Implementing a respirometry-based model into BioWin software to simulate wastewater treatment plant operations

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Abstract

The management of wastewater treatment plants to comply with new strict effluent criteria is a great concern: the activated sludge modeling, when supported by an accurate calibration process, could be an essential tool for this purpose. In the present paper, three WWTPs were characterized in order to support their up-grade. Influent characteristics and activated sludge performances were studied by application of respirometry. Plant operations were simulated by BioWin software (EnviroSim Associates Ltd., Canada). The goodness of the simulation, checked by the calculation of the average relative deviation between measured and simulated data, demonstrated that the model was able to predict the plant performances.

Keywords

Respirometry, Kinetic model, COD fractions, BioWin, activated sludge model

1. Introduction

In a recent paper, Insel et al. [1] rhetorically asked if the standard WWTP design methods are suitable for any municipal wastewater. Before the 1980, the answer to this question would probably have been positive: at that time, the goals required for wastewater treatment plant were the removal of solids and organic matter, so the plant design methods complied with these purposes. As is known, in the last two decades, the standards for wastewater constituent removal have changed: the new regulations request strict effluent criteria from wastewater treatment plants into the water bodies. Therefore, appropriate process design and control issues are of great importance to maintain sustainable and cost-effective treatment under variable environmental conditions [1].

Dynamic models of activated sludge processes have demonstrated to be an indispensable tool in plant design and management [1-4] however, their calibration appears to be the bottleneck in their widespread application [5]. According to Petersen et al. [6], the calibration is the adaptation of the model to fit a certain set of information obtained from the full-scale WWTP under study. The calibration methodology of activated sludge plant models may be different depending on the targets of modeling [7].

Sin et al [8] compared four calibration protocols for activated sludge models: the BIOMATH calibration protocol [9], the STOWA calibration protocol [10], the HSG guidelines [11] and the WERF protocol for model calibration [12]. As a result of the Sin et al ~~[8]~~ analysis, appeared that all the protocols have three major common point: the crucial influence of goal determinations in the calibration procedure, the significance of data collection, verification and reconciliation and the recommendation of validating the model with a data set obtained under different operating conditions than those of the calibration period. However, the four cited protocols diverged for three major aspects [8]: the planning

of the measurement campaign, the experimental methods for influent characterization and the calibration method (selection of parameter subset, how to calibrate).

One of the major problems in Activated Sludge Models (ASMs) application and calibration is to select a set of relevant parameters, which are necessary to achieve good prediction of the used model [7].

Mannina et al. [13] paid attention to the parameter subset selection. Their proposed calibration protocol consisted in two major phases performing several steps. In the first phase a preliminary sensitivity analysis is carried out, selecting different subset of parameters, in order to reduce the number of model parameters to be calibrated. In the second phase the model calibration is performed by means of a group-wise Monte Carlo technique.

Several Authors reported the lists of more sensitive parameters in ASM calibration [7, 14] including: the yield coefficient for heterotrophic biomass $Y_{H,}$ the yield coefficient for autotrophic biomass Y_A, the maximum heterotrophic growth rate μ_{maxH}, the heterotrophic decay rate b_H, the maximum autotrophic growth rate $\mu_{maxA,}$, the half-saturation constant for organic substrate K_S, the half-saturation constant for ammonia K_{NH4}, the half-saturation constant for dissolved oxygen (related to autotrophs) K_{OA} and the anoxic ratio η_H.

These parameters are usually evaluated by means of respirometric tests [4, 6, 15-18]. Indeed, respiration rate is directly linked to two important biochemical processes that must be controlled in a WWTP: biomass growth and substrate consumption [19].

The present paper is the result of the field research carried out in three wastewater treatment plants, located in the Friuli Venezia Giulia (FVG) region, operating different technologies and serving a wide range of Population Equivalent. The study had the aim to support the up-grade design of the plants because, at that time, they showed some critical

situations related to the nitrogen removal and/or to the variability on the influent pollutant load.

The WWTPs performances were studied by means of respirometric tests. The experimental results were used to calibrate a home-made activated sludge model that was further implemented in BioWin software (EnviroSim Associates Ltd., Canada).

2. Materials and methods

According to a study published by the Italian Statistic Institute [20], at the end of 2008, 693 WWTPs were in operation in the FVG region, with a served population of 1,772,906 Person Equivalent (P.E.). Secondary treatment was in place for 36% of these plants; while the 56% of the plants operated the primary treatment and only the 8% of the plants had the tertiary treatment.

This study focuses on three WWTPs, having secondary treatment and the characteristics (at the time of field study) reported below.

Plant #1 served a population of 7,000 P.E. operating a time-based alternate cycles process. Anoxic and aerobic processes took place in the same basin that had a volume of 525 m^3. After passing a coarse bar screen (15 mm), the influent flowrate was channeled to biological reactor where the alternance of aerobic and anoxic conditions was controlled by time. The duration of aerobic phase was set equal to 4 hours, while that of anoxic step was equal to 45 minutes.

Plant #2, serving 18,200 P.E., operated the activated sludge process with preanoxic MLE (Modified Ludzack-Ettinger) denitrification. Influent raw sewage was subjected to pass the pre-treatment units consisting of a grit screw and a horizontal-flow grit chamber. Primary sedimentation was no carried out in order to support the BNR process. In the

biological unit, the flowrate of aerated sludge recirculated from aerobic reactor to anoxic section had the same value that those of influent.

Plant #3 was characterized by a seasonal variation of the influent wastewater with a maximum served population of 120,000 PE during the summertime. The water treatment line was divided in two independent sections: the physical-chemical treatment (with addition of aluminum chloride) and the biological activated sludge process. After preliminary treatment (grit screw, horizontal-flow grit chamber and preliminary settling), the influent flowrate was halved and the two resulting flowrates were piped to the respective section (the present study takes in account only the biological treatment line).

The characteristics of the examined plants and of the influent wastewaters are reported in table 1.

2.1 Steps of the work

The work steps are depicted in Figure 1. As stated before, the purpose of the study was the investigation of pollutants removal kinetics. To obtain it, an activated sludge model was developed and calibrated following several steps:

1. Information were collected regarding to plants layout and operations, long-time influent characterization and operational parameters. Collected data were checked calculating mass balances. Dedicated measuring campaigns were planned and carried out;
2. The characterization of the biological section of the plants was accomplished by application of the respirometric test, consisting in OUR, AUR and NUR;
3. The structure of biological model was formulated;

4. The model was calibrated using the results coming from respirometric assays. The calibration methodology was partially automated, meaning that some parameters were evaluated using a home-made software (hereinafter described).

   Steps from 1 to 4 were carried out for all the three examined WWTPs;

5. Step 5 (and also 6) regarded only the plant #2. It was preparatory to the operations simulation and consisted in the definition of aeration devices, controllers, flows and other operational parameters;
6. The model was implemented into BioWin software and validated using a data set of 11 months.

2.2 Experimental set-up

The rate at which activated sludge consumes oxygen is called respiration rate and it is usually measured using respirometers [21]. The respirometer is a reactor in which biomass and substrate are put in contact. It varies from a very simple manually operated bottle to a full self-operating instrument.

The respirometer employed in this work at the Chemical Plants Lab of the Engineering and Architecture Dept. at the Trieste University, is a cylindrical plexiglass reactor with a volume of 1L, continuously stirred and thermally controlled (water bath). Dissolved Oxygen (DO) concentration is measured by electro-chemical Clark-type probes (Hanna Instruments HI 76407/4). Aeration is provided by membrane pumps (SCHEGO) controlled to maintain the DO concentration higher than 2 $mgO_2 \cdot L^{-1}$. For this purpose, the data acquisition unit (Agilent 349701A) also operates as automatic control system. The experimental set-up is represented in figure 2.

2.3 Oxygen Uptake Rate (OUR)

The activated sludge taken from the aerated basin of each studied WWT plant was aerated for a few hours before the use, in order to obtain the endogenous conditions at the beginning of the experiments. The desired concentration of Total Suspended Solids in the respirometer was about 2÷3 $gTSS \cdot L^{-1}$; for this reason, occasionally, dilution of the sludge with tap water was necessary.

The applied ratio (S_0/X_0) of the initial substrate concentration S_0 and the initial biomass concentration X_0 varied from 0.044 to 0.096 $gCOD \cdot gVSS^{-1}$.

According to IWA Task Group definition, the experimental procedure was LSS-type (static gas, static liquid) [5]. The automatic control system switched on the blowers when the DO concentration measured in the reactor reached the set lower limit (2 $mgO_2\ L^{-1}$). The aeration had a fixed desired duration (generally 1 minute). The OUR was estimated by measuring the decrease in DO as a function of time due to respiration.

2.4 Ammonia Uptake Rate (AUR) and Nitrate Uptake Rate (NUR)

The nitrogen removal process was investigated by means of AUR and NUR tests.

To determine AUR, an activated sludge volume of 800 mL was placed into the respirometer and was put in contact with 100 mL of ammonia solution with a $N\text{-}NH_4$ concentration of 25÷30 mg L^{-1}. The mixed liquor was kept in suspension by aeration through diffusors, which also provided the sludge with oxygen in a concentration of 5÷6 $mgO_2\ L^{-1}$. The experiments had a duration of 6 hours, during which approximately eight samples (three in the first hour and then one per hour) were taken and analyzed for ammonia and nitrate nitrogen content.

NUR was determined by the use of a completely stirred and closed to atmosphere respirometer in which 800 mL of activated sludge sample were mixed with 100 mL of

nitrate solution having a desired concentration. Acetate was also added in order to provide readily biodegradable COD. The experiments had a duration of 6 hours, during which approximately eight samples (three in the first hour and then one per hour) were withdrawn and analyzed for $N\text{-}NO_3$ content.

3 Activated sludge modeling

A mathematical model, named 4CODf+, based on the Activated Sludge Model No.1 [22], was developed and calibrated using the experimental results from respirometry.
The 4CODf+ model is a system of differential algebraic equations (DAE) solving the mass balances of the involved substrates. In his whole version, shown in table 2, the model accounts for four COD fractions, described below:

- the rbCOD fraction (readily biodegradable): it is soluble and includes the organic compounds that can be directly metabolized at a high rate under aerobic as well as anoxic conditions, such as VFA, carbohydrates, alcohols and amino acids [23];
- the mbCOD fraction (medium-rate biodegradable): it is that part of the organic matter which can be hydrolyzed under aerobic conditions in a few hours;
- the sbCOD fraction (slowly biodegradable): it is constituted by the part of organic matter with a slow hydrolysis rate. It includes also the dead biomass purged of his inorganic fraction;
- the iCOD fraction (inert fraction): it represents the non-biodegradable COD.

Kinetic reactions rates and stoichiometric parameters of the model are presented in table 2 (where: S_R = rbCOD; S_M = mbCOD; S_S = sbCOD).

As it can be seen, the hydrolysis that takes place on influent mbCOD and sbCOD was not modelled and the three biodegradable COD fractions were considered such as three different substrates, distinguished on the basis of their biodegradation time.

The nitrification was modelled as one-step process in order to shorten the calculation.

The rbCOD was assumed to be the electron donor fraction in the anoxic process.

As regards to the decay of heterotrophic biomass, the death-regeneration approach was followed, then also the hydrolysis of part of decaying biomass into slowly biodegradable substrate was included in the model.

3.2 OUR modeling

The 4CODf+ model was shortened (keeping intact his structure) in order to simulate the oxygen uptake rate. Depending on the aerobic conditions into the respirometer during the development of OUR test, two model modifications were introduced:

- the denitrification process was excluded in the calculation;
- the dissolved oxygen was not considered as a limiting factor in the heterotrophic and autotrophic processes.

Therefore the oxygen uptake rate was calculated as follows:

$$\frac{dO_2}{dt} = \frac{(1-Y_H)}{Y_H} \cdot \left(\mu_{\max,R} \frac{S_R}{(S_R + K_{SR})} + \mu_{\max,M} \frac{S_M}{(S_M + K_{SM})} + \mu_{\max,S} \frac{S_S}{(S_S + K_{SS})} \right) \cdot \theta^{(T-20)} \cdot X_H + \frac{(4.57-Y_A)}{Y_A} \cdot \mu_{\max,A} \cdot \frac{NH_4}{(NH_4 + K_{NH4})} \cdot \theta_A^{(T-20)} \cdot X_A \quad (1)$$

The model equations were implemented in a home-made *Evalua*tOUR software. The software, written in FORTRAN programming language, provides the dynamic simulation of the oxygen consumption during a respirometric test. Input parameters are the

197 respirometric experimental data (*i.e*. the time-course of dissolved oxygen and temperature)
198 and the data from characterization analysis, such as values of TSS, VSS, COD and NH_4 in
199 the wastewater (WW), in the activated sludge (AS) and in the mixed liquor at the end of
200 respirometry. The output values are the kinetic and stoichiometric parameters of the
201 activated sludge and the WW COD fractions.
202 The fitting curve is obtained numerically by solving the DAE system with a LSODA routine
203 and evaluating the parameters with hybrid method.
204 All the kinetic and stoichiometric parameters, involved in respiration process, can be
205 estimated by using the *Evaluat*OUR software; therefore it is possible to decide which
206 parameters have to be calculated, which parameters have to be assumed as constant
207 values during the simulation and which parameters can be manually tuned.
208 The comprehensive lists of input and output parameters are presented in table 3.
209

210 **4 Results and discussion**

211

212 The field study on the plants had a duration of several months, during which
213 samples of influent wastewater and activated sludge were withdrawn weekly. The
214 experimental work was conducted as follows:

215 – plant #1: two months of analysis with 20 respirometric tests, 5 OUR (in duplicate), 4
216 AUR and 6 NUR;
217 – plant #2: four months of analysis with 53 respirometric tests, 21 OUR (in duplicate),
218 6 AUR and 5 NUR;
219 – plant #3: two months of analysis with 30 respirometric tests, 6 OUR (in triplicate), 6
220 AUR and 6 NUR.

Then kinetic and stoichiometric parameters, obtained by respirometric assays, were implemented (with the 4CODf+ model) in BioWIN software in order to simulate the plant #2 operations.

4.1 Evaluations of kinetic and stoichiometric parameters

The kinetic and stoichiometric parameters were evaluated by processing the data coming from respirometric assays. In particular, the calibration with *Evaluat*OUR software concerned the maximum growth rates for heterotrophic bacteria, $\mu_{max,R}$, $\mu_{max,M}$, $\mu_{max,S}$ (for rbCOD, mbCOD and sbCOD, respectively) and the related half-saturation constants, K_{SR}, K_{SM} and K_{SS}. The other parameters were acquired from literature or calculated as illustrated hereinafter. The choice of the parameters to calibrate was no supported by an identification analysis, but it had a qualitative nature. With the help of the *Evaluat*OUR software, the parameters were varied one by one and the effects on the simulated respirogram were visually evaluated.

The heterotrophic decay rate b_H was calculated from the endogenous OUR profiles [24]. In the endogenous respiration concept, the biodegradable fraction (1-f_i) of decaying biomass is regarded as a homogeneous substrate that undergoes self-destruction in the absence of external substrate [25].

The endogenous respiration rate is modelled with equation (2):

$$OUR(t) = (1 - f_i) \cdot \frac{dX_H}{dt} \quad (2)$$

where f_i is the non-biodegradable fraction of biomass, set equal to 0.08 as suggested by [15] and

$$\frac{dX_H}{dt} = -b_H \cdot X_H \quad (3)$$

represents the first-order degradation process of the heterotrophic biomass.

The integration of equation (3) resulted in:

$$X_H(t) = X_H(0) \cdot e^{-b_H \cdot t} \quad (4)$$

that leads to:

$$OUR(t) = (1 - f_i) \cdot X_H(0) \cdot e^{-b_H \cdot t} \quad (5)$$

A plot of measured ln[OUR(t)] versus time gives a straight line with slope b_H.

To obtain the endogenous OUR profiles, respirometries were carried out without addition of exogenous substrate. Collected samples of AS (for each plant) were subjected to respirometric tests with a duration of 48÷72 hours and then obtained OURs were expressed as explained before. The values of b_H found in this study varied from 0.017 d^{-1} for plant #3 to 0.052 d^{-1} for plant #2 resulting lower than values reported in literature (varying in the range 0.059÷0.500 d^{-1} [25]. However, due to the wide range of values of the Van't Hoff-Arrhenius coefficient θ, it is difficult to compare decay rates calculated at different temperatures [25].

The heterotrophic yield Y_H was calculated, as suggested by Vanrolleghem et al. [26], from respirometric tests with addition of real wastewater. The measured OUR profiles, purged of the endogenous contribution, were integrated with respect to time, obtaining the oxygen consumed for substrate oxidation. Afterwards the Y_H was calculated as:

$$Y_H = \frac{COD_{\deg raded} - \int OUR(t)dt}{COD_{\deg raded}} \quad (6)$$

where the amount of degraded COD derived from mass balances. Experiments were carried out with ATU addition to avoid nitrification. Evaluated heterotrophic yield values varied from 0.471 $gCOD \cdot gCOD^{-1}$for plant #1 to 0.599 $gCOD \cdot gCOD^{-}1$ for plant #3, in agreement with literature [3].

$\mu_{max,A}$ and K_{NH4} values were evaluated by AUR tests with the maximum autotrophic growth rate determined by equation (7) [27]:

$$\mu_{\max A} = \frac{r_N \cdot Y_A}{X_A} \quad (7)$$

where r_N represents the nitrification rate, measured in AUR test, Y_A is the yield coefficient for autotrophic biomass acquired from literature [28] and X_A is the autotrophs concentration in the respirometer, estimated as the 4% of the total MLVSS [29].

From $\mu_{max,A}$, the half-saturation constant K_{NH4} was tuned in order to minimize the mean square deviation between measured and calculated ammonia uptake rate (expressed as Monod-type equation).

After setting the aforementioned parameters, $\mu_{max,R}$, $\mu_{max,M}$, $\mu_{max,S}$, K_{SR}, K_{SM} and K_{SS} values were estimated by *Evaluat*OUR software. Figure 3 shows some examples of the obtained respirograms. The fitted values of $\mu_{max,R}$, $\mu_{max,M}$, $\mu_{max,S}$, K_{SR}, K_{SM} and K_{SS} are difficult to compare with literature data, because the applied 4CODf+ model considers the three biodegradable COD fractions such as different substrates. However, by comparing the maximum heterotrophic growth rate on rbCOD, $\mu_{max,R}$, with the μ_{max} suggested by the IWA task group [15], a lower value of one order of magnitude is evidenced (see table 4). This condition is in agreement with the paper of Elshorbagy and Shawaqfah [4] in which typical values of the maximum specific growth rate for heterotrophic biomass can vary in the range 0.6÷13.2 d^{-1}. As regards the half-saturation constants for COD (K_{SR}, K_{SM} and K_{SS}), it is important to note that they vary moderately for each plant, showing the affinity of each biomass with its own wastewater.

Finally, the correction factor η, accounting for the reduction of $\mu_{max,R,}$ in anoxic conditions, was evaluated by means of NUR tests. The parameter was calculated as the ratio between NUR and OUR on an oxygen equivalent basis [15], as reported in equation (8):

$$\eta = \frac{2.86 \cdot NUR}{OUR_{rbCOD}} \quad (8)$$

where OUR_{rbCOD} represents the respirogram area proportional to the rbCOD depletion (on the assumption that denitrification takes place on rbCOD).

The values of the model parameters are reported in table 4.

In table 4, the shares of the COD fractions for each plant are provided. The rbCOD percentages vary from 6.6% of the total incoming COD for plant #1 to 13.4% for plant #2, in agreement with literature values obtained by both respirometric and physical-chemical characterizations [15, 30-32]. For the three studied plants, the greater constituent is the mbCOD fraction changing from 34.0% for plant #3 to the high value of 74.0% for plant #1. The latter value, however, could be affected by the operating conditions of the plant #1, in which alternating aerobic and anoxic steps in the same reactor are realized. For this reason it was not clear if the sudden depletion of rbCOD, in the OUR profiles obtained with samples from plant #1, was due to its complete oxidation or to intracellular storage phenomena.

4.2 Simulation of WWTP #2 with BioWin Software.

The model was validated by simulating the WWTP #2 with BioWin software (EnviroSim Associates Ltd., Canada).

BioWin 3.1 uses the integrated activated sludge/anaerobic digestion (AS/AD) model, which is referred to as the BioWin General Model. This model is a combination of the international ASM1, ASM2d and ASM3 proposed by the IWA with an anaerobic digestion model. The section *model builder reactor* enables the users to customize existing models or to implement their own, allowing the calibration of the model taken into account.

318 The plant layout is presented in figure 4. As mentioned earlier, plant #2 serves
319 18,200 P.E. and operates the activated sludge process with pre-anoxic denitrification: the
320 biological section consists of one anoxic reactor followed by two aerobic reactors and two
321 settling tanks.

322 The process data, such as influent concentrations and incoming flowrates, were
323 provided by the plant staff. As it is known, missing data are a frequent issue for WWTPs,
324 whereas continuous data series are needed to simulate the plant operation. Additionally,
325 the aforementioned process data have typical diurnal trends that are often excluded by
326 automatic samplers.

327 To obtain a continuous input series data starting from discrete measures, the
328 approach proposed by Mannina and Viviani [33] was followed. The assumption of this
329 method is that, having the influent characteristics a periodic behaviour, is possible to
330 evaluate the long-term time series by means of a Fourier series. The figure 5 shows the
331 typical daily patterns of the influent characteristics for the plant #2 employed to generate
332 the Fourier series. In particular, the generic input variable Y was modelled as:

333 $$Y = \mu \cdot \left(-\beta \cdot \sin\left(\omega \cdot \left(t+\alpha\right)+\varphi_1\right) - \frac{1}{2} \cdot \beta \cdot \sin\left(2\omega \cdot \left(t+\alpha\right)+\varphi_2\right) - \frac{1}{3} \cdot \beta \cdot \sin\left(3\omega \cdot \left(t+\alpha\right)+\varphi_3\right) \right) + \mu \quad (9)$$

334 where β, ω, α, φ_1, φ_2 φ_3 are the series parameters, μ represents the daily average value of
335 considered variable and t is the time. The series parameters were evaluated by minimising
336 the standard deviations between the simulated and measured input variables. For the days
337 without measures (therefore without measured μ), missing data were replaced considering
338 a linear relationship between the nearest previous and following observations, according to
339 [13]:

340 $$\mu(t) = \left(\frac{\mu(t_+) - \mu(t_-)}{t_+ - t_-} \right) \cdot \left(t - t_-\right) + \mu\left(t_-\right) \quad (10)$$

where $\mu(t_+)$ and $\mu(t_-)$ are the measured mean value at the time (t+1) and (t-1)., respectively.

The biological unit of the plant was simulated by implementing the calibrated 4CODf+ model into the *model builder reaction* section.

The BioWin controller tool was activated to simulate the on/off plant controller for the aeration device: the lower value of DO concentration for switching on the aeration was set equal to 1,5 $mgDO \cdot L^{-1}$, whereas the higher DO value, for switching off the aeration, was set equal to 3 $mgDO \cdot L^{-1}$, according with the actual plant setting. The oxygen half-saturation constants in heterotrophic and autotrophic processes were set according to literature [15], and equal to $K_{O,H}$ = 0.2 $mgO_2\ L^{-1}$ and $K_{O,A}$ = 0.4 $mgO_2\ L^{-1}$, respectively.

The two settling tanks of figure 4 were considered as ideal clarifiers.

The return activated sludge flow and the nitrate feed flow were set equal to the influent flow rate (in agreement with the actual plant settings).

Eleven months of operations were simulated (from January to November): then, the predicted results were compared with the values of the parameters measured on field by the plant personnel

The figure 6 shows the comparison bet*ween t*he simulated and measured effluent COD and $N\text{-}NH_4$ and the comparison between the simulated and measured MLVSS concentrations into the oxidation tank. As it can be seen, the simulation reproduced the WWTP operation in a reasonably way.

To check the goodness of the prediction, the Mean Average Error (MAE) and the Average Relative Deviation (ARD) were calculated according to the following equations:

$$MAE = \frac{1}{N}\sum_{i=1}^{N}\left|m_i - p_i\right| \tag{11}$$

$$ARD = \frac{1}{N}\sum_{i=1}^{N}\frac{\left|m_i - p_i\right|}{m_i}\times 100 \tag{12}$$

where m_i and p_i are the measured and the predicted values of the output variable and N is the number of the observations. The ARD value for COD (calculated for the whole simulation period) was equal to 12.8%, indicating a good agreement [3]. Instead the ARD for N-NH_4 was equal to 30.7%, exceeding the value of 20%, recognised as the threshold for a proper calibration process [3]. However, the low values of MAE, 4.22 mg·L^{-1} for COD and 3.38 mg·L^{-1} for N-NH_4, indicate that the model can be considered unbiased [13].

The measured COD effluent concentrations were always lower than the predicted ones and this aspect can be correlated with the important deviations attested in the simulation of the effluent nitrate. For the whole simulated period, the measured N-NO_3 effluent concentrations were on average 30% lower than the BioWin predicted values (data not shown) prompting that the actual denitrification process was different than that simulated in laboratory. This was confirmed by observations done in the WWTP #2 during the sampling period: frequent rising phenomena in the secondary settling tanks were stated, meaning that a COD consuming denitrification process was taking place.

5 Conclusions

In this paper, a home-made activated sludge model 4CODf+ (based on ASM1) was calibrated using respirometric results obtained from three WWTPs. After calibration, the 4CODf+ model was also implemented in BioWin software in order to simulate the operations of one of the aforementioned plant. The results of the simulation showed a satisfactory agreement with the actual effluent data (with regard to COD and ammonia) and with the trend of MLVSS concentration measured in the aerobic reactor. Calculated MAE value for COD and N-NH_4 were equal to 4.22 mg·L^{-1} and 3.38 mg·L^{-1}, respectively, with ARD of 12.7% and 30.7%. Furthermore, the deviation of the BioWin nitrogen

390 predicted values, from measured ones, reproduced the actual denitrification criticality
391 noticed in the plant, indicating even more the efficacy of the simulation.
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References

[1] G. Insel, B. Güder, G. Güneş, E. Ubay Cokgor, Are standard wastewater treatment plant design methods suitable for any municipal wastewater?, Water Sci. Technol. 66 (2) (2012) 328-334.

[2] D. Brdjanovic, M.C.M. van Loosdrecht, P. Versteeg, C.M. Hooijmans, G.J. Alaerts, J.J. Heijnen, Modeling COD, N and P removal in a full-scale WWTP Haarlem Waarderpolder, Wat. Res. 34 (3) (2000) 846-858.

[3] E. Liwarska-Bizukoic, R. Biernacki, D. Gendaszewska, S. Ledakowic,. Improving the operation of the full scale wastewater treatment plant with use of a complex activated sludge model, Environment Protection Engineering 39 (1) (2013) 183-195.

[4] W. E. Elshorbagy, M. Shawaqfah, Development of an ASM1 dynamic simulation model for an activated sludge process in United Arab Emirates, Desalin Water Treat (2014) 1-13.

[5] G. Sin, P. A. Vanrolleghem, Extensions to modeling aerobic carbon degradation using combined respirometric–titrimetric measurements in view of activated sludge model calibration, Water Res. 41 (15), (2007) 3345–3358.

[6] B. Petersen, K. Gernaey, M. Henze, P.A. Vanrolleghem, Evaluation of an ASM1 model calibration procedure on a municipal-industrial wastewater treatment plant, J. Hydroinform 4 (1), (2002) 15-38.

[7] E. Liwarska-Bizukoic, R. Biernacki, Identification of the most sensitive parameters in the activated sludge model implemented in BioWin software, Biores. Technol. 101 (2010) 7278-7285.

[8] G. Sin, S.W.H. van Hulle, D.J.W. De Pauw, A. van Griensven, P.A. Vanrolleghem, A critical comparison of systematic calibration protocols for activated sludge models: A SWOT analysis, Wat. Res. 39 (2005) 2459-2474.

418 [9] P. A. Vanrolleghem, G. Insel, B. Petersen, G. Sin, D. De Pauw, I. Nopens, S.
419 Weijers, K. Gernaey, A comprehensive model calibration procedure for activated
420 sludge models. In: Proceedings: WEFTEC 2003, 76th Annual Technical Exhibition
421 and Conference. October 11–15, 2003, Los Angeles, CA, USA.
422 [10] J.J.W. Hulsbeek, J. Kruit, P.J. Roeleveld, M.C.M. van Loosdrecht, A practical
423 protocol for dynamic modelling of activated sludge systems, Water Sci. Technol. 45
424 (6) (2002) 127–136.
425 [11] G. Langergraber, L. Rieger, S. Winkler, J. Alex, J. Wiese, C. Owerdieck, M. Ahnert,
426 J. Simon, M. Maurer, A guideline for simulation studies of wastewater treatment
427 plants, Water Sci. Technol. 50 (7) (2004) 131–138.
428 [12] H. Melcer, P.L. Dold, R.M. Jones, C.M. Bye, I. Takacs, D.H. Stensel, A.W. Wilson,
429 P. Sun, S. Bury, Methods for wastewater characterisation in activated sludge
430 modeling. Water Environment Research Foundation (WERF), Alexandria, VA, USA
431 (2003).
432 [13] G. Mannina, A. Cosenza, P.A. Vanrolleghem, G. Viviani, A practical protocol for
433 calibration of nutrient removal wastewater treatment model, J. Hydroinform 13 (4)
434 (2011) 575-595.
435 [14] M.A. Sedran, A.S. Mehrota, A.B. Pincince. The dangers of uncalibrated activated
436 sludge simulations packages, in: Paper presented at the 2006 Water Environment
437 Foundation Conference, Dallas, TX, 2006.
438 [15] M. Henze, W.T. Gujer, M. van Loosdrecht, Activated sludge models ASM1, ASM2,
439 ASM2d and ASM3. IWA Scientific and Technical Report No.9. IWA, London, 2000.
440 [16] M. A. Hoque, V. Aravinthan, N.M. Pradhan, Can we decode the messages of
441 activated sludge through the respirograms?, Water Air Soil Pollut. 9 (2009) 449-459.
442 [17] G. Liu, J. Wang, Probing the stoichiometry of the nitrification process using the
443 respirometric approach, Water Res. 46 (2012) 5954-5962.

444 [18] T. Katipoglu-Yazan, E. Ubay Cokgor, D. Orhon, Modeling sequential ammonia
445 oxidation kinetics in enriched nitrifying microbial culture, J. Chem. Technol.
446 Biotechnol. 90 (2015) 72–79.
447 [19] H. Spanjers, P. Vanrolleghem, G. Olsson, P. Dold, Respirometry in control of the
448 activated sludge process, Wat. Sci. Tech. 34 (3-4) (1996) 117-126.
449 [20] ISTAT, 2008. http://dati.istat.it Il Sistema di indagini sulle acque. Last accessed July
450 2014.
451 [21] H. Spanjers, P. A. Vanrolleghem, G. Olsson, P. L. Dold, Respirometry in control of
452 the activated sludge process: Principles. IAWQ Sci. and Tech. Report No.7. IAWQ,
453 London, UK, 1998.
454 [22] M. Henze, C.P.L. Jr Grady, W. Gujer, G.v.R. Marais, T. Matsuo T., Activated sludge
455 model No.1. IAWQ Sci. and Tech. Report No.1. IAWQ, London, UK, 1987.
456 [23] M. Henze. Characterization of wastewater for modelling of activated sludge
457 processes, Water Sci. Technol. 25 (6) (1992) 1-15.
458 [24] A. Ramdani, P. Dold, P. Deleris, D. Lamarre, A. Gadbois. Biodegradation of the
459 endogenous residue of activated sludge. Water Res. 44 (7) (2010) 2179-2188.
460 [25] M. Friedrich, I. Takács, A new interpretation of endogenous respiration profiles for
461 the evaluation of the endogenous decay rate of heterotrophic biomass in activated
462 sludge, Water Res. 47 (2013) 5639-5646.
463 [26] P. A. Vanrolleghem, H. Spanjers, B. Petersen, P. Ginestet, I. Takacs. Estimating
464 (combination of) activated sludge model no.1 parameters and components by
465 respirometry, Water Science and Technology 39 (1) (1999) 195-214.
466 [27] O. Nowak, P. Schweighofer, K. Svardal, Nitrification inhibition. A method for the
467 estimation of actual maximum autotrophic growth rates in activated sludge systems,
468 Water Sci. Technol. 30 (6) (1994) 9-19.

469 [28] J.B. Copp, K.L. Murphy, Estimation of the active nitrifying biomass in activated
470 sludge, Water Res. 29 (8) (1995) 1855-1862.
471 [29] R. Vismara, Depurazione biologica. Teoria e processi, 2nd edition, Hoepli.,
472 Milano,1988.
473 [30] F. Lagarde, M.H. Tusseau-Vuillemin, P. Lessard, A. Héduit, F. Dutrop, J.M.
474 Mouchel, Variability estimation of urban wastewater biodegradable fractions by
475 respirometry. Water Res. 39 (19) (2005) 4768–4778.
476 [31] I. Pasztor, P. Thury, J. Pulai, Chemical oxygen demand fractions of municipal
477 wastewater for modelling of wastewater treatment. Int. J. Environ. Sci. Tech 6 (11)
478 (2009) 51-56.
479 [32] P. Lu, X. Zhang, D. Zhang. An integrated system for wastewater COD
480 characterization and a case study. Water Sci. Technol. 62 (4) (2010) 866-874.
481 [33] G. Mannina, G. Viviani, Hybrid moving bed biofilm reactors: an effective solution for
482 upgrading a large wastewater treatment plant, Wat. Sci. Tech. 60 (5) (2009) 1103-
483 1116.
484

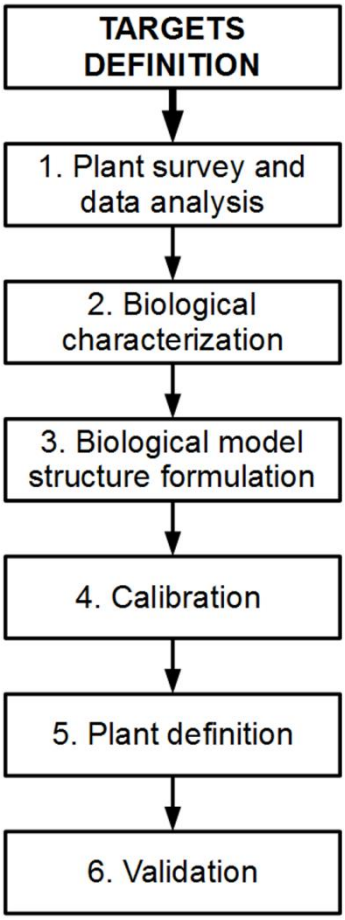
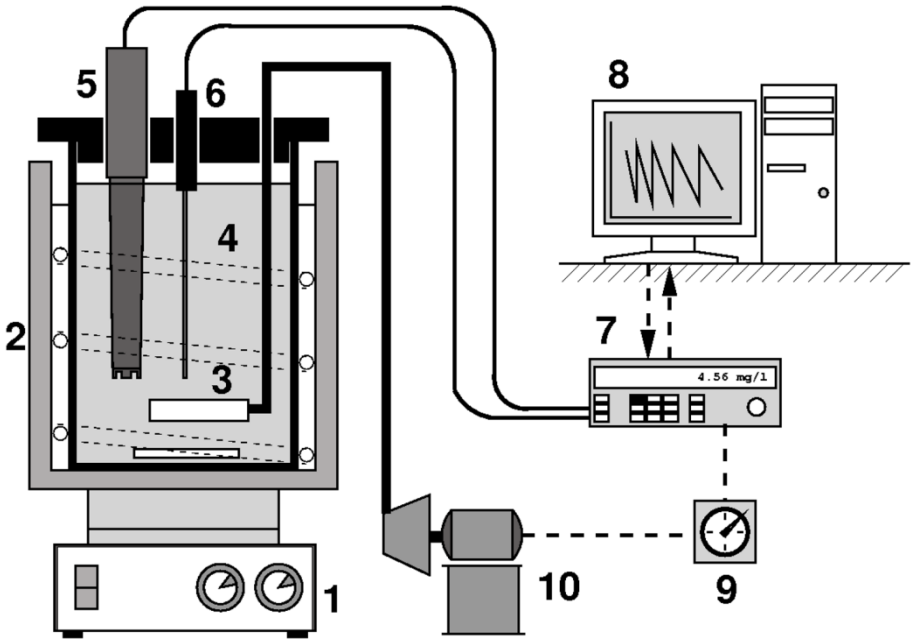

TARGETS DEFINITION
1. Plant survey and data analysis
2. Biological characterization
3. Biological model structure formulation
4. Calibration
5. Plant definition
6. Validation

Figure 1



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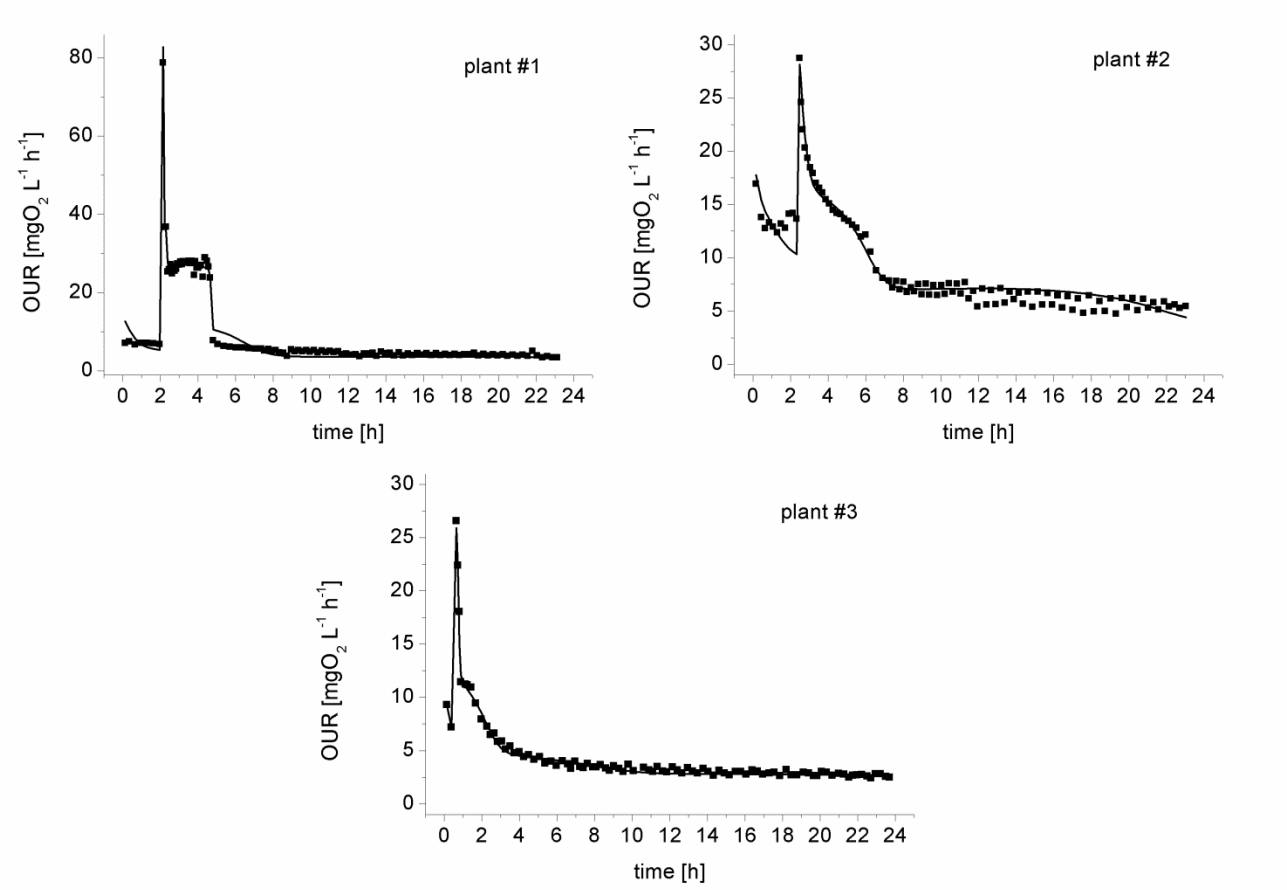
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time [h]
plant #2
OUR [mgO2 L-1 h-1]
time [h]
plant #3
OUR [mgO2 L-1 h-1]
time [h]

Figure 3

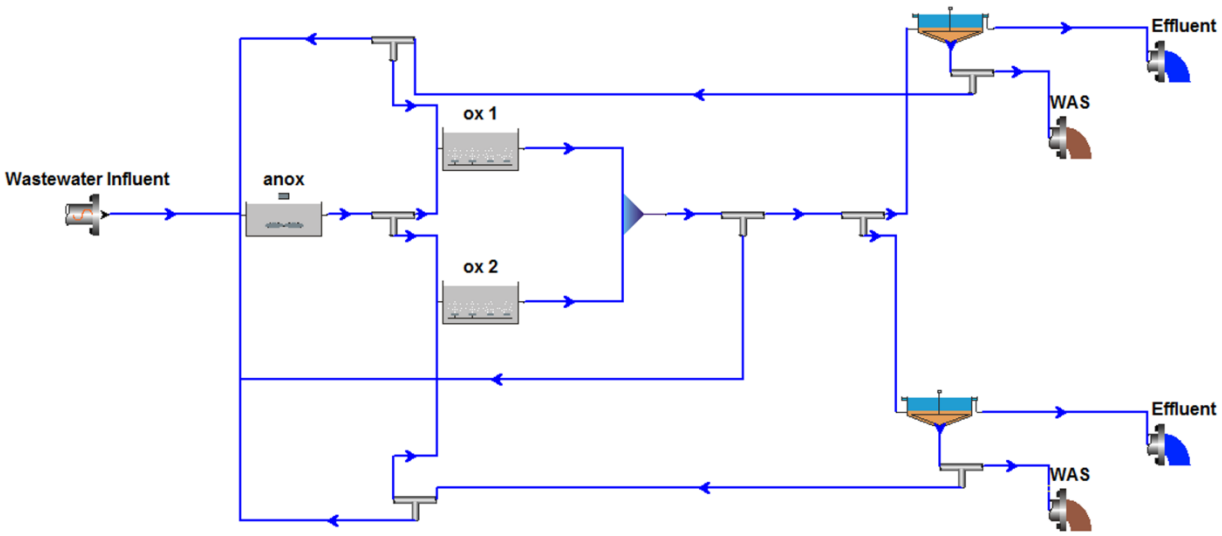
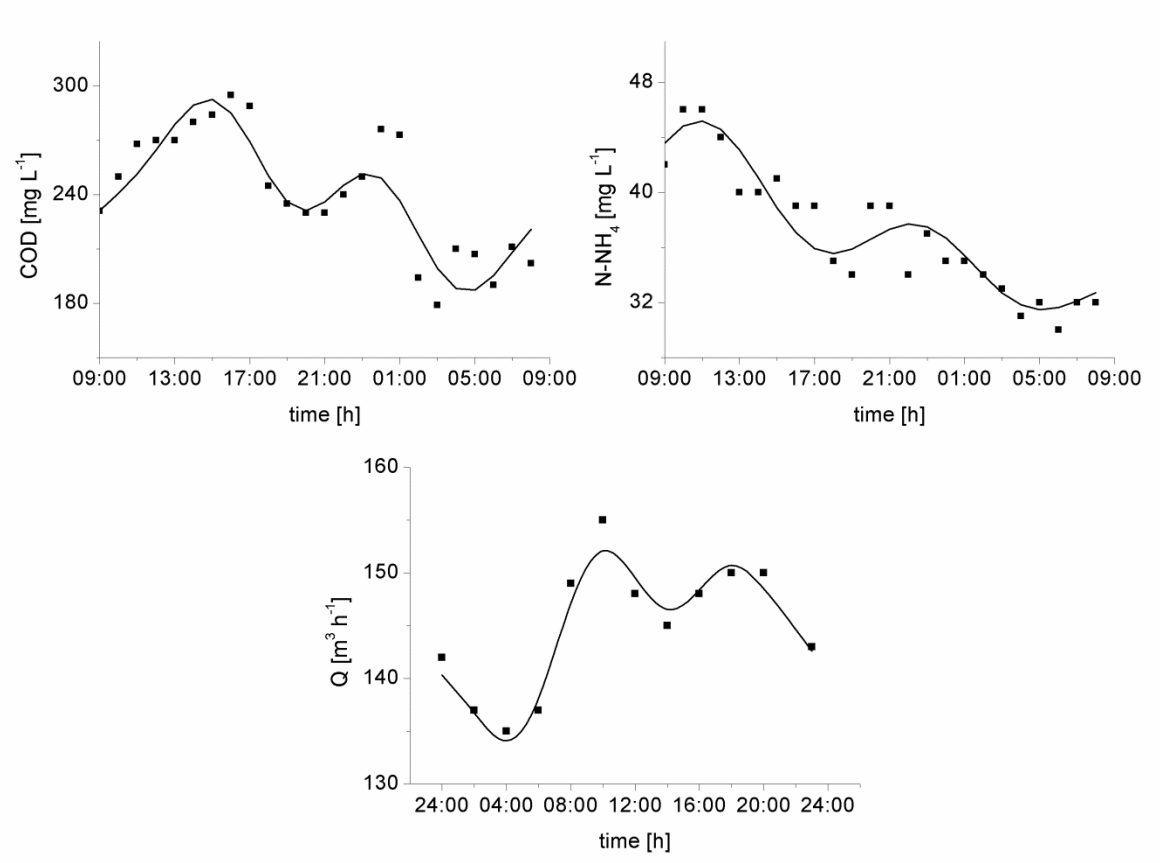

Wastewater Influent
anox
ox 1
ox 2
Effluent
WAS
Effluent
WAS

Figure 4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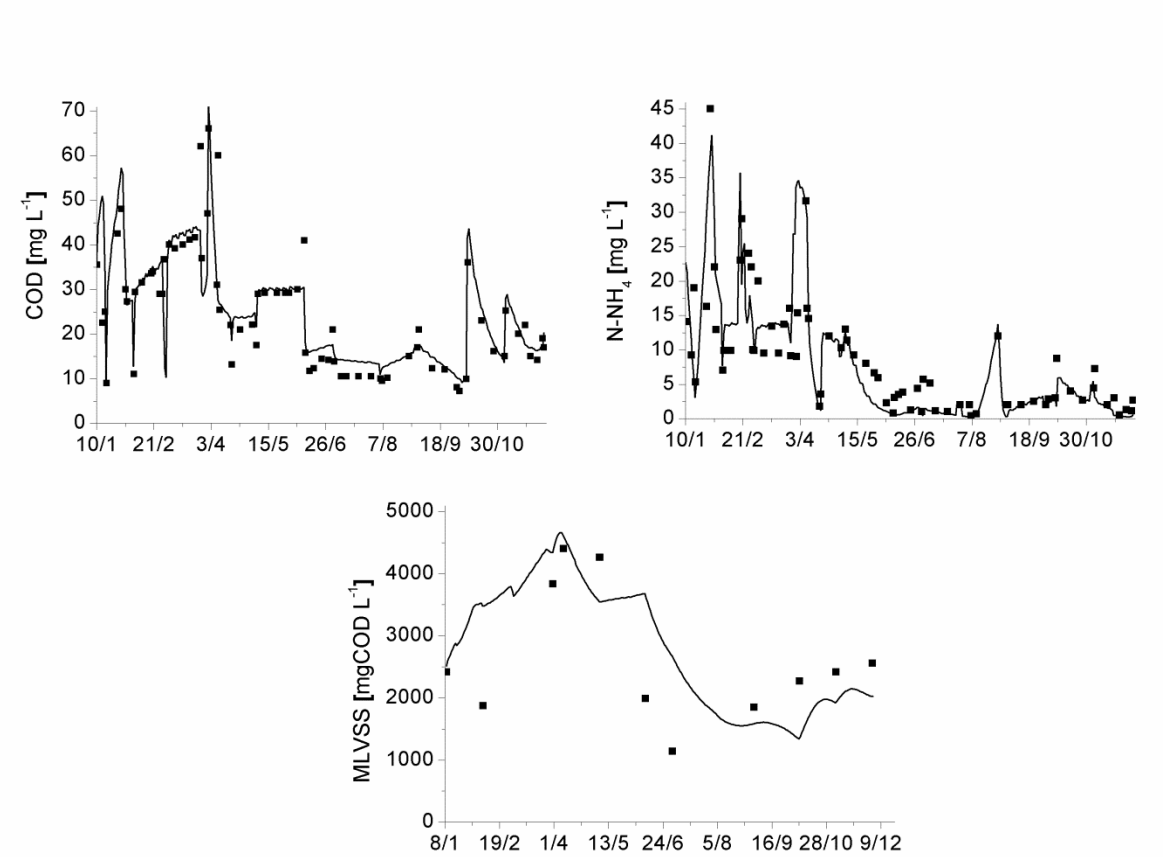
240
180
09:00 13:00 17:00 21:00 01:00 05:00 09:00
time [h]
N-NH4 [mg L-1]
48
40
32
09:00 13:00 17:00 21:00 01:00 05:00 09:00
time [h]
Q [m3 h-1]
160
150
140
130
24:00 04:00 08:00 12:00 16:00 20:00 24:00
time [h]

Figure 5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60
50
40
30
20
10
0
10/1 21/2 3/4 15/5 26/6 7/8 18/9 30/10
N-NH4 [mg L-1]
45
40
35
30
25
20
15
10
5
0
10/1 21/2 3/4 15/5 26/6 7/8 18/9 30/10
MLVSS [mgCOD L-1]
5000
4000
3000
2000
1000
0
8/1 19/2 1/4 13/5 24/6 5/8 16/9 28/10 9/12

Figure 6

Figure captions

Figure 1 Calibration flow-chart

Figure 2 Experimental respirometer: (1) Magnetic stirrer; (2) Thermostatic water-bath; (3) Oxygen porous diffuser; (4) Mixed liquor; (5) OD probe; (6) T probe; (7) Data-logger, acquisition data system; (8) PC; (9) Timer; (10) Membrane pump.

Figure 3 Examples of respirograms: (▪) measured values, (—) fitted values

Figure 4 Plant #2 layout for simulation in BioWin

Figure 5 Daily trends of influent characteristics: (▪) measured values, (—) simulated Fourier series

Figure 6 Simulation results: (▪) measured values, (—) simulated values.

Table 1. WWTPs and influent flowrates characteristics

Parameter	Unit	Value Plant #1	Plant #2	Plant #3
Influent WWs characteristics				
Total Suspended Solids	[mgTSS·L^{-1}]	110 (64÷148)	48 (17÷108)	166 (65÷282)
Chemical Oxygen Demand	[mgCOD·L^{-1}]	314 (197÷417)	240 (53÷373)	357 (163÷622)
Ammonium nitrogen	[mgN·L^{-1}]	35 (8÷57)	20 (7÷48)	32 (22÷38)
Nitrate nitrogen	[mgN·L^{-1}]	0.5 (0.0÷1.3)	3.9 (2.0÷8.0)	0.4 (0.0÷1.1)
Flow rates				
Influent flow rate (average), Q_{IN}	[m^3 d^{-1}]	1,400	3,642	14,688
Recirculation of activated sludge (ratio), RAS	-	1	1	2
Recirculation of aerated sludge (ratio), R	-	n.a.	1	n.a.
Volumes/Size				
Anoxic reactor	[m^3]	525 (alternating)	208	n.a.
Aerobic reactor	[m^3]		514x2	2350
Final settling tank diameter	[m]	11.0	14.4	35.0
Side water depth of clarifier	[m]	2.5	2.5	3.0
Biological section operation				
MLVSS	[mgVSS·L^{-1}]	2115	2883	4434
Solids Retention Time, SRT	[d]	13	8	6.5
Hydraulic Retention Time, HRT	[h]		11.8	
Total blower capacity, Q_{AIR}	[Nm^3 h^{-1}]	400	732	

Table 2. 4CODf+ Model – Stoichiometry and process kinetics

	Heterotrophic Bacteria (HB)									
	O_2	S_R	S_M	S_S	NH_4	NO_3	X_H	X_A	X_I	Process kinetics
growth on rbCOD	$-\frac{(1-Y_H)}{Y_H}$	$-\frac{1}{Y_H}$					1			$\mu_{\max R}\frac{S_R}{(S_R+K_{SR})}\frac{O_2}{(O_2+K_{O2})}\vartheta^{(T-20)}X_H$
growth on mbCOD	$-\frac{(1-Y_H)}{Y_H}$		$-\frac{1}{Y_H}$				1			$\mu_{\max M}\frac{S_M}{(S_M+K_{SM})}\frac{O_2}{(O_2+K_{O2})}\vartheta^{(T-20)}X_H$
growth on sbCOD	$-\frac{(1-Y_H)}{Y_H}$			$-\frac{1}{Y_H}$			1			$\mu_{\max S}\frac{S_S}{(S_S+K_{SS})}\frac{O_2}{(O_2+K_{O2})}\vartheta^{(T-20)}X_H$
anoxic growth		$-\frac{1}{Y_H}$				$-\frac{(1-Y_H)}{2.86\,Y_H}$	1			$\eta\mu_{\max R}\frac{S_R}{(S_R+K_{SR})}\frac{K_{O2}}{(K_{O2}+S_{O2})}\frac{NO_3}{(NO_3+K_{NO3})}\vartheta^{(T-20)}X_H$
endogenous respiration				$+(1-f_I)$			-1		f_I	$b_H\vartheta_b^{(T-20)}X_H$
	Autotrophic Bacteria (AB)									
	O_2	S_R	S_M	S_S	NH_4	NO_3	X_H	X_A	X_I	Process kinetics
aerobic growth	$-\frac{(4.57-Y_A)}{Y_A}$				$-\frac{1}{Y_A}$	$+\frac{(1-Y_A)}{Y_A}$		1		$\mu_{\max A}\frac{NH_4}{(NH_4+\mathrm{K_{NH4}})}\frac{O_2}{(O_2+K_{O2\,A})}\vartheta^{(T-20)}X_A$
endogenous respiration				$+(1-f_I)$				-1	f_I	$b_A\vartheta_b^{(T-20)}X_A$

Note: The previous is the whole model; when accounting for the respirometry only, anoxic growth and oxygen limitation have to be erased.

Table 3. Input and output parameters in *Evaluat*OUR SW

Input Data	Output Data
time-course of OUR and T (file *.txt)	$\mu_{max,R}$ max growth rate of HB on the rbCOD [d^{-1}]
sludge volume [mL]	$\mu_{max,M}$ max growth rate of HB on the mbCOD [d^{-1}]
wastewater volume [mL]	$\mu_{max,S}$ max growth rate of HB on the sbCOD [d^{-1}]
water volume (if added) [mL]	$\mu_{max,A}$ max growth rate of AB [d^{-1}]
TSS in the sludge [mg·L^{-1}]	b_H decay rate of HB [d^{-1}]
VSS in the sludge [mg·L^{-1}]	b_A decay rate of AB [d^{-1}]
COD in the sludge [mg·L^{-1}]	Y_H heterotrophic yield [gSSV·$gCOD^{-1}$]
COD in the wastewater [mg·L^{-1}]	Y_A autotrophic yield [gSSV·$gCOD^{-1}$]
COD at the end of the experiment [mg·L^{-1}]	$K_{S,R}$ half saturation constant for HB growth on rbCOD [mg·L^{-1}]
N-NH_4 in the sludge [mg·L^{-1}]	$K_{S,M}$ half saturation constant for HB growth on mbCO [mg·L^{-1}]
N-NH_4 in the wastewater [mg·L^{-1}]	$K_{S,S}$ half saturation constant for HB growth on sbCOD [mg·L^{-1}]
time of addition of wastewater [s]	K_{NH4} half saturation constant for AB growth [mg·L^{-1}]
addition of ATU: 0 = no, 1 = yes	$rbCOD_{WW}$ readily biodegradable COD in ww [mg·L^{-1}]
number of ww fractions (3 or 4)	$mbCOD_{WW}$ medium rate biodegradable COD in ww [mg·L^{-1}]
	$sbCOD_{WW}$ slowly biodegradable COD in ww [mg·L^{-1}]
	$rbCOD_S$ readily biodegradable COD in AS [mg·L^{-1}]
	$mbCOD_S$ medium rate biodegradable COD in AS [mg·L^{-1}]
	$sbCOD_S$ slowly biodegradable COD in AS [mg·L^{-1}]

Table 4. Respirometric tests results

Parameter		Unit	Plant #1	Plant #2	Plant #3
$\mu_{max,R}$	(a)	[d^{-1}]	0.251	0.516	0.422
$\mu_{max,M}$	(a)	[d^{-1}]	0.106	0.191	0.115
$\mu_{max,S}$	(a)	[d^{-1}]	0.058	0.082	0.069
$\mu_{max,A}$	(b)	[d^{-1}]	0.145	0.240	0.251
b_H	(b)	[d^{-1}]	0.033	0.052	0.017
b_A	(c)	[d^{-1}]	0.050	0.050	0.050
Y_H	(b)	[$gCOD \cdot gCOD^{-1}$]	0.471	0.531	0.599
Y_A	(c)	[$gCOD\ gN^{-1}$]	0.185	0.185	0.185
$K_{S,R}$	(a)	[$mg \cdot L^{-1}$]	0.23	10.73	4.40
$K_{S,M}$	(a)	[$mg \cdot L^{-1}$]	0.12	7.26	4.11
$K_{S,S}$	(a)	[$mg \cdot L^{-1}$]	1.60	7.96	3.04
K_{NH4}	(a)	[$mg \cdot L^{-1}$]	1.47	0.99	0.561
K_{NO3}	(c)	[$mg \cdot L^{-1}$]	0.50	0.50	0.50
η	(a)	-	0.28	0.50	0.56
f_i	(c)	-	0.08	0.08	0.08
rb COD	(a)	[%]	6.6	13.4	7.0
mb COD	(a)	[%]	74.0	54.4	34.0
sb COD	(a)	[%]	8.2	10.1	28.9
i COD	(a)	[%]	11.2	22.1	30.1

(a) evaluated; (b) calculated; (c) from literature