An Approach to the Simulation of a Batch-respirometer

D. Goi, G. Di Giorgio, I. Cimarosti, M. Mion,* and G. Dolcetti
Dipartimento di Scienze e Tecnologie Chimiche, University of Udine, Via Cotonificio 108, 33100 Udine – Italy, E-mail: clsgoi@ uniud.it
*AMGA SpA Azienda Multiservizi, Via Cotonificio 60, 33100 Udine – Italy, E-mail: mmion@amga.udine.it

Original scientific paper
Received: November 11, 2005
Accepted: March 15, 2006

Dynamic models in activated sludge processes have demonstrated to be a reliable and useful instrument in design and management of wastewater treatment plants. The biochemical nature of the processes involved the models which need a specific calibration to local conditions. A common method to determine kinetic and stoichiometric parameters of the biomass or wastewater/sludge fractionations is respirometry. Theoretically, nearly all biomass parameters and fractions can be estimated by respirometry, but a lot of difficulties rise when some parameters, such as saturation and hydrolysis rate constants, have to be drawn from experimental data.

The aim of our work is the setting up of a simple method to calibrate Activated Sludge Model No. 1 applying traditional batch respirometric tests together with dynamic simulations of the respirometer itself.

Key words:
Respirometry, ASM1, simulation, activated sludge, modeling

Introduction

The Activated Sludge Model No. 1 (ASM1),[1] presented by the IAWQ Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment Processes, has become a major reference for many scientific and practical applications.[2-5]

Setting up and running ASM1 simulations mean the determination of kinetic and stoichiometric parameters with the assumption of some conversion factors. Since oxygen consumption is the most macroscopic and direct expression of the biomass activity and manifestation of inhibitory effects,[6] the respirometry is usually adopted to evaluate kinetic and stoichiometric parameters in order to model typical processes of wastewater treatment. These processes have a biochemical nature, so the characteristics of each wastewater treatment process need to be determined according to the local situation.[7]

The key to obtain a useful model application is the correct assessment of basic model parameters by accurate, reproducible, and economic techniques able to guarantee the best equivalence between real data and simulation.

Respirometric techniques are recognized as reliable laboratory experiences to arrange main model parameters and they are often used when wastewater treatment plant simulation must be carried out and only few data about biomass quality are available.[8]

Some of the more sensitive and fundamental parameters of the ASM1 model (e.g. specific growth rate, yield) can be carried out by simple respirometric tests, nevertheless, their values can influence largely final wastewater treatment plant simulation.

Even if some methods have been proposed, and widely used, to calculate main model parameters and components running a series of numerical transformations on respirometric data,[9,10] less experiences have been conducted on the simulation of respirometric own measurements.[11]

In this note a simulation of a respirometer is attempted, main parameters are deducted from traditional computations on respirometric data, and other ASM1 model parameters are estimated by simulations. A best fitting between experimental and simulation data was sought in the assessment of the unknown parameters by the implementation of ASM1 on the software GPS-X®.

Materials and methods

The respirometric system employed in our experiences was a batch closed reactor assembled in 1 litre transparent plastic bottle. A lid, having three openings for the insertion of the air diffuser, the dissolved oxygen probe and the guide for the addi-

Corresponding author:
D. Goi, E-mail: clsgoi@uniud.it

tion of substrates or reagents, hermetically seals the reactor. Inside the reactor there was a micro porous diffuser connected to a 3 L min^{-1} flow rate capacity compressor by a tube, to supply oxygen to activated sludge. The reactor was equipped with a magnetic stirrer rotating at about $n = 400$ min^{-1} and a thermostatic mantel with water recirculation. For the purpose of measurement of dissolved oxygen mass concentration progress in activated sludge samples, a galvanic oxymeter has been used. Oxymeter was able to store the measured dissolved oxygen concentration data.

The Chemical Oxygen Demand (COD) and the Volatile Suspended Solids concentration (VSS) have been carried out using the Standard Methods for Examination of Water and Wastewater.[12] In all biomass calculations, γ_{X_T} (total active biomass) and γ_{X_H} (heterotrophic active biomass) were expressed by means of COD using the conversion factor 1.45 m_{COD}/m_{VSS} (mg mg^{-1}).

Respirometric trials for the assessment of kinetic and stoichiometric parameters were set up using activated sludge drawn from a biological reactor of a medium size wastewater treatment plant which treats municipal sewage. After the withdrawal, the activated sludge was aerated for some hours to remove all biodegradable COD and ammonia nitrogen contained in the sample. This operation allowed reaching the requested biomass endogenous condition, that must be guaranteed before starting any endogenous-base test.

The activated sludge used in respirometric tests has arranged in a mass concentration of about 1.5 g L^{-1} VSS. To evaluate heterotrophic biomass activity only, autotrophic biomass activity was inhibited adding 10-15 mg L^{-1} of allylthiourea.

Activated sludge temperature was maintained at 20 °C exactly during each test.

The whole volume of the respirometer was filled by mixed sludge, this allowed a high liquid/gas volume ratio, and so the oxygen transfer from the small volume gas phase of the headspace of the reactor was considered negligible.

Experimental

The experimental session was carried out to fix some of the fundamental parameters of the ASM No. 1 model, then simulations and sensitivity analyses were tried to achieve the best fitting between actual and simulated data,[13] so other parameters were carried out.

The oxygen uptake rate (OUR or γ_O) for the activated sludge sample, contained in the batch closed respirometer, was expressed by means of the following equation:

$$\frac{d\gamma_{S_0}}{dt} = -\Gamma_0(t) \quad (1)$$

The main respirometric parameters were found following the procedures reported below.

Assessment of heterotrophic endogenous decay coefficient (b_H) and initial heterotrophic active biomass amount (γ_{H_0})

The allylthiourea was added to the pre-aerated activated sludge sample contained into the closed batch reactor at constant temperature. The biomass endogenous condition, obtained by pre-aeration of the sample, was kept by no external substrate addition during this test.

Continuous phases of aeration and not-aeration were created in the respirometer to obtain the required series of OUR values (respirogram).

To describe the true heterotrophic biomass endogenous decay, a large number of endogenous OUR points were collected, in this way aerobic digestion in the batch reactor was continued for several days.

Using the same respirogram, it is possible to evaluate both b_H and γ_{H0}. The viability ratio ($\gamma_{X_{H0}}/\gamma_{X_{T0}}$) can be calculated when the initial VSS mass concentration ($\gamma_{X_{T0}}$) is measured.

In an activated sludge reactor containing no external substrate, the integrated rate expression for heterotrophic endogenous decay is the following:

$$\gamma_{X_H}(t) = \gamma_{X_{H0}} \cdot e^{-b_H t} \quad (2)$$

The loss of biomass due to endogenous decay is commonly considered as an oxidation process. Consequently, the rate of dissolved oxygen consumption under aerobic conditions may be defined as follows:

$$\frac{d\gamma_{S_0}}{dt} = -(1 - w_{X,ex})\, b_H \cdot \gamma_{X_H} \quad (3)$$

Substituting the value of γ_{X_H} from [2] to above equation it is possible to obtain two equations:

$$\frac{d\gamma_{S_0}}{dt} = -(1 - w_{X,ex})\, b_H \cdot \gamma_{X_{H0}} \cdot e^{-b_H t} \quad (4)$$

$$\ln(\Gamma_0(t)) = \ln[(1 - w_{X,ex})\, b_H \gamma_{X_{H_0}}] \cdot b_H \quad (5)$$

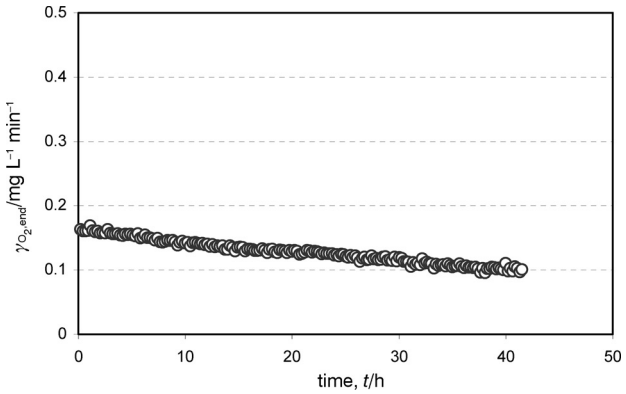
Equation [5] shows that it is possible to evaluate b_H as the slope of a plot of $\ln(\Gamma_O(t))$ versus time. For $t = 0$, eq. 5 can be reduced to:

$$\Gamma_0(t_0) = (1 - w_{x,ex}) \cdot b_H \gamma_{X_{H_0}} \quad (6)$$

The estimated value of b_H must be used to evaluate $\gamma_{X_{H0}}$, when $\gamma_O(t_0)$ is experimentally determined from the respirogram as the *y*-axis intercept of eq. 6 (Fig. 1). The active biomass concentration ($\gamma_{X_{H0}}$), initially contained in the reactor, can be calculated as:

$$\gamma_{X_{H_0}} = \frac{\Gamma_0(t_0)}{b_H(1-w_{X,ex})} \quad (7)$$

A typical value of 0.2 can be assumed for $w_{x,ex}$.



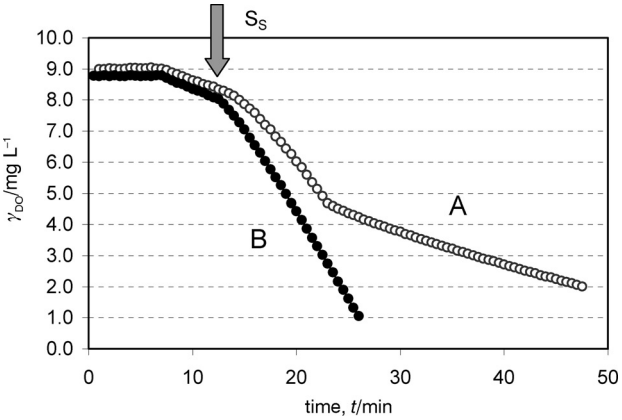
F i g . 1 – *Endogenous respirogram for the evaluation of* $\gamma_{X_{H0}}$ *and* b_H

Assessment of the heterotrophic yield (Y_H)

The closed batch reactor was filled with pre-aerated activated sludge. The sludge contained in the reactor was aerated until reaching the maximum dissolved oxygen concentration (saturation). Then, the aeration was interrupted and dissolved oxygen concentration started to drop. The first endogenous part of the dissolved oxygen concentration drop was measured. An amount of about 15 mg L^{-1} COD of sodium acetate was added to the activated sludge as readily biodegradable substrate (γ_{S_S}). This mass concentration was calibrated in order to observe the end of the substrate oxidation before all the oxygen in the activated sludge was used. The introduction of the substrate immediately produced a clear increase of the oxygen uptake rate. The end of the substrate degradation is graphically pointed out by the return of the OUR close to the endogenous value measured before the addition of the substrate (Figure 2, curve A).

In the same figure, the endogenous respiration rate (γ_{end}) and the total respiration rate (γ_{tot}) were estimated according to equation 1 as the slope of the diagram of the dissolved oxygen concentration versus time.

The oxygen balance for the degradation of readily biodegradable substrates, referred to the volume unit of the reactor, is:



F i g . 2 – *Respirometric tests for the evaluation of* Y_H *(curve A) and* μ_H *(curve B)*

$$\gamma_{O_2,tot} = \gamma_{O_2,ex} + \gamma_{O_2,end} \quad (8)$$

where

$\gamma_{O_2,tot}$ = total oxygen consumption, mg L^{-1}

$\gamma_{O_2,ex}$ = oxygen consumption for the substrate removal, mg L^{-1}

$\gamma_{O_2,end}$ = endogenous oxygen consumption, mg L^{-1}.

$\gamma_{O_2,tot}$ and $\gamma_{O_2,end}$ are calculated by the following integrals:

$$\gamma_{O_2,tot} = \int_0^{t_e} \Gamma_{tot}\,dt \qquad \gamma_{O_2,end} = \int_0^{t_e} \Gamma_{end}\,dt \quad (9)$$

where t_e is the length of the substrate oxidation that can be estimated graphically in Fig. 2, curve A.

Because the mass concentration of the readily biodegradable substrate is known, the calculation of Y_H is obtained using the following equation:

$$Y_H = 1 - \frac{\int_0^{t_e} \Gamma_{ex}\,dt}{\gamma_{S_S}} = 1 - \frac{\gamma_{O_2,ex}}{\gamma_{S_S}} \quad (10)$$

Assessment of maximum heterotrophic specific growth rate ($\mu_{H,max}$)

The experimental procedure for the assessment of the maximum specific growth rate was the same as employed for the evaluation of the yield, except for the amount of the added substrate. In fact, in this second test, a mass concentration of about 150 mg L^{-1} COD of sodium acetate was put into the reactor running in the endogenous phase, this amount allowed the whole dissolved oxygen exhaustion by the substrate.

After the readily biodegradable substrate addition, the OUR immediately increases and the following relation can be written:

$$\Gamma_{tot} = \Gamma_{end} + \Gamma_{ex} \quad (11)$$

Γ_{tot} is given as the slope of the plot of the dissolved oxygen concentration versus time (Fig. 2 B). Γ_{end} is evaluated from the first endogenous part of the dissolved oxygen decrease. In this condition the evaluation of μ_{max} was carried out considering Γ_{ex} both was not substrate limited and proportional to γ_{X_H}, so the simplified equation 12 can be used:

$$\mu_{H,max} = \frac{\Gamma_{ex} \cdot Y_H}{(1 - Y_H)\gamma_{X_H}} \quad (12)$$

The values of the parameters estimated from respirometric tests are summarized in Table 1 with the fundamental relationships from which they can be drawn.

Results and discussions

The A.S.M. No.1 was implemented utilizing the worldwide known software GPS-X®.

The closed batch respirometer has been modelled as a simple 1 L volume CSTR, characterised by diffused aeration with a pumped flow rate of 2 L min^{-1}. In the basic data of the model, an activated sludge mass concentration of 1,500 mg L^{-1} S_S and a 19 °C temperature were imposed. The addition of the substrate has been represented as an injection into a batch influent unit.

The dynamic simulation of A.S.M. No. 1 was performed considering the initial concentrations of the Mixed Liquor COD fractions showed in the Table 2, in the same table are reported other main parameters required by the model.

The model has been completed using the stoichiometric and kinetic parameters Y_H, $\mu_{H,max}$ and b_H obtained by respirometric batch tests (Table 1). As shown in eq. 12, $\mu_{H,max}$ is dependent on γ_{X_H}, nevertheless sensitivity analysis on the unknown parameters γ_{X_H}, γ_{X_I} and γ_{X_S} confirmed that variations of γ_{X_H} influence the modelled system more than changes in γ_{X_I} and γ_{X_S}.

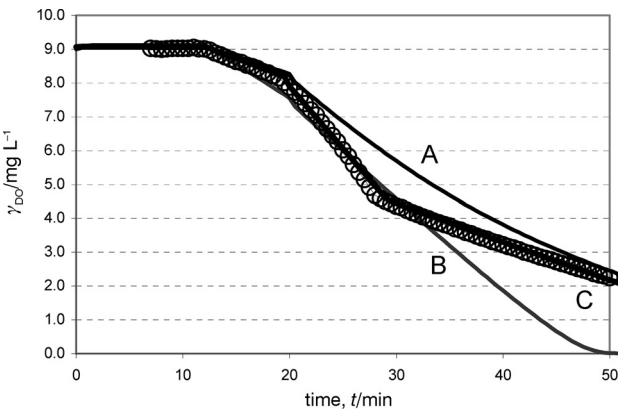
A sensitivity analysis on k_H, K_X, K_{OH} and K_S was performed obtaining several simulation curves for the respirometric dissolved oxygen runnings. Starting from initial values, all not experimentally found values were determined considering the best fitting between experimental and simulation data. In Fig. 3 are reported the respirometric data (dots), two approximate curves (curve A, B) and the best fitting curve, this final curve was obtained by the model optimisation.

T a b l e 1 – *Parameters evaluated by respirometric test*

Parameter	Fundamental equation	Value
b_H	$\frac{d\gamma_{S_0}}{dt} = -(1 - w_{X,ex})b_H\gamma_{X,H_0} \cdot e^{-b_H t}$	0.52 d^{-1}
viability ratio $\gamma_{X_{H0}}/\gamma_{X_{T0}}$	$\gamma_{X,H_0} = \frac{\Gamma_0(t_0)}{b_H(1 - w_{x,ex})}$	30 %
Y_H	$Y_H = 1 - \frac{\gamma_{O_2,ex}}{\gamma_{S_S}(0)}$	0.73 mg_{O_2} mg_{COD}^{-1}
$\mu_{H,max}$	$\mu_{H,max} = \frac{\Gamma_{ex} \cdot Y_H}{(1 - Y_H)\gamma_{X_H}}$	3.53 d^{-1}

T a b l e 2 – *Initial values arranged for main parameters of the model*

Parameter	Initial value	Note
$\gamma_{X,BH}$	30 %	Deduced from endogenous respirogram results.
γ_{S_S}	≅ 0	Because of the long sample pre-aeration provided.
γ_{S_I}	≅ 0	Because of the long sample pre-aeration provided.
$\gamma_{X,BA}$	0	Considering the injection of the nitrification inhibitor.
$\gamma_{X,U}$	0	It is assumed $\gamma_{X_T}=\gamma_{X_{BH}}+\gamma_{X_I}+\gamma_{X_S}$, so γ_{X_U} is incorporated into inert particulate fraction
γ_{X_I}	unknown	Initially $\gamma_{X_I}=\gamma_{X_S}$.
$\gamma_{X,S}$	unknown	Initially $\gamma_{X_I}=\gamma_{X_S}$.
k_H	3.0 d^{-1}	According to IAWQ Task Group.
K_X	0.03 gCOD $gCOD^{-1}$	According to IAWQ Task Group.
K_{OH}	0.2 mg L^{-1} O_2	According to IAWQ Task Group.
K_S	20 mg L^{-1} COD	According to IAWQ Task Group.



F i g . 3 – *Graphical representation of the simulation trials (A, B) and the best fitting curve (C)*

The respirometric oxygen depletion, due to injection of 15 mg L^{-1} COD sodium acetate, was modelled with the best fitting (with a 1.5 % relative error), using the parameters of the curve C (best curve values) reported in the Table 3.

Table 3 – *Values of the parameters used for the simulation of the oxygen trends shown in figure 3 obtained from the sensitivity analysis*

Kinetic parameters	Symbol	Unit	Curve A	Curve B	Curve C
substrate saturation constant	K_S	mg L^{-1} COD	5.64	5.64	0.50
oxygen saturation constant	K_{OH}	mg L^{-1} O_2	0.20	0.20	0.20
hydrolysis rate coefficient	k_H	d^{-1}	3.00	2.00	2.00
hydrolysis saturation constant	K_X	mg mg^{-1}	0.03	0.02	0.03

Conclusion

This work shows an experience of the use of a simple respirometric test, coupled with its dynamic simulation, for the evaluation of main activated sludge process parameters of a biomass from a medium size wastewater treatment plant.

Some conclusive considerations can be presented:

– Our laboratory experience has confirmed that respirometric tests are a valid and reliable instrument to evaluate only some traditional kinetic and stoichiometric activated sludge constants.

– Data from basic respirometric tests are often incomplete for the ASM1 implementation, so the substantial difficulty in determining the whole number of main parameters of ASM1, suggests to achieve some other way to set up these components.

– In this work, an attempt to calibrate the ASM1 model coupling the respirometric tests and an optimization procedure on dynamic simulation of experimental data, was carried out. The fitting of measured dissolved oxygen mass concentration values with the dynamic simulation results has resulted in getting parameters which can not be drawn easily from respirometric tests.

– The results obtained indicates, that the simple batch respirometric test coupled with the fitting of simulations and conducted implementing theoretic models (e.g. ASM1) followed by a sensitivity analysis on specific unknown parameters, may be a valuable instrument to have rapid and reliable information on the activated sludge system performance.

It can be recognized, that if a reasonably close agreement is obtained between the measures of dissolved oxygen mass concentrations, coming from a respirometer and the respective simulations, the developed model can be reasonably considered a good representation of the real wastewater treatment plant biomass performance.

ACKNOWLEDGEMENTS

The authors wish to thank Dr. Ruggero Borghese of the ARPA-FVG Department of Udine and Ing. Cristiana Gregoris for their support during the research project.

Symbols and abbreviations

b_H – heterotrophic endogenous decay coefficient, d^{-1}
k_d – endogenous decay coefficient, d^{-1}
k_H – hydrolysis rate coefficient, d^{-1}
K_{OH} – oxygen half saturation constant for heterotrophic biomass, mg L^{-1}
K_S – half saturation constant for readily biodegradable substrate, mg COD L^{-1}
K_X – hydrolysis saturation constant, mg COD mg COD^{-1}
m – mass, mg
n – stirrer speed, min^{-1}
t – time, min
$w_{x,ex}$ – inert fraction of the biomass, 1
Γ_{O_2} – dissolved oxygen consumption rate or OUR, mg L^{-1} min^{-1}
Γ_{tot} – total measurable dissolved oxygen consumption rate, mg L^{-1} min^{-1}
Γ_{end} – endogenous dissolved oxygen consumption rate, mg L^{-1} min^{-1}
Γ_{ex} – exogenous dissolved oxygen consumption rate, mg L^{-1} min^{-1}
γ_{S_I} – inert organic soluble matter mass concentration, mg COD L^{-1}
γ_{S_O} – dissolved oxygen concentration, mg L^{-1}
γ_{S_S} – readily biodegradable substrate concentration, mg COD L^{-1}
γ_X – biomass concentration, mg L^{-1} COD or mg L^{-1} TSS or mg L^{-1} VSS
$\gamma_{X_{BA}}$ – autotrophic biomass concentration, mg L^{-1} COD
$\gamma_{X_{BH}}$ – heterotrophic biomass concentration, mg L^{-1} COD
γ_{X_H} – heterotrophic biomass concentration, mg L^{-1} COD
$\gamma_{X_{H0}}$ – initial heterotrophic biomass concentration, mg L^{-1} COD
γ_{X_I} – inert biomass concentration, mg L^{-1} COD
γ_{X_P} – particulate matter due to endogenous decay concentration, mg L^{-1} COD
γ_{X_S} – slowly biodegradable particulate matter concentration, mg L^{-1} COD

γ_{X_T} – total suspended solids concentration of mixed liquor, mg L^{-1} COD or mg L^{-1} TSS or mg L^{-1} VSS

$\gamma_{X_{T0}}$ – initial total suspended solids concentration of mixed liquor, mg L^{-1} COD or mg L^{-1} TSS or mg L^{-1} VSS

γ_{X_U} – not-biodegradable particulate matter coming from cellular decay, mg L^{-1} COD or mg L^{-1} TSS or mg L^{-1} VSS

Y_H – heterotrophic yield coefficient, mg mg^{-1}

μ_H – the specific growth rate for heterotrophic biomass, d^{-1}

$\mu_{H,max}$ – the maximum specific heterotrophic growth rate, d^{-1}

$\gamma_{O_2,end}$ – endogenous dissolved oxygen consumption, mg L^{-1}

$\gamma_{O_2,ex}$ – exogenous dissolved oxygen consumption, mg L^{-1}

$\gamma_{O_2,tot}$ – total dissolved oxygen consumption, mg L^{-1}

γ_{COD} – chemical oxygen demand, mg L^{-1}

γ_{DO} – dissolved oxygen mass concentration, mg L^{-1}

OUR – oxygen uptake rate or Γ_O, mg L^{-1} min^{-1}

TSS – total suspended solids

VSS – volatile suspended solids

References

1. *Henze, M., Grady, L. C. P., Jr., Gujer, W., Marais, G. V. R.*, Activated Sludge Model No.1. – IAWPRC Scientific and Technical Report No. 1, IAWPRC, London, England, (1987).
2. *Kolisch, G., Londong, J.,* Water Sci. Technol. **38** (3) (1998) 71.
3. *Lennox, J. A., Yuan, Z., Harmand, J.,* Water Sci. Technol. **43** (7) (2001) 367.
4. *Drolka, M., Plazl, I., Koloini, T.,* Chem. Biochem. Eng. Q. **15** (2) (2001) 71.
5. *Nuhoglu, A, Keskinler, B, Yildiz, E.,* Process Biochem. **40** (7) (2005) 2467.
6. *Mrafkova, L., Goi, D., Gallo, V., Colussi, I.,* Chem. Biochem. Eng. Q. **17** (3) (2003) 217.
7. *Vanrolleghem, P. A., Spanjers, H., Petersen, B., Ginestet, P., Takacs, I.,* Water Sci. Technol. **39** (1) (1999) 195.
8. *Boursier, H, Beline, F, Paul, E,* Water Sci. Technol. **49** (5-6) (2004) 389.
9. *Banes, O., Spanjers, H., Holba, M.,* Water Sci. Technol. **46** (4-5) (2002) 1.
10. *Ricco, G, Tomei, M. C.,* IA Ingegneria Ambientale **28** (1999) 502.
11. *Giroux, E. Y., Spanjers, H, Patry, G. G., Takacs, I.,* Water Sci. Technol. **33** (1) (1996) 297.
12. Standard methods for the examination of Water and Wastewater. APHA, AWWA, WPCF, Washington, DC, 1992.
13. *Orhon, D., Artan, N.,* Modelling of activated sludge systems. Technomic Publishing AG Inc., Basel, Switzerland 1994.