Dynamic modelling of activated sludge process
II. Linearized kinetic models

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In this paper the transient behaviour of an activated sludge process is studied. A simplified model using a linearization solution method, is verified and compared with a nonlinear one. Some qualitative evaluation of system responses to a step feed concentration change is presented. The model availability in the elaboration of the process control strategy is discussed.

В этой статье разбирается динамика процесса аэрации с активным илом. Проверяется упрощенная математическая модель при использовании метода линеаризации и сравнивается с нелинейной моделью. Приводится качественная оценка отклика системы на использование ступенчатого изменения концентрации субстрата во входном потоке. Обсуждается возможность использования модели для составления стратегии управления процесса.

Mathematical models are useful for the treatment process design and are particularly helpful for evaluation and control of activated sludge process. There are many different approaches to mathematical modelling of this process in literature. The wide-spread one is based on using kinetic equation originally formulated to describe processes involving pure cultures of microorganisms that metabolize a single organic compound. This continuous cultivation theory has been extended to describe the activated sludge process even though a many types of microorganisms and a waste water with many different soluble and nonsoluble organic compounds are presented. Thus, microbial growth is usually described with a Monod equation or modified Monod equation in term of endogenous decay coefficient [1, 2]. Although the inconvenience of this approach has been claimed [3—5] the approach of many authors [1, 2, 6—8] is still based on this concept. The Michaelis—Menten equation for kinetics of substrate removal is usually used, but also kinetic equations analogous to chemical kinetics have been employed [2, 8]. Some other kinetic equations of substrate utilization have been published by *Fair* [9], *Grau* [10], *Vavilin* [11], and Moser [12].

The common feature of the majority of activated sludge mathematical modelling approaches consists in steady-state process consideration. However, this assumption is rarely valid in real process operation realizing the complexity of activated sludge process. Therefore the attention of many investigators has been focused on the dynamic behaviour of activated sludge process.

In the previous paper [13] we presented the results of dynamic modelling of the activated sludge process using nonlinear kinetic models of Michaelis—Menten and Monod type. One of the reasons for dynamic modelling of activated sludge process, which could lead to useful applications, is the process identification and an adaptive control strategies elaboration in order to improve the plant treatment efficiency.

The major object of this research is to develop and verify the linearized dynamic model of activated sludge process. Another aim is the qualitative evaluation of system response to a step shock change in feed concentration.

Theoretical

Mathematical model

In the previous paper [13] we presented a simplified mathematical model of activated sludge process based on material balances for substrate

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \Theta^{-1}(S_0 - S) + r_s \tag{1}$$

and biomass

$$\frac{\mathrm{d}X}{\mathrm{d}t} = r_g - \frac{V_x}{V_a} X \tag{2}$$

The rate of the substrate utilization r_s was expressed by the equation

$$r_s = -\frac{\mu_{max}}{Y_{obs}} \frac{XS}{K_s + S} \tag{3}$$

For biomass growth rate description, we adapted both the Monod equation

$$r_g = \mu_{max} \frac{XS}{K_s + S} \tag{4}$$

and a modified Monod equation expressed by

$$r_g = \mu_{max} \frac{XS}{K_s + S} - k_d X \tag{5}$$

The explicit fourth-order Runge—Kutta—Merson method has been used to integrate the set of nonlinear differential equations (*1*) and (*2*). In this paper the method of linearization using the Taylor series [14] is used, and as a result of this approach the computational time is reasonably reduced.

The oscillation of substrate and biomass concentration values ranging above and below new steady-state values, after the step change of the feed concentration employed, has been considered. Thus, the set of linear differential equations for the deviations S_l and X_l from steady-state substrate concentration S_u and biomass concentration X_u has been obtained. The matrix form of these equations can be written as

$$\frac{d}{dt}\begin{pmatrix} S_l \\ X_l \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} S_l \\ X_l \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \tag{6}$$

where

$$S_l = S - S_u$$
$$X_l = X - X_u$$

Solution and computing methods

An analytical solution of the differential equations set (*6*) has the form [15]

$$\begin{aligned} S_l(t) &= c_1 e^{\lambda_1 t} + c_2 e^{\lambda_2 t} + A \\ X_l(t) &= c_1 \eta_{12} e^{\lambda_1 t} + c_2 \eta_{22} e^{\lambda_2 t} + B \end{aligned} \tag{7}$$

After substituting the following initial conditions

$$S_l = 0 \quad X_l = 0 \quad \text{for } t = 0 \tag{8}$$

in eqn (*7*) we get

$$\begin{aligned} c_1 &= \frac{-A\eta_{22} + B}{\eta_{22} - \eta_{12}} \\ c_2 &= \frac{-B + A\eta_{12}}{\eta_{22} - \eta_{12}} \end{aligned} \tag{9}$$

Values λ_1 and λ_2 were obtained by the formula

$$\lambda_{1,2} = \frac{a_{11} + a_{22}}{2} \pm \frac{1}{2}(a_{11}^2 - 2a_{11}a_{22} + 4a_{21}a_{12} + a_{22}^2)^{\frac{1}{2}} \tag{10}$$

Following the linear differential equations by the solution method [15] the expressions for η_{12} and η_{22} vector components have also been obtained

$$\eta_{12} = -\frac{a_{11} - \lambda_1}{a_{12}}$$
$$\eta_{22} = -\frac{a_{11} - \lambda_2}{a_{12}} \tag{11}$$

For a step type of the feed substrate concentration change we get particular solution of differential equations set (*6*) in the form

$$A = \frac{-b_1 a_{22} + b_2 a_{12}}{a_{11}a_{22} - a_{12}a_{21}}$$
$$B = \frac{-b_2 a_{11} + b_1 a_{21}}{a_{11}a_{22} - a_{12}a_{21}} \tag{12}$$

Inserting eqns (*3*) and (*4*) into eqns (*1*) and (*2*) and applying the above solution procedure leads to

$$a_{11} = -\Theta^{-1} - \left[\frac{\mu_{\text{max}}}{Y_{\text{obs}}}\left(\frac{X_{\text{u}}}{K_{\text{s}} + S_{\text{u}}} - \frac{S_{\text{u}}X_{\text{u}}}{(K_{\text{s}} + S_{\text{u}})^2}\right)\right]$$
$$a_{12} = -\frac{\mu_{\text{max}}}{Y_{\text{obs}}}\frac{S_{\text{u}}}{K_{\text{s}} + S_{\text{u}}}$$
$$a_{21} = \frac{\mu_{\text{max}}X_{\text{u}}}{K_{\text{s}} + S_{\text{u}}} - \frac{\mu_{\text{max}}S_{\text{u}}X_{\text{u}}}{(K_{\text{s}} + S_{\text{u}})^2} \tag{13}$$
$$a_{22} = -\frac{V_{\text{x}}}{V_{\text{a}}} + \mu_{\text{max}}\frac{S_{\text{u}}}{K_{\text{s}} + S_{\text{u}}}$$

and

$$b_1 = \Theta^{-1}(S_0 - S_{\text{u}}) - \frac{\mu_{\text{max}}}{Y_{\text{obs}}}\frac{S_{\text{u}}X_{\text{u}}}{K_{\text{s}} + S_{\text{u}}} \tag{14}$$

$$b_2 = -\frac{V_x}{V_a} X_u + \frac{\mu_{max} S_u X_u}{K_s + S_u}$$

By the same solution method one can obtain

$$a_{22} = \frac{\mu_{max} S_u}{K_s + S_u} - k_d - \frac{V_x}{V_a} \tag{15}$$

$$b_2 = -\frac{V_x}{V_a} X_u - k_d X_u + \frac{\mu_{max} S_u X_u}{K_s + S_u} \tag{16}$$

when applying a modified Monod equation (*5*). The forms of expressions for evaluation of other matrix components are identical to those described above, *i.e.* eqns (*13*) and (*14*). The simplex optimization technique [16] has been applied to determine the parameter values of kinetic equations (*3*) and (*4*) or (*5*). Minimization function has the form

$$\omega = \sum_{i=1}^{M} [(S_{exp} - S_{calc})^2 + (X_{exp} - X_{calc})^2] \tag{17}$$

Results and discussion

The experiments were performed in laboratory equipment of an activated sludge process. The details of this technique, the operational parameters and analytical methods used were presented in our previous paper [13]. The shock step changes of substrate concentration in the feed were carried out in order to simulate experimentally and mathematically transient behaviour of the process.

Different system responses to shock load imposed have been observed for individual variables examined during the experimental runs. As shown in Fig. 1, there is a time delay in COD concentration system response obvious and evident COD concentration increase in outlet of the system. Fig. 2 illustrates the instantaneous biomass concentration response to twofold decrease of biomass load in the inlet of the system. During the first 14 days of transient run the biomass concentration X reached the minimum. An oscillating behaviour above and below the new steady-state biomass concentration value was observed in the following stage of the experiment. The new steady-state was judged to be reached more than 25 days after shock load was imposed. The average biomass concentration value during the steady-state behaviour was 3.39 kg m^{-3} and the standard deviation 0.093 kg m^{-3}. The corresponding average biomass concentration before substrate concentration step change carried out was 6.2 kg m^{-3} and the standard deviation 0.083 kg m^{-3}. A twofold increase of substrate

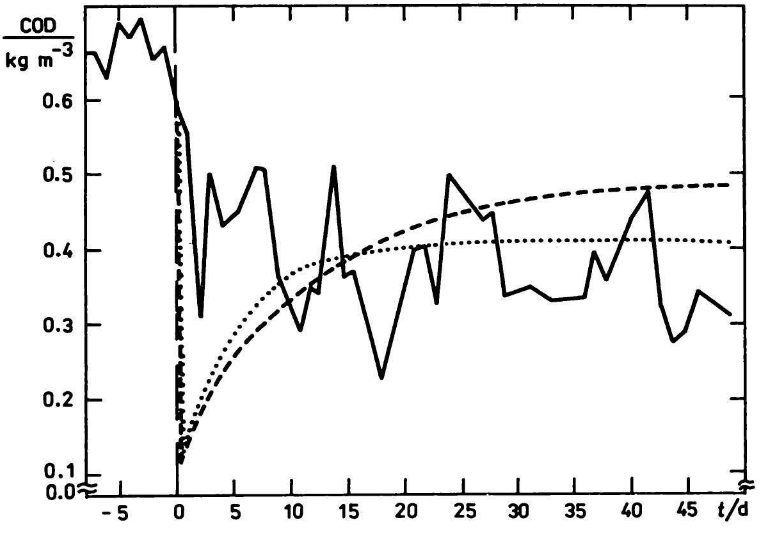

Fig. 1. COD concentration responses of activated sludge process to twofold decreasing of feed concentration.
——— Experimental; – – – calculated using Monod equation; ······ calculated using modified Monod equation.

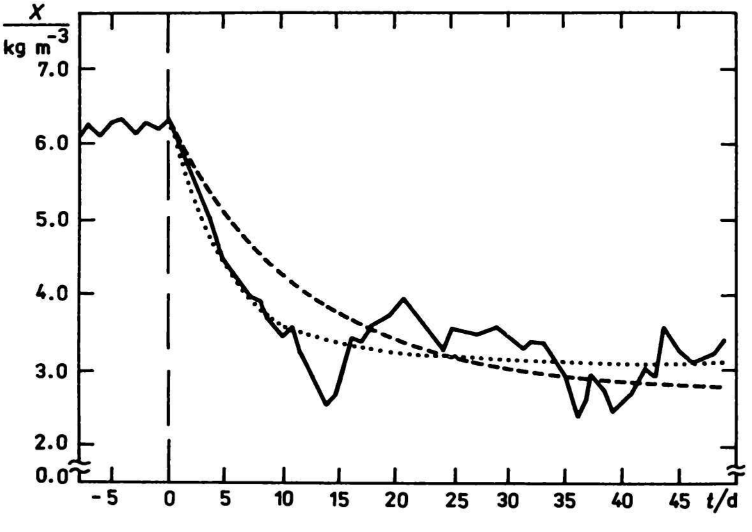

Fig. 2. Biomass concentration responses of activated sludge process to twofold decreasing of feed concentration.
——— Experimental; – – – calculated using Monod equation; ······ calculated using modified Monod equation.

concentration in the feed was achieved in the next experimental run. A more expressive COD response was observed. In less than four days after the shock was carried out, COD concentration in the aerated tank increased significantly with treatment efficiency decreasing to 65 %. An instantaneous biomass concentration system response was observed in this run. New steady-state was obtained in 18 days after step change. The average biomass concentration value in the next 10 days of run was 6.15 $kg\,m^{-3}$ and the standard deviation value 0.0319 $kg\,m^{-3}$. There is a close fit of average biomass concentration with those maintained before the first transient experimental run referred to above. In less than 10 days after shock imposed, changes of biomass colour and flocs macroscopic appearance were observed. After new steady-state was reached the initial biomass colour was observed, but no changes in magnitude of sludge flocs had occurred. Little foaming was observed during this transient experimental run.

Responses observed in actual experiments were compared to those predicted using linearized models derived in the previous stage of this paper. In Figs. 1 and 2 calculated profiles *vs.* time of both the outlet substrate concentration and biomass concentration are plotted. The optimal parameter values for both Monod and modified Monod equations obtained using the analytical solution in connection with simplex optimization method are summarized in Table 1. Identically, as stated in our previous work, the greatest differences between experimental and simulated values were observed during the first stage of the experimental run in the case of COD responses. On the other hand, there is a very good average fit of experimental biomass concentration profile and those calculated, using the modified Monod equation (*5*) for biological growth in connection with eqn (*3*), for substrate utilization.

Table 1

Biokinetic parameter values

Kinetic model	Parameters				
	$\frac{\mu_{max}}{d^{-1}}$	Y_{obs}	$\frac{K_s}{kg\,m^{-3}}$	$\frac{k_d}{d^{-1}}$	ω eqn (*17*)
Monod eqn (*4*)	0.25	0.21	0.72	—	17.51
Modified Monod eqn (*5*)	0.95	0.68	0.71	0.19	7.52

The highest value of the minimization function was obtained applying the Monod equation (*4*) for biological growth based on the comparison of results obtained using both linearized and nonlinear solution methods of dynamic model equations. These results provide evidence that also linearized Monod kinetic equation is inadequate for predicting actual transient responses in biomass and substrate concentrations. The best agreement between experimental and computer-simulated responses was obtained using a modified Monod equation, which is comparable with those obtained using nonlinear solution procedure. The disadvantage of linearized modified Monod model is the high value of yield coefficient Y_{obs}. Experimental values of this parameter obtained during the performed dynamic measurements were in the range of 0.1—0.36 of COD. In the consequence of this fact it is convenient to consider the linearized modified Monod equation as the regression model without straightforward physical interpretation of parameter values. The model derived above is based on considerable simplifications in the description of such a complex process as that which represents biological waste water treatment process. The advantage of the linearized solution method employed consists in the computational time reduction approximately by 20 times, in comparison with the nonlinear solution technique presented in our previous paper [13]. Another advantage is the straightforward applying possibility in process control. It can be easily mechanized on a small process computer and used as a process state observer.

Based on the results of our work, it can be concluded that the modified Monod kinetic model is suitable to predict actual transient biomass and substrate concentrations. The influent concentration changes in a real activated sludge plant usually do not suffer such wild fluctuations as examined in our work. Thus, a linearized dynamic model based on Michaelis—Menten and modified Monod equations can contribute to the implementation of more advanced control strategies such as adaptive control, to improve the plant treatment efficiency.

Conclusion

Different activated sludge system responses to step feed concentration change for individual variables were observed. The time delay of about four days in COD concentration responses occurred both during the step decreasing and increasing of feed substrate concentration. Instantaneous biomass concentration system responses were observed.

Computations showed that the Monod equation is not accurate in the prediction of transient behaviour of an activated sludge process. Close results were obtained using both nonlinear and linearization methods in solution of the simplified dynamic model derived by applying modified Monod kinetic equations.

Due to the significant computational time reduction in parameters model estimation procedure the linearized model can contribute to the activated sludge process control. From the practical point of view, as well as linearized model the statistical one could be available for the process control. The results obtained by applying this approach will be presented later.

Symbols

COD	chemical oxygen demand	$kg\,m^{-3}$
k_d	endogenous decay coefficient	h^{-1}
K_s	substrate saturation constant	$kg\,m^{-3}$
M	number of measurements	
r_g	biomass growth rate	$kg\,m^{-3}h^{-1}$
r_s	rate of substrate utilization	$kg\,m^{-3}h^{-1}$
S	effluent substrate concentration	$kg\,m^{-3}$
S_0	feed substrate concentration	$kg\,m^{-3}$
S_u	steady-state substrate concentration	$kg\,m^{-3}$
t	time	h
V_a	volume of aeration tank	m^3
V_x	waste sludge flow-rate	m^3h^{-1}
X	biomass concentration	$kg\,m^{-3}$
X_u	steady-state biomass concentration	$kg\,m^{-3}$
Y_{obs}	observed yield coefficient of biomass per unit of COD removed	
μ_{max}	maximum specific growth rate of microorganisms	h^{-1}
ω	minimization function	
Θ	hydraulic detention time	h

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