,1}\right)Y_H}{X_{H,1}\cdot V_1}\right)\left(\frac{S_O + K_{O,H}}{S_O}\right)\left(\frac{S_{COD,1} + K_S}{S_{COD,1}}\right), \tag{18}$$

which is derived from the mass balance of heterotrophic organisms (Eq. 2) arranged for steady-state operation, considering again the simple flow relation (Eq. 11), substrate concentration equality ($S_{COD,1}$=$S_{COD,2}$), and condition $X_{H,2}$=$2X_{H,1}$ (Eq. 16). Finally, equation 18 is obtained after simple mathematical procedures considering the expressions for b_H (Eq. 17) and Q_2 (Eq. 12).

g) The maximum value of N content of biomass, $i_{X,max}$, is determined from the condition of positive growth rate at defined operational conditions (see Eq. 21):

$$i_X \le i_{X,\max} = \frac{Q_0\left(A_0 - A_1\right)}{R_H V_1}. \tag{19}$$

If the initial value of i_X is bigger than $i_{X,max}$, the procedure is then repeated from step c) until satisfying system solution (Eq. 22). The study of parametric sensitivity of the dynamic model has shown that the influence of i_X on system stability is very high. After a number of iterations the final value, $i_X = 0.001\ gN\ (gCOD)^{-1}$, was found for our experimental conditions at which the system error is negligible.

h) The value for the maximum growth rate of autotrophic organisms, $\mu_{max,A}$, can be calculated from the equation (Eq. 20):

$$\mu_{\max,A} = \frac{\left[Q_0\left(A_0 - A_1\right)Y_A - i_X Q_0\left(S_{COD,0} - S_{COD,1}\right)Y_H Y_A\right]\left(A_1 + K_A\right)\left(S_O + K_{O,A}\right)}{X_{H,1} A_1 S_O V_1\left(1 + i_X Y_A\right)}, \tag{20}$$

which is derived from the mass balance of ammonium (Eq. 3) arranged for steady-state operation, considering again the simple flow relation (Eq. 11), ammonium concentration equality (A_1=A_2), and condition $X_{A,2}$=$2X_{A,1}$ (Eq. 16). After some simple arrangements, R_A can be expressed:

$$R_A = \frac{Q_0\left(A_0 - A_1\right)Y_A}{V_1\left(1 + i_X Y_A\right)} - \frac{i_X R_H V_1 Y_A}{V_1\left(1 + i_X Y_A\right)}, \tag{21}$$

and by replacing the growth rate of heterotrophs, R_H with Equation 9 considering the expression for $\mu_{max,H}$ (Eq. 18), Equation 20 can be obtained.

i) The system error considering the initial value of b_A can be determined from the following equation (Eq. 22):

$$0 = Q_2 X_{A,2} - Q_1 X_{A,1} + R_A V_1 - b_A X_{A,1} V_1, \qquad (22)$$

which is derived from the mass balance of autotrophic organisms (Eq. 4) arranged for steady-state operation. From Equation 22 the new value for b_A can be obtained. The procedure is then repeated from step d) to i) until reaching system solution.

Results and Discussion

On the basis of the described method the calibrated parameters defined for steady-state activated sludge process taking place in a pilot single-stage wastewater treatment plant (Table 1) can now be used for successful process simulation based on the dynamic model (Eq. 1- 16). The calibrated parameters used in the dynamic model are presented in Table 3.

Table 3. Estimated and typical literature values for some kinetic and stoichiometric coefficients (Hence *et al.*, 1994).

Parameter	Steady-state model calibration	Literature data	Units
b_H	*0.0079*	*0.008-0.016*	h^{-1}
b_A	*0.0018*	*0.002-0.006*	h^{-1}
i_X	*0.001(0.066)*	*0.07*	$gN\ (gCOD)^{-1}$
$\mu_{max,H}$	*0.0146(0.0324)*	*0.125-0.25*	h^{-1}
$\mu_{max,A}$	*0.0218*	*0.015-0.042*	h^{-1}

The substantial deviation can be seen for $i_X = 0.001$ and $\mu_{max,H} = 0.0146$ in case the system calibration error is practically zero. However, for practical purposes which still allowed stability of the system (system error determined from Eq. 22 is -0.015) at acceptable agreement with experimental data, the value $0.066\ gN\ (gCOD)^{-1}$ for i_X and the value $0.0324\ h^{-1}$ for $\mu_{max,H}[K_S=60\ gCOD\ m^{-3}]$ were calculated. Some examples of dynamic model experimental confirmation for the single-stage wastewater treatment plant (*JP Vodovod Kanalizacija Ltd., Ljubljana*) are presented in Figures 2 and 3. It is quite remarkable that the dynamic model predictions are in agreement with the experimental data for steady-state activated sludge process. Some dynamic simulations of the activated sludge process are presented in Figures 4-7 for sinuous and “real” disturbances of inlet wastewater flow.

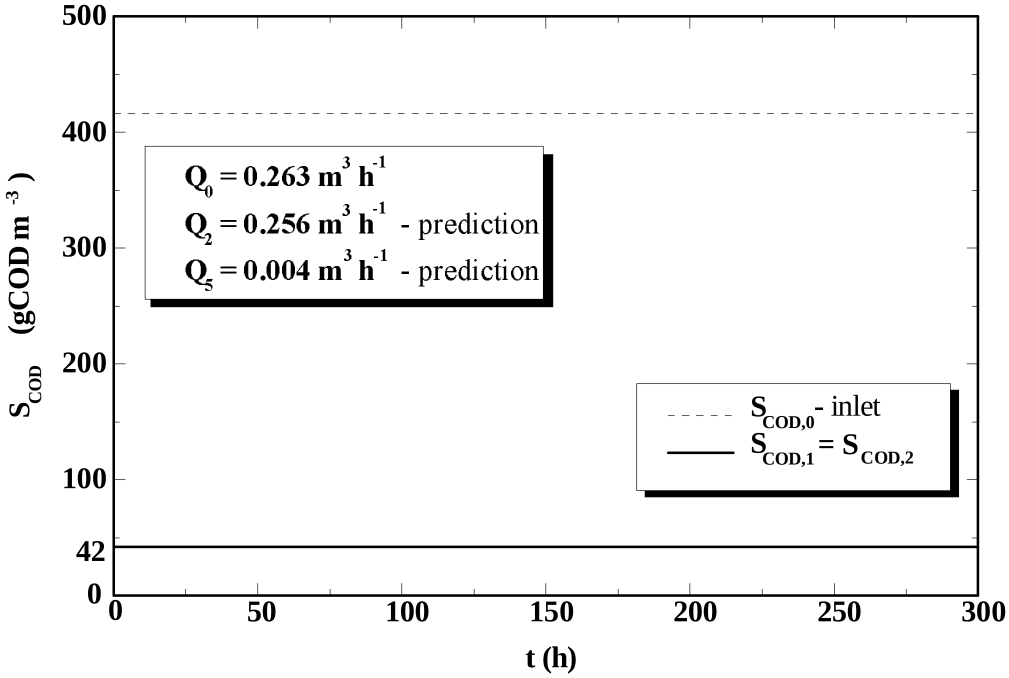

Figure 2. Dynamic model prediction of substrate concetration for the steady-state activated sludge process taking place in a single-stage wastewater treatment plant.

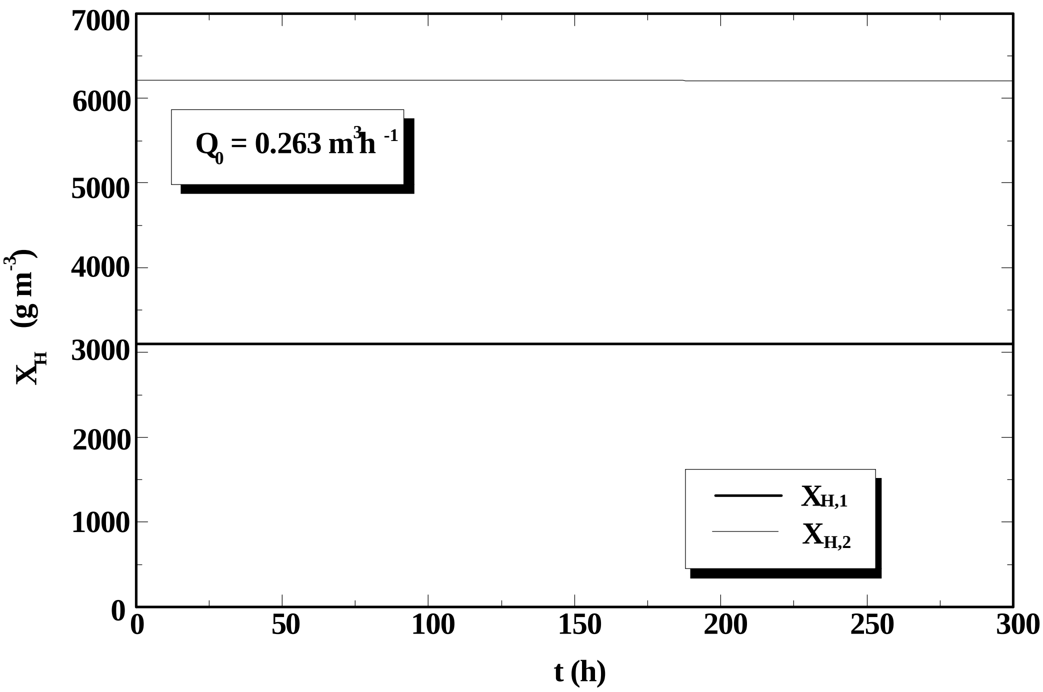

Figure 3. Dynamic model prediction of heterotrophs for the steady-state activated sludge process taking place in a single-stage wastewater treatment plant.

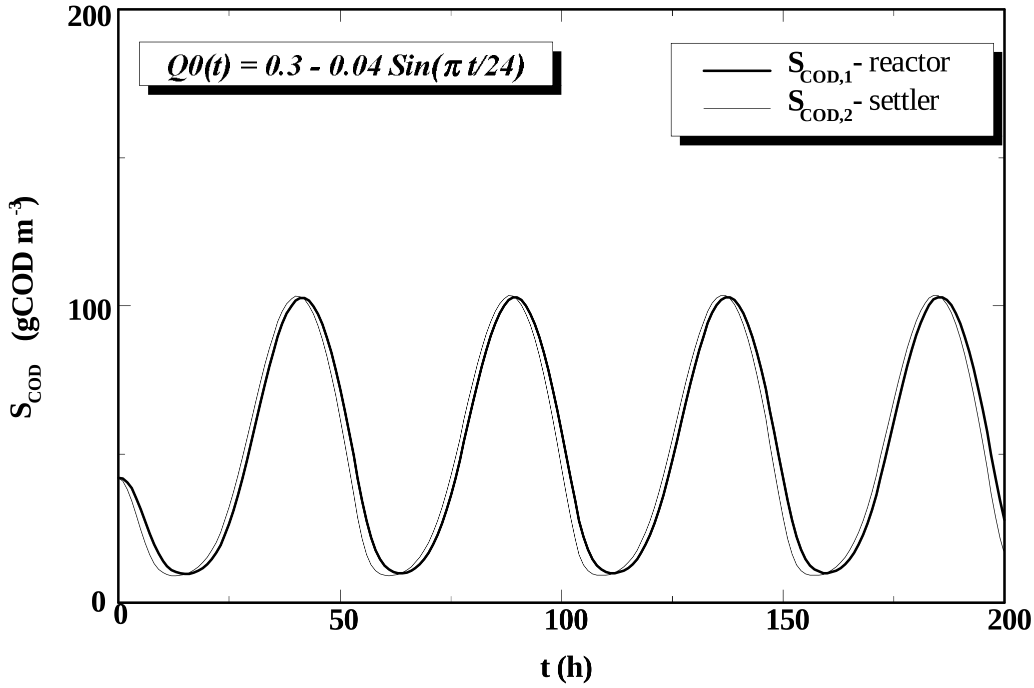

Figure 4. Dynamic response of substrate concentration in the reactor and settler at sinuous simulation of inlet wastewater flow.

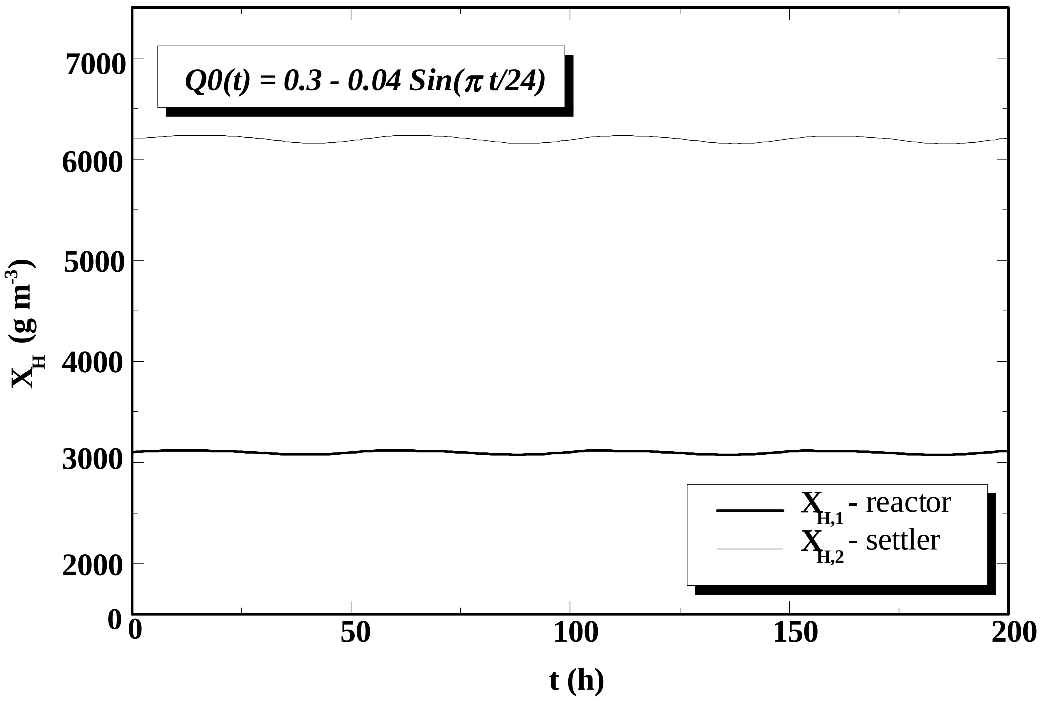

Figure 5. Dynamic response of heterotrophs concentration in the reactor and settler at sinuous simulation of inlet wastewater flow.

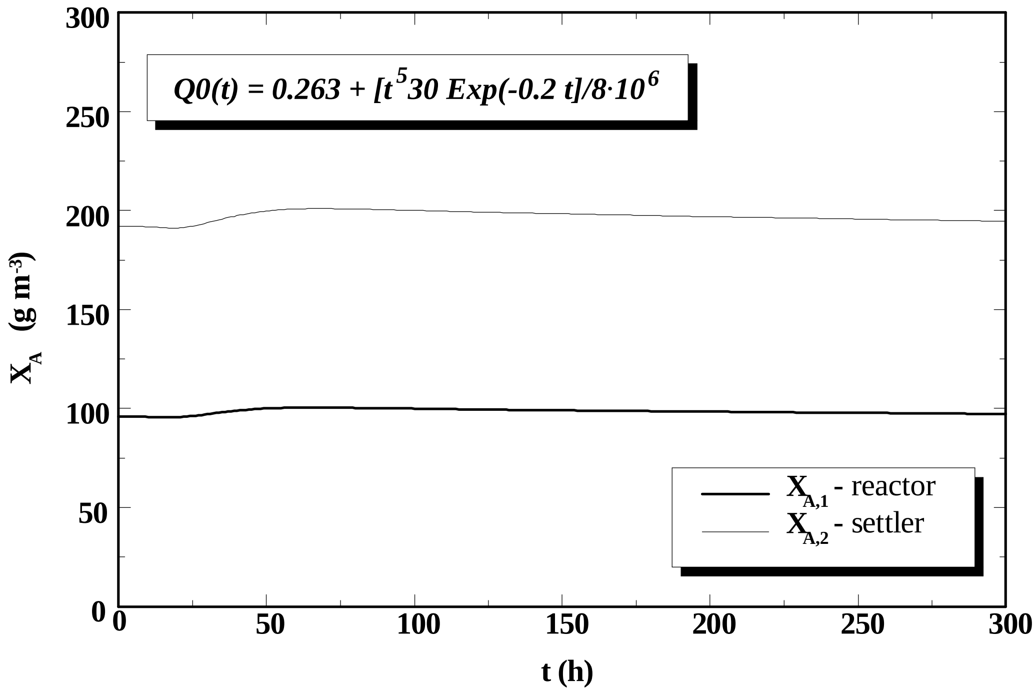

Figure 6. Dynamic response of ammonium concentration in the reactor and settler at simulation of “real” two-day disturbation of inlet wastewater flow.

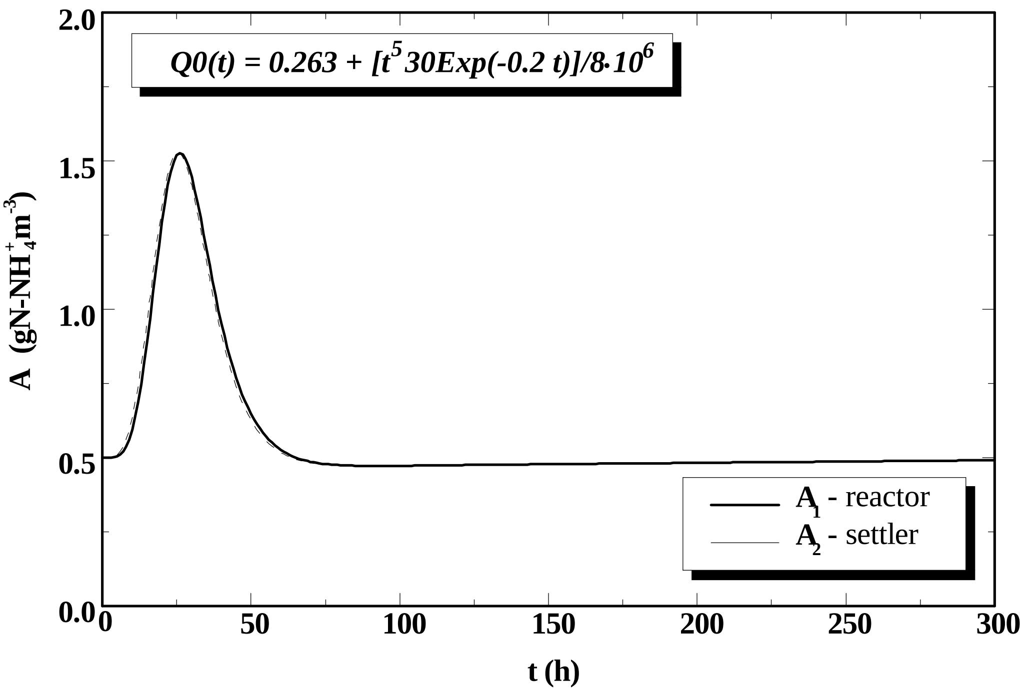

Figure 7. Dynamic response of autotrophs in the reactor and settler at simulation of “real” two-day disturbation of inlet wastewater flow.

Conclusions

A mathematical model of the activated sludge process taking place in a pilot single-stage wastewater treatment plant was built. A relatively simple procedure for kinetic and stoichiometric coefficients evaluation is proposed. The dynamic model calibration was successfully experimentally confirmed for steady-state operational conditions.

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Povzetek

Simulacijski modeli čistilnih naprav so zelo uporabna orodja pri optimiranju obstoječih in pri načrtovanju in optimiranju novih čis tilnih naprav. Prav tako je lahko matematični model v veliko pomoč pri razumevanju kompleksnih procesov čiščenja, izobraževanju in treningu, kot tudi pri uvajanju automatizacije procesov. Vendarle, pa je uporaba modela za večino čistilnih naprav omejena s poznavanjem vrednosti nekaterih parametrov, ki jih zahteva model. Čeprav v literaturi obstaja precej eksperimentalno določenih podatkov za posamezne parametre pa lahko ugotovimo, da je razpon objavljenih vrednosti nekaterih parametrov zelo širok. Po drugi strani pa je parametrična občutljivost dinamičnega modela izredno velika. Uveljavilo se je spoznanje, da vrednost nekaterih parametrov v veliki meri zavisi od narave določene čistilne naprave.

Pričujoče delo predstavlja dinamični model enostopenjske čistilne naprave, ki je bil uspešno testiran na pilotni čistilni napravi Ljubljana. Pri študiju smo posebno pozornost namenili določitvi realnih parametrov za posamezno čistilno napravo in parametrični občutljivosti dinamičnega modela.