DOI: 10.1002/jctb.1085

Modelling and optimisation of a chemical industry wastewater treatment plant subjected to varying production schedules

Stijn WH Van Hulle and Peter A Vanrolleghem*
BIOMATH, Department of Applied Mathematics, Biometrics and Process Control, Ghent University, Coupure Links 653, B-9000 Gent, Belgium

Abstract: Industrial wastewater treatment plants (WWTPs) have to provide 100% reliability and availability for the discharging facilities at an industrial site. Varying production schedules at these facilities and specific components occurring in the industrial wastewater considerably hinder the optimisation of industrial WWTPs. In this context it is shown in this paper that model-based optimisation is an efficient and cost-reducing way to ensure that an industrial WWTP functions well. The aim of the study presented was two-fold. The first step was to show the usefulness of a proposed procedure to build and calibrate a model for the industrial WWTP. The second objective was to use the model for optimisation of the WWTP. As an example, a large set of possible production schedules in the different discharging facilities was simulated. Based on these simulations it could be predicted which schedules allow the effluent standards to be met and which do not. The calibrated and validated model was also used to investigate different operating strategies such as the in-series operation of the two available aeration tanks. In fact, with the model it was shown that a 20% reduction of the degradable COD concentration in the effluent could be achieved by operating the tanks in series instead of in parallel. This case study shows how the approach presented can lead to fast and cost effective modelling and optimisation of an industrial WWTP.

Keywords: industrial wastewater treatment plant; activated sludge model; model-based optimisation; scenario analysis; calibration

NOTATION

b_H	Decay rate for heterotrophs (day^{-1})
K_S	Half saturation constant for heterotrophic growth (mgCOD dm^{-3})
K_{SIM}	Inhibition constant for fictive component (mgCOD dm^{-3})
K_{SSP}	Inhibition constant for specific component (mgCOD dm^{-3})
OUR	Oxygen uptake rate (mgO$_2$ dm^{-3} d^{-1})
Q	Flow rate through the pump (m^3 d^{-1})
S_{O2}	Oxygen concentration (mgO$_2$ dm^{-3})
S_S	Substrate concentration (mgCOD dm^{-3})
t	Time (d)
V	Volume (m^3)
WWTP	Wastewater treatment plant
X_H	Active heterotrophic biomass (mgcellCOD dm^{-3})
Y_H	Heterotrophic yield coefficient (mg cellCOD mgCOD^{-1})
μ_H	Maximum heterotrophic growth rate (day^{-1})
ρ	Process rate (mgCOD dm^{-3} d^{-1})
X_I	Inert biomass (mgcellCOD dm^{-3})
X_S	Slowly biodegradable biomass (mgcellCOD dm^{-3})

INTRODUCTION

One way of dealing with industrial wastewater is to discharge it to a municipal wastewater treatment plant (WWTP) where it is treated together with domestic wastewater. This brings some advantages, such as the smoothing of peakloads due to the diurnal load changes in a purely municipal system. However, in view of the uncoupling policy of the Flemish Government, this type of operation is no longer allowed in the northern part of Belgium. Furthermore, large companies, such as the company under study, would be a major contributor to a municipal WWTP and may cause overloading. Therefore companies are increasingly forced to have their own WWTP which is subject to stringent effluent standards. These WWTPs have to provide 100% reliability and availability for the discharging facilities.[1]

* Correspondence to: Peter A Vanrolleghem, BIOMATH, Department of Applied Mathematics, Biometrics and Process Control, Ghent University, Coupure Links 653, B-9000 Gent, Belgium
E-mail: peter.vanrolleghem@ugent.be
Contract/grant sponsor: Hemmis NV
(*Received 28 October 2003; revised version received 2 March 2004; accepted 2 March 2004*)
Published online 28 July 2004

The industrial WWTP under study treats wastewater in the same way most municipal WWTPs do, ie with an activated sludge process. However, some differences can be pointed out. The first problematic difference is that domestic wastewater normally has a more or less constant composition, although weekly or diurnal variations occur.[2] The composition of industrial wastewater on the other hand fluctuates considerably more because of the variations in the schedules of the production facilities at the industrial site discharging to the single WWTP. This complexity of the wastewater composition hinders the optimisation of the WWTP considerably. Model-based optimisation however is able to deal with this and can be considered as an efficient, cost reducing and elegant way to ensure that an industrial WWTP functions well.[3,4]

A second problem is that some components occur in the industrial wastewater that are normally not present in domestic wastewater. They may be toxic (eg cyanide), have self-inhibitory degradation kinetics (eg phenol) or have specific physico-chemical properties (eg volatile organics). This makes it necessary to extend the normally applied Activated Sludge Model Nr 1[5] (ASM1) to cope with these specific components.

The aim of this study was two-fold. The first was the building and calibration of a model for the industrial WWTP. It is based on a previously proposed calibration protocol,[4] that has to be extended to take into account the specific components in the wastewater. On the other hand some simplifications could be made to the procedure since no nitrification occurs in the WWTP.

The second objective of the study was to use the model for optimisation of the WWTP. By simulating with the calibrated and validated model it could, for example, be estimated how much reduction of the degradable COD concentration in the effluent could be achieved by making design or operational changes. Also a large set of possible schedules in the production facilities at the industrial site was simulated, allowing prediction of which schedules allow the effluent standards to be met and which do not.

METHODS

Description of the WWTP

The schematic lay-out of the WWTP as implemented graphically in the modelling and simulation environment WEST®[6] (Hemmis NV, Kortrijk, Belgium) is given in Fig 1. Two production facilities are discharging to the plant. In particular, facility 1 has a varying production schedule. In total 11 products are produced and every product has a certain amount of polluted water associated with it, as can be seen from Table 1. In this polluted water the total COD (as indicated in Table 1) can be divided into a readily biodegradable fraction and a fraction that consists of a specific component that is produced in production facility 1. For confidentiality reasons, the products will be named with the letters A, B, C, D, E, F, G, H, K, M and S. Not all product combinations are possible: the production facility can only produce A or B. Also it can only produce G, H, K or M and C or S. So a product combination such as A, C, D and G is possible while a product combination such as A, B, C, K and G is not. This leads to a total of 359 possible product combinations. Because the COD load is so high, a chemical pre-treatment that eliminated approximately 80% of the COD was constructed so that on average 500 mg COD dm^{-3} of product was discharged from production facility 1.

The plant also treats the rainwater collected at the production site and water coming from a landfill, but the flow rate and pollutants load of this last discharge is very low. Average flow rates, temperatures and COD concentrations of the different flows are summarised in Table 2.

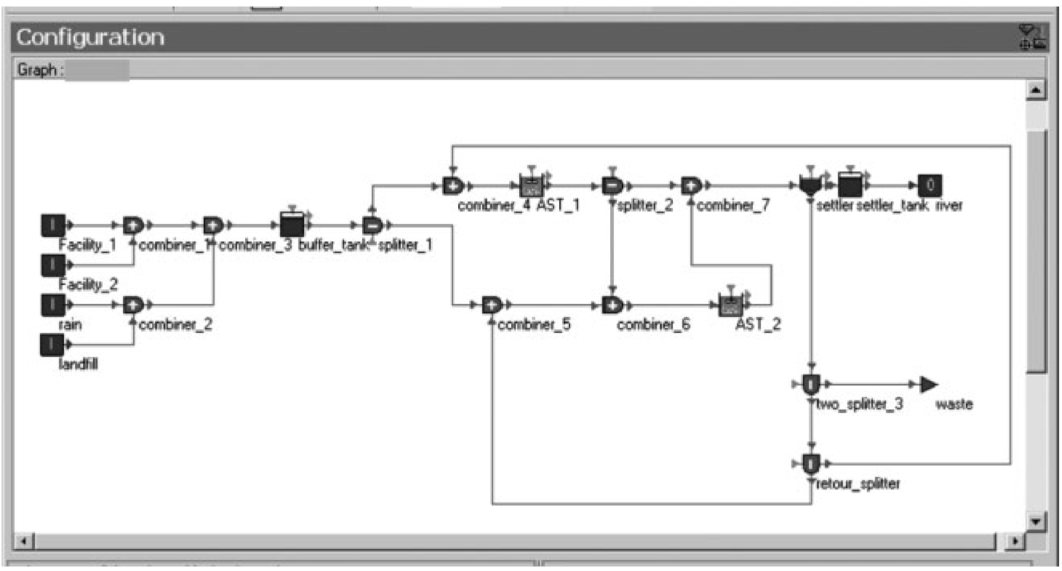

Figure 1. The schematic lay-out of the WWTP under study.

Table 1. Amount of water and pollution associated with the products produced by production facility 1

Product	Average flow rate ($m^3\,d^{-1}$)	COD (mgCOD dm^{-3})	Specific component concentration (mgCOD dm^{-3})
A	720.0	7480.0	2846.0
B	763.2	6740.0	3399.0
C	266.4	4650.0	99.0
D	64.8	23 233.0	17 420.0
E	482.4	4813.0	1528.0
F	355.2	1223.0	1017.0
G	508.8	7603.0	5795.0
H	204.0	1258.0	1041.6
K	458.4	1258.0	1041.6
M	223.2	1278.0	1225.0
S	355.2	6178.0	4324.0

Table 2. Average flow rates, temperatures and COD concentrations of the different flows to the WWTP

Stream	Average flow rate ($m^3\,d^{-1}$)	COD concentration (mgCOD dm^{-3})	Temperature (°C)
Facility 1	1460	1250	40
Facility 2	530	160	Ambient
Rainwater	1400	—	Ambient
Landfill water	31	—	Ambient

After mixing of the different streams in a 300 m^3 buffertank the wastewater is sent via splitter 1 (Fig 1) to two parallel activated sludge tanks (AST) with a volume of 3000 m^3 each. Although the ASTs have a very large volume, they can still be considered as ideally mixed as a result of the long retention time. In the model implemented in WEST® a connection between the two ASTs is foreseen to anticipate a partial or total serial operation of the AST. This connection goes via splitter 2 and combiner 6, but does not exist yet at the actual plant, although it has been suggested to be a feasible upgrade scenario.

The treated wastewater coming from the two AST is combined in combiner 7 and sent to a clarifier which has excellent performance. The point settler model selected from the WEST® modelbase has no volume. Hence, in order to mimic the residence time in the settler, a buffertank with the same volume is placed after the settler. The effluent of the settler is discharged to the river and the return sludge is recycled to both ASTs through the retour splitter and combiners 4 and 5. Part of the return sludge is wasted. The average hydraulic residence time (HRT) and the average sludge residence time (SRT) of the installation are confirmed to be 1.5 days and 45 days, respectively. Despite this long SRT only carbon is removed and no nitrification occurs, because nitrification is inhibited by specific components in the influent of the WWTP. Approximately 400 mgCOD dm^{-3} of substrate is degraded.

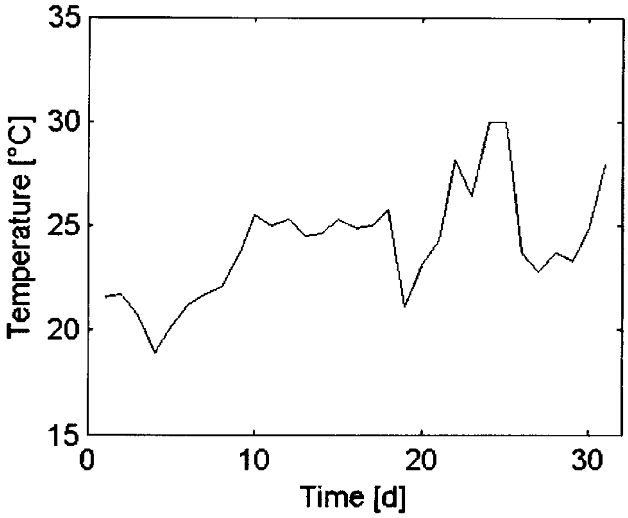

Figure 2. The temperature in one of the ASTs over a 30-day period.

Extension of ASM1

ASM1[5] was extended with two extra components; S_{SP} and S_{IM}, to take into account specific components that are present in the wastewater. The first component is representative for a specific component in the wastewater that is coming from production facility 1 and which shows an inhibitory effect on the degradation. The second component is a fictive component that could be discharged from a new, additional production facility. In this way the influence of an additional production facility can now be evaluated with the model without the requirement to extend the model further. The inhibitory influence of both components on the COD degradation kinetics of the activated sludge can be modelled by including two additional switching functions $K/(K+S)$ in the process rate formulation:

$$\rho = \rho' \frac{K_{SSP}}{K_{SSP} + S_{SP}} \frac{K_{SIM}}{K_{SIM} + S_{IM}}$$

In this equation ρ is the process rate when both new components are taken into account, ρ' is the original ASM1 process rate without the effect of S_{SP} and S_{IM}. K_{SSP} and K_{SIM} are the inhibition constants for S_{SP} and S_{IM}. Of course, if it turns out that other kinetics are appropriate for the new fictive component, these kinetics can easily be implemented. Note also that it was assumed that both S_{SP} and S_{IM} only have an influence on the kinetics, but that they are not degraded themselves.

A second, more traditional, extension of the standard ASM1 is the insertion of a temperature dependency of the kinetics, because, as reported by the operators, the temperature in the AST may vary up to 10 °C in a relatively short time. This is illustrated in Fig 2 where the temperature in one of the ASTs is depicted over a 30-day period. By applying an Arrhenius type of equation,[5] the temperature dependency is included in the model:

$$\rho(T) = \rho(T_{ref}) e^{\theta(T - T_{ref})}$$

where T is the actual reactor temperature, T_{ref} is the reference temperature, which was 25 °C in this study, and θ is the Arrhenius constant. Also the oxygen transfer coefficient[7] and the oxygen saturation concentration[8] were made dependant on the temperature.

The BIOMATH calibration protocol[4]

Model calibration and validation was based on a calibration protocol[4] that is summarised in Fig 3. This protocol is composed of four main stages and 10 modules (see Fig 3). The first stage is the definition of the target(s) of the modelling exercise followed by decision-making on the necessary information for the WWTP. Some of the modules (1–10) can be skipped depending on the general evaluation of whether the targets are reached. The second stage is the collection of detailed information on the WWTP. The mass transfer (hydraulic and oxygen transfer), biological, settling and the influent characterisations are included in this step. In addition, the experimental or laboratory-scale work is incorporated. By averaging the influent and operational characteristics, steady-state modelling is performed for the mass transfer, settler and the biological model. The third step includes the complete calibration of the activated sludge model using the dynamic influent data incorporating the parameter values obtained from laboratory-scale experiments or full-scale data. At the last stage, decisions will be made upon eventual re-iteration of the modules.

Experimental setup

The characterisation of the sludge biokinetics was based on respirometry and full-scale data. A hybrid respirometry set-up[9] was used for determination of the maximum specific growth rate for the heterotrophic biomass (μ_H) and the heterotrophic yield coefficient (Y_H). This hybrid set-up consists of two reactors, an aerated and a non-aerated one, that are connected in such a way that activated sludge can be circulated continuously from one to the other. In the non-aerated reactor the oxygen transfer coefficient is 0 and therefore the following oxygen mass balance can be used for this reactor:

$$\frac{dS_{O2}^{NA}}{dt} = \frac{Q}{V}(S_{O2}^{A} - S_{O2}^{NA}) - OUR$$

where Q is the flow rate through the pump, V is the volume of the non-aerated reactor, OUR is the oxygen uptake rate and S_{O2}^{NA} and S_{O2}^{A} are the oxygen concentration in the non-aerated reactor and the aerated reactor respectively. Since both the oxygen concentration in the aerated reactor and the non-aerated reactor are measured, the only unknown in this equation is the OUR. Thus, the OUR can easily be calculated. Batch experiments were performed leading to respirograms that can be interpreted

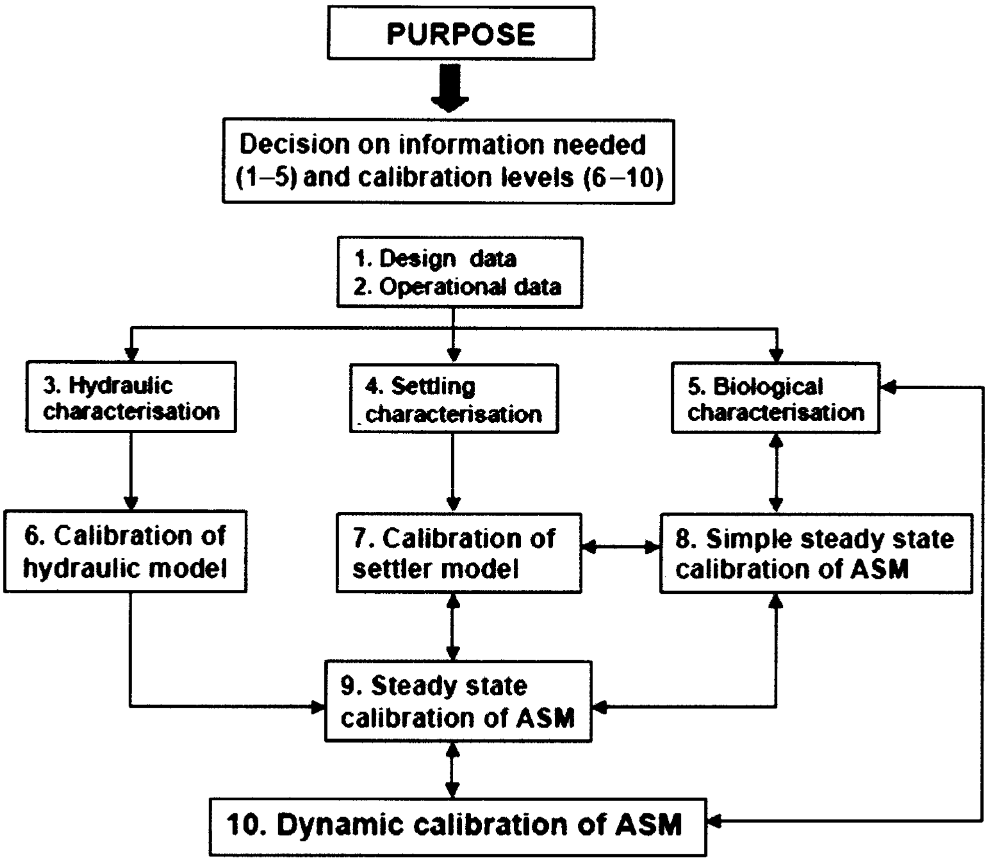

Figure 3. The applied calibration protocol[4].

for the characterisation of the wastewater and the biodegradation kinetics.

For determination of the decay coefficient (b_H) a different respirometric method[10] was used. In this respirometric test the *OUR* of a sludge sample is measured over a period of several days. No substrate is added and the *OUR* of the first day is not considered since on the first day residual substrate is degraded.

RESULTS AND DISCUSSION

Model calibration and validation

After investigating the design and a year of operational data (steps 1 and 2 in Fig 3), some measurement errors were found by making mass balances for water and COD. These errors were reported to the operators and subsequently corrected on the basis of logbook information. Both the hydraulic and settling characterisation (steps 3 and 4 in Fig 3) have already been tackled during the basic description of the WWTP. Indeed, the ASTs can be considered as completely mixed and are therefore modelled as completely stirred reactors (CSTR). The aeration coefficient in the ASTs was set to $50\,d^{-1}$ on basis of the off-gas analysis. The sludge settles extremely well, so a point settler with a non-settleable fraction of the biomass (f_{ns}) is considered as an appropriate model for the settler.

Since in this case a specific industrial wastewater was investigated was not possible to use the default values of the biological parameters of ASM1 as indicated in the IWA report[5] and therefore a thorough biological characterisation was necessary (step 5 in Fig 3). Since no nitrification occurs, only aerobic heterotrophic activity had to be investigated. The decay coefficient was determined by a respirometric method[10] and subsequently corrected for use in the ASM model.[11] The slope of the natural logarithm of the measured *OUR*-evolution as function of the time is equal to the heterotrophic decay coefficient (b'_H). This coefficient however has to be corrected for use in the ASM1 model according to the following equation:[5]

$$b_H = \frac{b'_H}{(1 - Y_H(1 - f_P))}$$

where f_P represents the inert fraction of the biomass. A value of $0.42\,d^{-1}$ at 25 °C was obtained.

Both the heterotrophic yield and the maximum specific growth rate for the heterotrophic biomass (μ_H) were derived from an oxygen uptake rate (*OUR*) profile as explained below. An *OUR* profile was recorded from a batch experiment with the hybrid respirometric set-up.[9] First the endogenous respiration was subtracted from this profile. The resulting substrate oxidation-related *OUR* profile was used for determination of Y_H and μ_H (Fig 4).

The surface under the profile is a measure for Y_H according to the following formula:[11]

$$Y_H = 1 - \frac{\int OUR\,dt}{S_S(t = 0)}$$

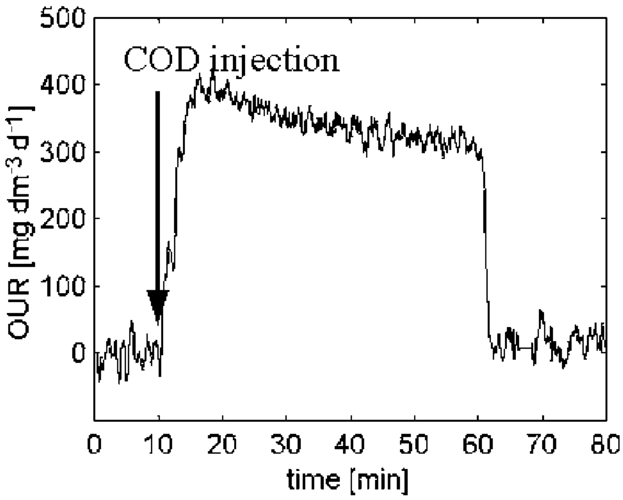

Figure 4. The substrate oxidation-related *OUR* profile for the determination of Y_H and μ_H.

In this formula the surface under the OUR profile is represented by the integral and $S_S(t = 0)$ is the initial substrate concentration. With a surface of $8.58\,mg\,dm^{-3}$ and an initial substrate concentration of $33\,mgCOD\,dm^{-3}$, a heterotrophic yield of 0.74 mg cell COD (mg substrate COD^{-1}) is obtained.

Combining the heterotrophic biomass concentration, which was assumed to be $600\,mgCOD\,dm^{-3}$ in the batch experiment, with the maximum *OUR* (OUR_{max}), which was $403\,mg\,dm^{-3}\,d^{-1}$, leads to the calculation of μ_H:[4]

$$\mu_H = \frac{OUR_{max} Y_H}{(1 - Y_H)X_H} = 1.9\ d^{-1}$$

The values obtained for Y_H and b_H are rather high for the studied WWTP. However, all three parameter values are well within an acceptable range.

After the biological characterisation a steady state calibration was performed (step 9 in Fig 3). For this the average influent and effluent data of the plant were collected. No particulates enter the WWTP, so only soluble components, either degradable or specific, had to be considered in the influent. The available influent data were used as such as input for the simulation. After comparing the measured and calculated data three more parameters of ASM1 were adjusted to improve the fit. The inert fraction of the biomass (f_P) which has a default value of 0.08 in ASM1 was set to 0.06 and the non-settleable fraction of the biomass (f_{ns}) was set to 0.014, ie 1.4% of the incoming sludge leaves the settler via the effluent. The value of K_{SSP} was set to $250\,mgCOD\,dm^{-3}$. This steady state analysis gave rise to the following sludge composition: $X_H = 1.2\,gCOD\,dm^{-3}$ and $X_I = 1.5\,gCOD\,dm^{-3}$. The value of X_S was very low ($5\,mgCOD\,dm^{-3}$). The concentration of heterotrophic biomass is about twice as high as the value used for the calculation of μ_H, since the sludge concentration for biological characterisation was halved for practical reasons.

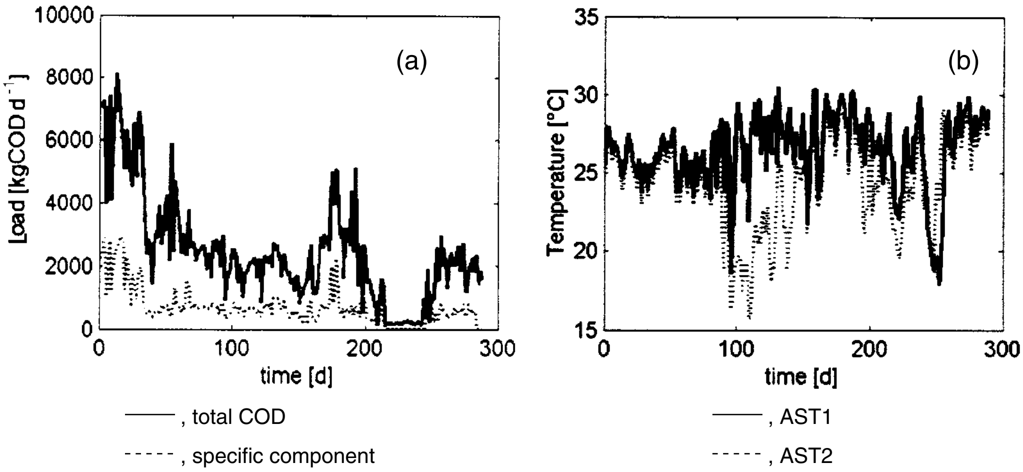

Figure 5. The influent load of total COD and specific component to the WWTP (a) and the temperature in the ASTs (b) over the 288-day calibration period.

Step 10 in the calibration protocol, the dynamic calibration, was skipped as the model was directly validated with the data set obtained from detailed measurement over 288 days. In Fig 5 the influent load of total COD and specific component to the WWTP and the temperature in the ASTs over the 288 days is depicted. This influent load varies because of production schedule fluctuations. From days 210 to 240, which corresponds with the month August, there was a production shut-down. In this period the incoming load is considerably smaller and only one AST was operated. The sludge of both ASTs was transported to this AST. The temperature in both ASTs varies, but is on average 25 °C.

In Fig 6 it is shown that the calculated and measured variables agree well, in spite of the strong variations of influent composition. The measured degradable COD (a) and specific component (b) in the effluent, measured effluent suspended solids (c) and biomass in one of the ASTs (d) show good agreement with the simulated results.[12] Degradable COD was calculated by subtracting the measured concentration of specific component (in mgCOD dm^{-3}) from the measured total soluble COD concentration. The increase in biomass concentration between days 210 and 240 is due to the maintenance shut-down. All the biomass was moved to this AST.

Model-based optimisation and scenario analysis

After calibration and validation the model could subsequently be used to investigate different operating strategies such as the in-series operation of the AST. In fact, with the model it was shown that a 20% reduction of the degradable COD concentration in the effluent could be achieved by operating the AST in series instead of in parallel as it is now (results not shown). In this way the flow regime in the AST has a more plugflow-like character and hence the removal efficiency will be higher despite the potential for increased toxicity.[13] Based on the simulation results, the in-series operation of the ASTs has been effectively implemented since November 2002.

Also, it was investigated what the effect would be of a complete shut-down of one of the two ASTs during production stops for maintenance purposes or holidays. The simulated degradable COD concentration in the effluent of this scenario is compared in Fig 7 with the corresponding simulated values of the normal operation, ie two ASTs in parallel. From Fig 7 it can be seen that considerably more degradable COD is discharged when only one AST is used, except of course for periods such as August where a significantly lower discharge occurs due to the production shut-down. In this period maintenance works can be planned without deterioration in the quality of the effluent.

Waste design

The calibrated model can also be used to quantify the effect of different production schedules of the different production facilities. Indeed, in many chemical industries the total yearly production can be obtained in different ways. However, some products are made on the same reactor sequence which puts constraint on the number of possible schedules. For now, only a steady state analysis was conducted in which the influence of 359 possible production schedules on the WWTP performance was investigated. However, in the future dynamic sequences of discharges can also be studied with the available model. Part of the results is summarised in Table 3. None of the product combinations exceeds 450 mgCOD dm^{-3}, which was the limit in the new discharge licence of the WWTP under consideration. Among the two top ranked product combinations a synergistic effect occurs, because the addition of product E to the production schedule leads to a lower effluent concentration. This is due to the fact that product E makes more readily biodegradable substrate available and that an increased flow rate is available for dilution.

Based on the ranking in Table 1, production facility 1 may adjust its production schedule in order to have a discharge that is as low as possible. This so-called waste design, of course, has to be combined

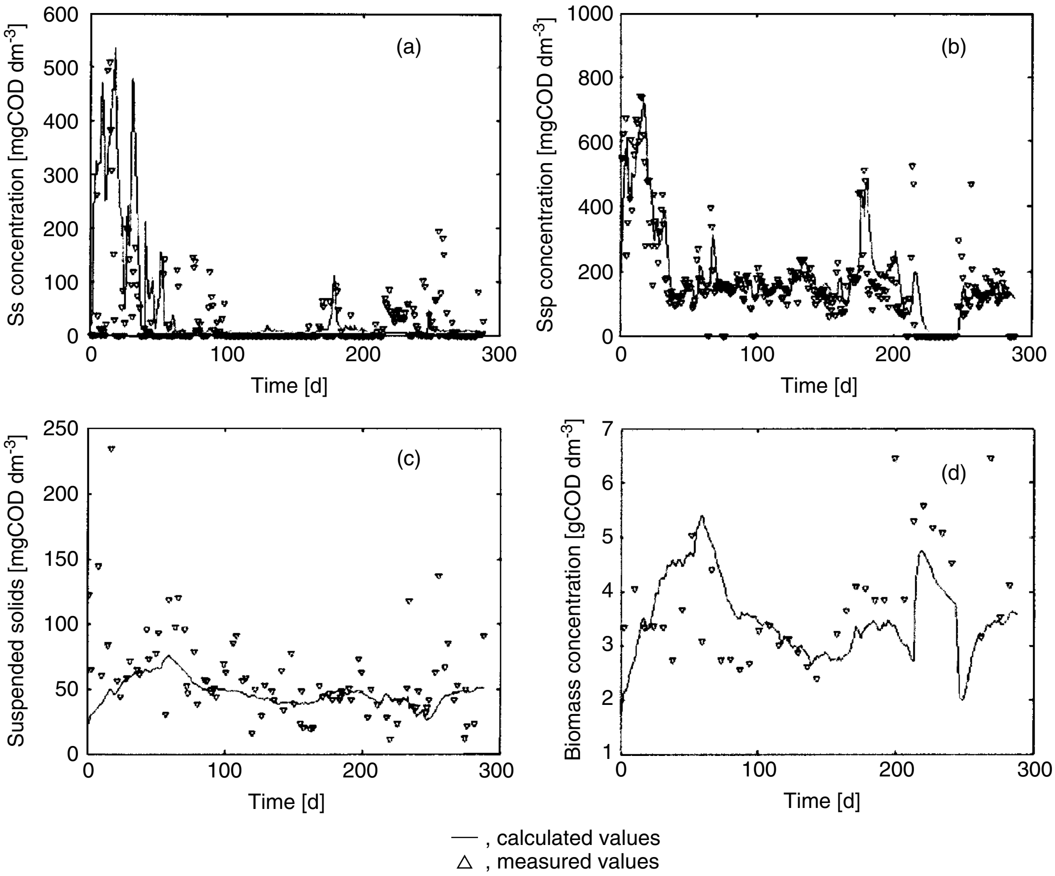

Figure 6. The calculated and measured degradable COD (a) and specific component (b), measured effluent suspended solids (c) and biomass in one of the ASTs (d) in the effluent.

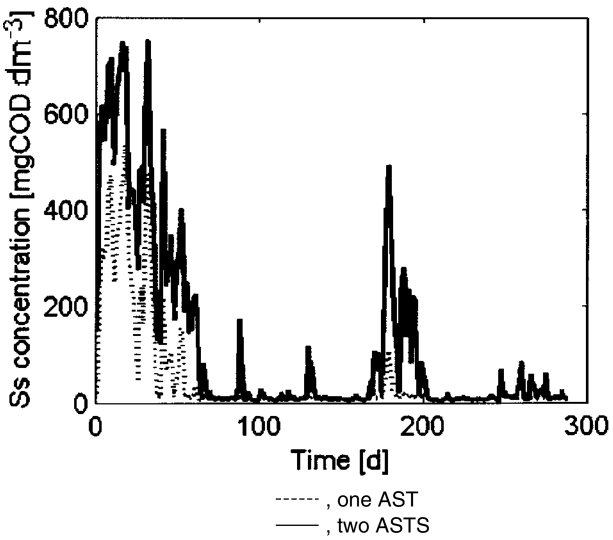

Figure 7. The effluent degradable COD for one and two ASTs.

Table 3. Average effluent COD as function of the product combination

Combination number	Product combination	COD in effluent (mgCOD dm^{-3})
1	G + B + D + S	420
2	E + G + B + D + S	413
3	F + G + B + D + S	402
4	G + A + D + S	401
5	E + F + G + B + D + S	398
6	E + G + A + D + S	396
7	F + G + A + D + S	385
8	E + F + G + A + D + S	382
9	G + B + D	376
10	E + G + B + D	373
	....	
355	F	33
356	M + C	30
357	H + C	29
358	H	23
359	C	14

with economic considerations such as market demand and production costs. However, even in current legislative conditions, waste design itself can be an economic consideration since a reduction in the effluent concentrations directly leads to a reduction in (considerable) effluent fines. Further, the model can be used to predict the effect on the behaviour of the WWTP of a future production facility discharging the fictive component described above. In this way, a selection can be made on which production facility can be implemented, also considering its environmental impact via discharge of the treated wastewater.

CONCLUSIONS

A model for an industrial WWTP was constructed and subsequently calibrated and validated. Special attention was given to the specific characteristics of industrial wastewater. A thorough biological characterisation was conducted following a recently developed calibration protocol.[4] The ASM1[5] model had to be extended to take into account the specific industrial components in the wastewater. A fictive component was also introduced to enable the prediction of the influence of a new production facility at the industrial site. The model has proven to be able to predict the course of strong variations in effluent composition. Subsequently, the model was used to simulate different scenarios. One of the scenarios tested showed a 20% improvement in effluent quality by transforming the in-parallel into an in-series configuration of the two available aeration tanks. Hundreds of possible production schedules of the discharging facilities were also investigated and ranked according to their subsequent average effluent concentration. This so-called waste design has a clear economic benefit, but requires a more holistic evaluation (market requests, production costs, etc) before it can be adopted. The study presented clearly shows the advantages of the use of models for optimisation and upgrading of industrial WWTPs.

ACKNOWLEDGEMENTS

The authors would like to thank G Sin for the help with the experiments. This study was partially supported by Hemmis NV (Kortrijk, Belgium, www.hemmis.com).

REFERENCES

1 Bury SJ, Groot CK, Huth C and Hardt N, Dynamic simulations of chemical wastewater treatment plants. *Water Science & Technology* **45**:355–363 (2002).

2 Henze M, Harremoës P, LaCour Jansen J and Arvin E, *Wastewater Treatment: Biological and Chemical Processes*. Springer, New York (1995).

3 Coen F, Vanderhaegen B, Boonen I, Vanrolleghem PA and Van Meenen P, Nitrogen removal upgrade of a WWTP within existing reactor volumes: a simulation supported scenario analysis. *Water Science & Technology* **34**:339–346 (1996).

4 Petersen B, Gernaey K, Henze M and Vanrolleghem PA, Evaluation of an ASM1 model calibration procedure on a municipal-industrial wastewater treatment plant. *Journal of Hydroinformatics* **4**:15–38 (2002).

5 Henze M, Gujer W, Matsuo T and Van Loosdrecht M, *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3*, Scientific and Technical Reports. IWA Publishing, London, UK (2000).

6 Vanhooren H, Meirlaen J, Amerlinck Y, Claeys F, Vangheluwe H and Vanrolleghem PA, WEST: Modelling biological wastewater treatment. *Journal of Hydroinformatics* **5**:27–50 (2003).

7 American Society of Civil Engineers, *ASCE Standard Measurement of Oxygen Transfer in Clean Water*. American Society of Civil Engineers, New York (1992).

8 APHA, *Standard Methods for the Examination of Water and Wastewater*, 18th edn. American Public Health Association, Inc, New York (1992).

9 Vanrolleghem PA and Spanjers H, A hybrid respirometric method for more reliable assessment of activated sludge model. *Water Science & Technology* **37**:237–246 (1998).

10 Ekama GA, Dold PL and Marais GvR, Procedures for determining influent COD fractions and the maximum specific growth rate of heterotrophs in activated sludge systems. *Water Science & Technology* **18**:91–114 (1986).

11 Petersen B, Gernaey K, Henze M and Vanrolleghem PA, Calibration of activated sludge models: a critical review of experimental designs, in *Biotechnology for the Environment: Wastewater Treatment and Modeling, Waste Gas Handling*, ed by Agathos SN and Reineke W. Kluwer Academic Publishers, Dordrecht, The Netherlands, pp 101–186 (2003).

12 Van Hulle SWH and Vanrolleghem PA, Modelling an industrial WWTP using a calibration protocol. Biomath Technical report. Ghent University, Belgium, pp 32 (2002).

13 Froment GF and Bishoff KB, *Chemical Reaction Engineering*. Wiley, New York (1990).