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MODEL-BASED CHARACTERISATION OF HYDRAULIC, KINETIC AND INFLUENT PROPERTIES OF AN INDUSTRIAL WWTP

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ABSTRACT

This paper illustrates the modelling of a full-scale industrial wastewater treatment plant. First, the hydraulics of the plant were characterised by a model-based interpretation of the results of a tracer test. The plant consists of three parallel reactors. The hydraulics of each reactor could be modelled by two tanks in series with non-equal volume. These results were confirmed by calculation of the single pass residence time distribution. Also it was found that the influent flow and the recycle flow were not distributed equally to the three reactors, resulting in different loading rates. Secondly, off-line respirometric experiments were performed to characterise the influent and to determine the sludge kinetics. The same model structure could be applied to describe the influent characteristics and the biokinetics over a period of 1 year. It was found that all wastewaters could be fractionated into three fractions and that one of the fractions was acetate-like. Concentrations of the fractions changed significantly over the year. From on-line respirometric experiments the diurnal dynamics of the influent characteristics and the kinetics of the sludge were assessed. Analysis of the respirograms showed that the wastewater composition and kinetics of the sludge did not change significantly over a short-term period of 40 hours. © 1998 Published by Elsevier Science Ltd. All rights reserved

KEYWORDS

Activated sludge; identification; mathematical modelling; mixing; respirometry.

INTRODUCTION

The efficiency of the activated sludge process is dependent both upon the amount of substrate removed in the aeration tank, and upon the ability of the particulate matter to flocculate and settle in the secondary clarifier. In recent years simulation has proven to be a useful tool in optimisation of wastewater treatment plants (WWTPs). The model most typically used to describe the biological processes in an activated sludge system is the Activated Sludge Model No.1 (ASM1) (Henze *et al.*, 1987). ASM1 has been developed for systems treating municipal wastewater, with only minor impact from industrial discharges and should therefore only be considered as a guideline to modelling industrial activated sludge systems. Especially for

industrial WWTP the information about influent characteristics and kinetics of the sludge may be very plant specific due to the higher variability of industrial wastewater compared to municipal wastewater.

However the behaviour of a WWTP is not only determined by biological processes but also by physical processes (e.g. mixing, aeration). Typically, the mixing properties in the activated sludge reactors are modelled by the tanks-in-series approach. The experimental technique widely applied to characterise the hydraulic properties is the tracer test. Performing a tracer test on a reactor gives the fraction of the fluid that has a certain residence time in the reactor (Danckwerts, 1953). However, in the case of wastewater treatment recycling of the settled sludge makes it difficult to interpret the tracer test results.

The first part of this paper focuses on the determination of the hydraulic characteristics of the aeration tank while in the second part the determination of biokinetic parameters and influent characterisation is highlighted. The study is performed on an industrial WWTP removing only COD. The hydraulic information of the aeration tank was extracted from a tracer test using two different approaches. One approach was based on simulation of the system with recycle, the other one used straightforward calculation of the residence time distribution (RTD). The results of both approaches were compared. Respirometry was used for the on-line monitoring of the short-term BOD to obtain information on the diurnal dynamics of the influent characteristics and the kinetics of the sludge. Furthermore batch experiments were carried out off-line to determine the most appropriate model structure for influent characterisation and biodegradation kinetics of the sludge. Using the model structure developed on the basis of the off-line respirometric data, it was tried to automatically analyse the respirometric data collected at the influent line of the activated sludge plant.

MATERIALS AND METHODS

A tracer test was performed at an industrial WWTP (Figure 1). The plant consists of a small distribution tank (DT) where return sludge and influent are mixed, three parallel activated sludge reactors (AS1, 1930 m^3; AS2, 3050 m^3; and AS3, 3050 m^3) and one rectangular settler (300 m^3). The influent flow rate was measured and the recycle flow rate was kept constant at 125 m^3/h. The distribution of the influent and recycle flow from the distribution tank to the 3 reactors was not known. Lithium chloride was used as a tracer. A pulse of 20 kg of LiCl was dosed in the distribution tank. Samples were taken in the effluent of each biological reactor. In Figure 1 the LiCl dosing point and sampling points are indicated.

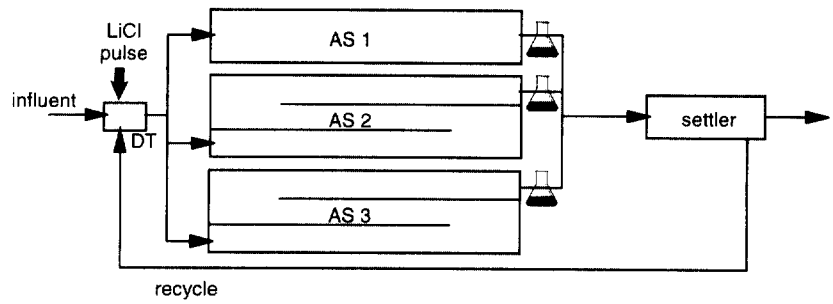

Figure 1. Schematic representation of the industrial WWTP.

The off-line batch experiments were carried out with a RODTOX device (Kelma bvba, Niel, Belgium) installed in the laboratory. The RODTOX consists of a constantly aerated, completely mixed batch reactor containing 10 litre of sludge. For a more detailed description of the principles see Vanrolleghem *et al.*, (1994). The dissolved oxygen (DO) concentration, from which the respiration rate is obtained, is measured by a DO electrode and collected on a PC. The temperature was controlled at 25°C and the pH at 7.5. Off-line experiments were carried out at five different dates during two measuring campaigns in spring and autumn/winter 1996 with influent and sludge sampled at the same time from the influent line and the activated sludge tanks of the full-scale WWTP. Acetate was used as calibration solution. During the two

measuring campaigns a RODTOX device was also installed on-line for continuous monitoring of short-term BOD in the influent to the activated sludge tanks. Here too an acetate solution was used for calibration of the device. Every fifth injection of wastewater was followed by a calibration cycle. Due to the moderate changes of the influent concentration the injected wastewater sample volumes could be fixed to 250 ml and a decantation cycle was initiated after 12 wastewater injections. The sludge in the reactor was replaced every week during the maintenance check.

RESULTS AND DISCUSSION: HYDRAULIC MODELLING

The results of the tracer experiment are given in Figure 2. The interpretation of the tracer test was complicated because the tracer recycle is fed into the three different activated sludge reactors. This means that the measurements performed in the effluent of AS1 were not only determined by the hydraulic characteristics of AS1 but were also influenced by the residence time distribution of AS2 and AS3. Moreover, the mixing in the distribution tank is not perfect. This was concluded from measurements of the sludge concentrations in the three activated sludge reactors over a one month period. The sludge concentration in AS2 (3.5 kg SS/m^3) differed significantly (5% t-test) from the sludge concentration in AS1 (3.1 kg SS/m^3) and AS3 (3.0 kg SS/m^3). To account for this imperfect mixing it was assumed that the three reactors each received different fractions of influent flow (f_{in1}, f_{in2}, f_{in3}) and recycle flow (f_{r1}, f_{r2}, f_{r3}). To determine these fractions mass balances for the tracer lithium and for the sludge were made.

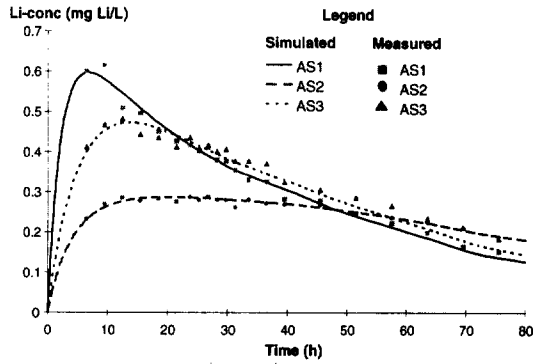

Figure 2. Measured and simulated concentration profiles of the tracer experiment.

Mass balance for lithium

A mass balance for lithium over the activated sludge system gives:

$$\int_0^{t_m} f_{in1}\, Q_{in}(t)\, C_1(t)\, dt + \int_0^{t_m} f_{in2}\, Q_{in}(t)\, C_2(t)\, dt + \int_0^{t_m} f_{in3}\, Q_{in}(t)\, C_3(t)\, dt = M - M_r \qquad (1)$$

The influent flow is denoted as Q_{in}. The concentrations C_1, C_2 and C_3 are the outlet concentrations of each reactor. The fractions f_{in1}, f_{in2}, f_{in3} are fractions of the influent flow to each reactor. M is the mass of lithium dosed. The measurements of C_1, C_2, C_3 were performed over a finite time t_m (= 76 hours), during which only part of the tracer had reached the effluent. M_r is the amount of lithium in the reactors after a time t_m. To calculate this amount it was assumed that the concentrations C_1, C_2 and C_3 were identical to the concentrations in the reactor. This assumption will be validated below. Calculation revealed that 31% of the lithium was still in the system after 76 h. The conservation of influent flow is expressed in equation (2).

$$f_{in1} + f_{in2} + f_{in3} = 1 \qquad (2)$$

Mass balance for sludge

A mass balance for sludge over the distribution tank gives the following set of equations. The contribution of particulate matter in the influent could be neglected.

$$X_r f_{r1} Q_r = X_1 (f_{in1} Q_{in} + f_{r1} Q_r) \quad (3)$$
$$X_r f_{r2} Q_r = X_2 (f_{in2} Q_{in} + f_{r2} Q_r) \quad (4)$$
$$X_r f_{r3} Q_r = X_3 (f_{in3} Q_{in} + f_{r3} Q_r) \quad (5)$$

The conservation of recycle flow is expressed in equation (6).

$$f_{r1} + f_{r2} + f_{r3} = 1 \quad (6)$$

Solution of the set of equations (1-6) with given M, calculated M_r and measured Q_{in}, Q_r and X_r gave the fractions summarised in Table 1. The loading of the three reactors was unequal. In view of the foreseen increase in load of the industrial WWTP an important optimisation would be the improvement of the mixing in the distribution tank.

Table 1. Distribution fractions of the influent and the recycle flow to the three activated sludge reactors. Estimated volume for the two tanks in series representing the hydraulics of the bioreactors

	AS1		AS2		AS3	
influent fractions f_{in}	0.36		0.24		0.40	
sludge fractions f_r	0.35		0.31		0.34	
Volume (m3)	tank 1	tank 2	tank 1	tank 2	tank 1	tank 2
Method 1	175	1570	250	2555	430	2010
Method 2	165	1620	220	2760	280	2300

Simulation of the tracer test (Method 1)

The technique of simulation and non-linear parameter estimation was needed to interpret the tracer test results. The model used for simulation of the tracer test was based on the concept of the ideally mixed 'tanks-in-series' model. The parameters of the model were the number of tanks in series and the volumes of the tanks (which are normally of equal size in the conventional 'tanks-in-series' model). A non-linear parameter estimation routine (Brent, 1973) was used to find the optimal set of parameters. The best fit to the experimental results was obtained by describing the hydraulics of each reactor by two tanks in series. The results (see Figure 2) were significantly better compared to 1 and 3 reactors (F-test with 5% hypothesis). The optimal volumes of the tanks in series are given in Table 1.

From these results the dead space in reactors AS1, AS2, AS3 is found to be respectively 9%, 8% and 20% of the reactor volume. The flow pattern in the reactors is described by the hydraulic model of a small tank followed by a larger tank. The RTD expresses only the time that the various fractions of the fluid have spent in the reactor. It provides no information on the mixing details. For instance, also the opposite set-up – a large tank followed by a small tank – will give the same hydraulic pattern but the biological conversion might be totally different.

Calculation of the single pass RTD (Method 2)

A straightforward technique to calculate the single pass RTD of any reactor operated with recycle of the effluent stream is described in Battaglia *et al.* (1993). This second method is applied here to check independently the results obtained from the simulation of the tracer test (Method1). In the case of a pulse dosage of tracer in the influent the concentration of tracer entering the reactor on each time instant is equal to:

$$C_{in}(t)=\frac{M}{Q_{in}+Q_r}\delta(t)+\frac{Q_r}{Q_{in}+Q_r}C_{out}(t) \tag{7}$$

The second term on the right-hand side is due to recycling of the effluent flow. The effluent tracer concentration leaving a reactor at time t is given by the convolution integral of the influent concentration with the single pass RTD $E_s(t)$. Substituting the above equation into the convolution integral and rearranging yields equation 8. This implicit equation in $E_s(t)$ can be solved numerically for $E_s(t)$ by successive approximations.

$$E_s(t)=\frac{Q_{in}+Q_r}{M}C_{out}(t)-\frac{Q_r}{Q_{in}+Q_r}\int_0^t C(t-t')E_s(t')dt' \tag{8}$$

For the industrial WWTP the fractions of the sludge recycle to each reactor are known from independent calculations (Table 1). Consequently, the coupled system of three reactors could be uncoupled into three independent systems with recycle. The method of Battaglia *et al.* (1993) was applied to the tracer test results to calculate the single pass concentration profiles of each reactor. These are the hypothetical tracer concentrations in the outlet of the reactor when there would be no recycle of tracer over the reactor. Parameter estimation with the tanks-in-series model shows the best fitting (see Figure 3) for 2 tanks in series. The optimal volumes are reported in Table 1. The volumes of the three reactors estimated with the single pass simulation are slightly different compared to the volumes derived from the simulation of the total WWTP. This may be due to the calculation method of the single pass concentrations where a mean flow rate was used instead of the actual flow measurements used for simulation of the three-reactor system.

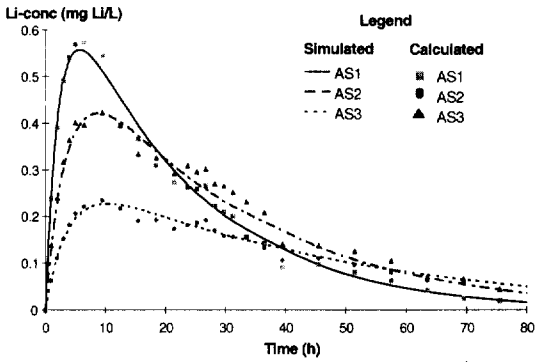

Figure 3. Calculated and simulated single pass concentration profiles.

RESULTS AND DISCUSSION: BIOKINETIC MODELLING

The model structure defined for the kinetics and influent characterisation was based on the profiles of substrate degradation related Oxygen Uptake Rate (OUR) which are obtained from the DO profiles (Vanrolleghem *et al.*, 1994). The OUR profiles are shown as a function of time in Figure 4 together with the model fit. In all five cases three distinctive shoulders can be seen. This shape of the OUR profiles indicates that the organic substrate in the wastewater could be divided into three fractions since the shoulders end in a distinguishable sharp way. A sharp shoulder indicates that the affinity for the substrate is high (Vanrolleghem and Van Daele, 1994).

The model used for influent characterisation and biodegradation kinetics of the sludge included COD removal only and was a modified version of the Activated Sludge Model No.1 (Henze *et al.*, 1987). ASM1 is based on Monod kinetics and fractionation of the biodegradable organic substrate into soluble readily biodegradable substrate and particulate hydrolysable substrate. However, to describe the phenomena observed in the respirometric data obtained for this industrial case study, the substrate division of ASM1 had

to be modified by dividing the soluble readily biodegradable substrate into three fractions (referred to as S_1, S_2 and S_3).

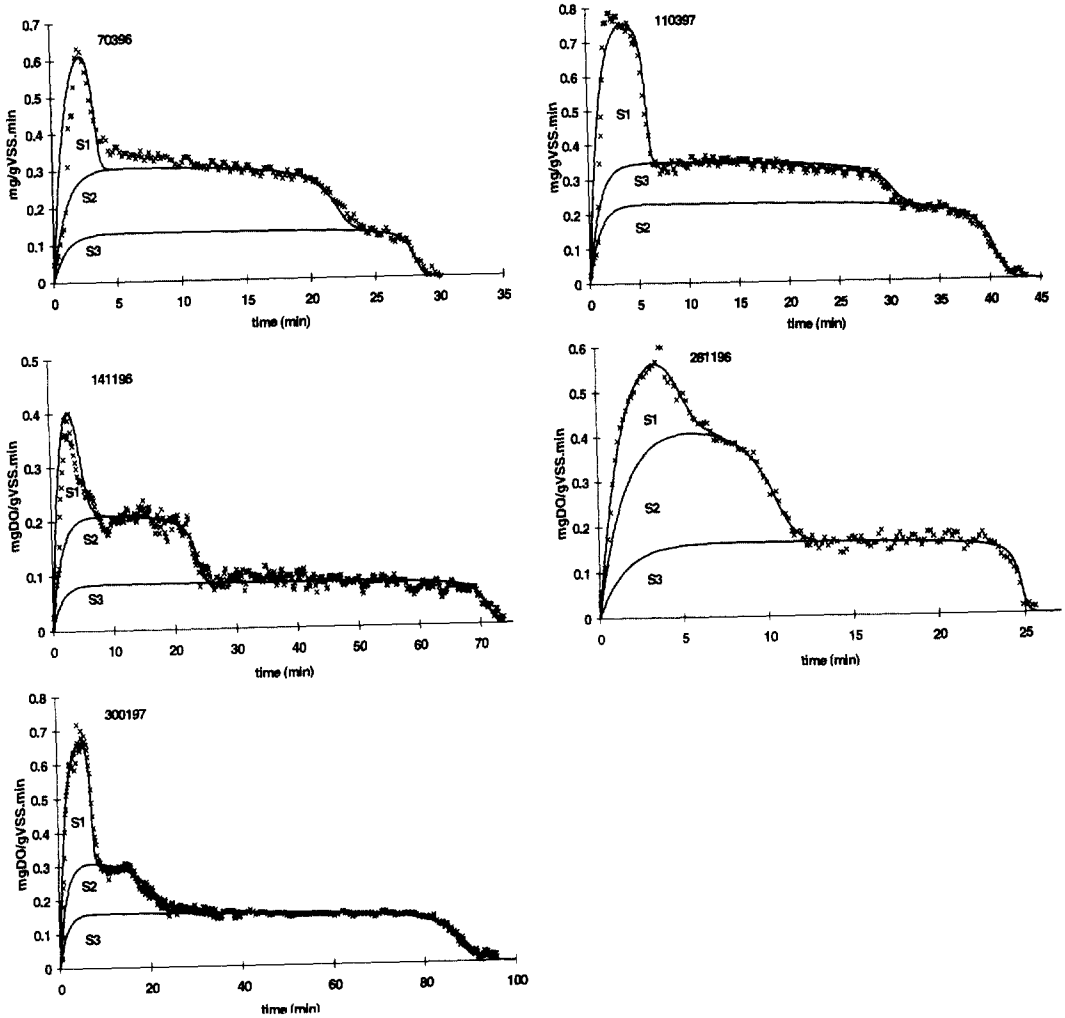

Figure 4. Results of off-line RODTOX experiments. Measured OUR as mgDO/gVSS.min as a function of time for five influent samples (symbols) and model fits (lines).

The following parameter combinations are theoretically identifiable from respirometric data: (1-Y)/Y•μ_{max}•K_{BH}, (1-Y)•K_S and (1-Y)•S (Dochain *et al.*, 1995). The parameter estimation was performed with a fixed yield (Y) of 0.67 mg COD/l and concentration of active biomass (X_{BH}) in order to estimate the specific maximum growth rate (μ_{max}), the half saturation coefficient (K_S) and the initial substrate concentrations (S). Using the above parameter combinations one can recalculate these parameter values for different assumptions of Y and X_{BH}. Another modification of the model was required to describe the biological start-up phenomenon found in these batch experiments (Coen and Vanrolleghem, 1997). A first order correction factor for the growth rate ($1-e^{-t/tau}$) was used to reasonably describe this phenomenon. Typical estimates of this start-up time constant (tau) lie between 0.5 and 2 minutes.

The parameter estimation was carried out with the parameter estimation program Mosifit (Kong *et al.*, 1996). The same model structure was applied to all influent samples. The model fits are shown in Figure 4,

also showing results of simulations performed to illustrate the contribution of each substrate to the OUR profile. Table 2 shows the estimated specific maximum growth rates (μ_{max}) and the half saturation coefficients (K_S). Table 3 shows the estimated concentrations of the three soluble substrate fractions in the five influent samples, the estimated sum of soluble COD ($\Sigma S_{ESTIMATE}$), the ratio between the estimated three substrates, the area under the OUR profiles corresponding to the 3 different substrates divided by (1-Y) gives ΣS_{RODTOX}, together with the chemical analyses of soluble-, total-COD and VFA.

Table 2. Estimated specific maximum growth rates (μ_{max}) and the half saturation coefficients (K_S). Estimates between brackets are not unique, see text

date	μ_1 (d^{-1})	K_{S1} (mg COD/l)	μ_2 (d^{-1})	K_{S2} (mg COD/l)	μ_3 (d^{-1})	K_{S3} (mg COD/l)
070396	(3.93)	(0.37)	1.68	0.36	0.96	0.13
110396	3.93	0.37	1.97	0.57	1.02	0.27
141196	(3.36)	(2.50)	0.86	0.50	0.57	0.41
281196	(2.03)	(2.32)	1.93	2.39	1.10	0.39
300197	2.83	0.38	1.13	0.85	1.09	1.11

Table 3. Estimated substrate fractions and chemical analyses of the five influents, all in mg/l

date	S_1	S_2	S_3	$\Sigma S_{ESTIMATE}$	S_1:S_2:S_3	ΣS_{RODTOX}	CODt	CODs	VFA
070396	158	504	1348	2010	8:25:67	2100	3624	3446	113
110396	205	656	533	1394	15:47:38	1230	1921	1604	123
141196	167	464	997	1628	11:28:61	1509	1456	1294	82
281196	498	1397	2427	4322	12:32:56	4179	3981	3883	336
300197	358	430	2154	2942	12:15:73	2870	4167	3693	563

From Table 2 it can be seen that the kinetic parameters of the three substrates are comparable within a factor two among the five sampling dates indicating that the kinetics of the influent fractions are comparable. However, problems with the practical identifiability (Vanrolleghem *et al.*, 1995) of the kinetics of substrate one were encountered with three of the influents (070396, 141196 and 281196) due to a lack of data points of the first shoulder in the OUR profile providing information on μ_1 and K_{S1}. From the kinetic parameters of substrate S_1 obtained for sample 110397 and 300197 it could be concluded that substrate one was acetate-like since the estimated kinetics were very comparable to the biodegradation kinetics of acetate obtained from calibration experiments with the same sludge samples. Presence of acetate was further confirmed by chemical analysis of volatile fatty acids (Table 3). Thus, the parameters of substrate one in sample 070396 were fixed on the values derived from sample 110396, leading to a reasonable fit. However, applying the same kinetic parameters to experiments 141196 and 281196 did not work since too pronounced a tailing was observed that could not be described. A higher K_S value can be used to describe this slower decrease of degradation rate. However, as seen from the chemical analyses these two samples did also contain volatile fatty acids which indicated that substrate one was also acetate-like and it may be hypothesised that the more pronounced tailing after substrate one must be due to other compounds contained in the wastewater or processes not considered in the chosen model.

From Table 3 it can be seen that the estimated sums of substrate match the area under the OUR profiles (divided by 1-Y) and that this sum of soluble readily biodegradable substrate is comparable to the measured COD. The small difference may be either due to inert matter or substrate not biodegraded within the time frame of the experiments. While for the kinetic parameters quite large confidence regions apply, the estimation of substrates is much more accurate (Vanrolleghem and Keesman, 1996). This higher accuracy allows us to state that the observed changes in substrate concentrations and especially the ratios between the substrates are significant for this WWTP.

The above mentioned comparability of the kinetic parameters and influent composition is remarkable since the industry under study operates with a batch production mode, i.e. regularly shifts in the type of products made and by this one would expect considerable differences in waste products. In spite of this the soluble readily biodegradable substrate could consistently be divided into three fractions with comparable kinetics. Furthermore, the sharpness of the OUR profiles leads to the conclusion that the main composition of the

influent to the activated sludge tanks consists of the same three specific chemical compounds, however with varying ratios. Using the model structure developed on the basis of the off-line OUR profiles, it was tried to automatically analyse the DO profiles collected at the influent line of the activated sludge plant.

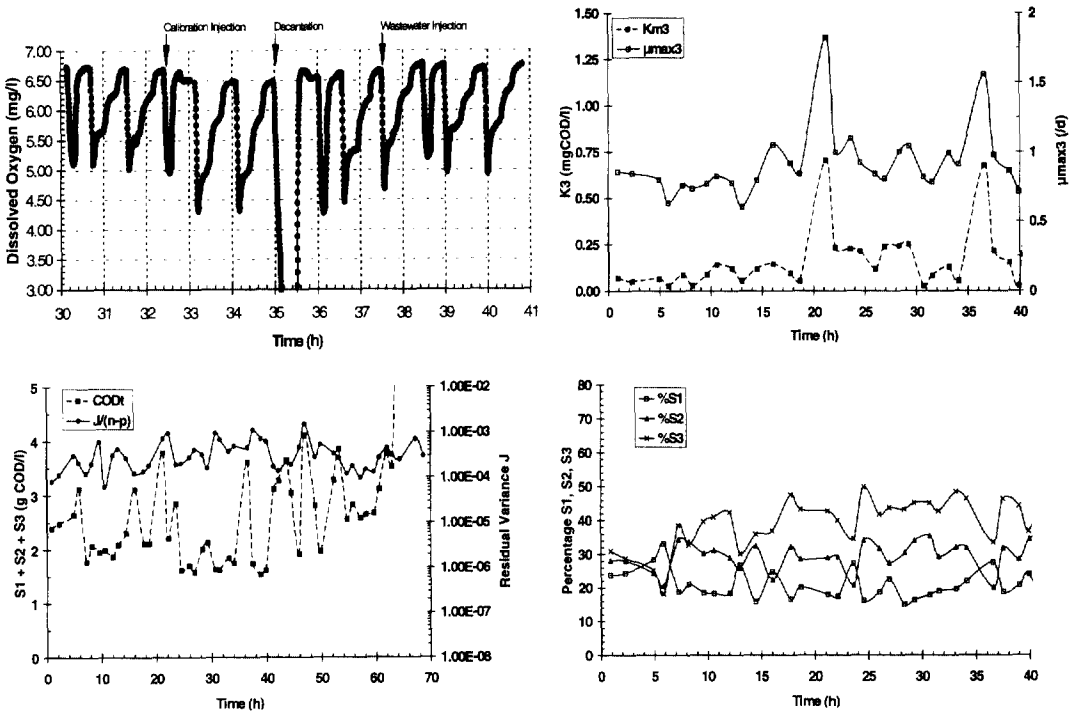

Figure 5. Raw Dissolved Oxygen sequence (top left), example of kinetics of substrate 3 (top right), total COD and residual variance (bottom left) and substrate fractions (bottom right).

In Figure 5 (top, left) a typical sequence of raw dissolved oxygen data for 8 batch experiments with wastewater, 4 calibration experiments and 1 decantation cycle are given. These data were divided into respirograms that were subsequently interpreted using an on-line version of Mosifit. Calibration and wastewater respirograms were interpreted with different models, i.e. for the calibration cycle a single Monod model was sufficient, while for the wastewater samples, the triple Monod model developed on the basis of the off-line experiments was identified. For the calibration cycles, no problems were to be expected as this is a fairly easy identification problem. For the wastewater respirograms, however, it was obvious from the off-line interpretations that good initial estimates of the parameters were necessary to allow reliable identification. Indeed, no less than 13 degrees of freedom were available, i.e. 2 mass transfer parameters, 3 substrate concentrations in the wastewater, 3 max. growth rates, 3 affinity constants, the initial oxygen concentration and the start-up phenomenon parameter. The procedure adopted was to manually support the estimation on the first respirogram so that it gave a good fit and then use the estimates of a previous respirogram as initial values for identification of the next one. It is quite obvious that wastewater composition or sludge biokinetics did not change that drastically, so that the identification algorithm is allowed to slowly "follow" the changes. Indeed, except for a few respirograms, it was found that this procedure was quite reliable. Some illustrative results for the kinetics (of substrate 3) and the total substrate concentration and composition ratios are reported in Figure 5 (top right and bottom left). The fit (Figure 5, bottom right) was always very good and the residual variance is only slightly above the typical measurement variance, indicating an appropriate model structure and good performance of the numerical algorithm. It is, however, clear that the identification results of the respirograms at t=20h and at t=36h deviate from the ones before and after. This was a recurring phenomenon that appeared to be related to the presence of a decantation cycle just before these deviating wastewater cycles (Figure 5, top left). This aspect certainly

warrants further research. The total readily biodegradable substrate concentration appears to be quite constant over this 2 day period and the ratio between the different substrates does not change dramatically (Figure 5, bottom right).

Consequently the substrate concentrations do not change over short-term periods but do change over long-term periods as seen in Table 3. This makes the proposed procedure of on-line interpretation of the respirometric data realistic in the industrial case studied.

CONCLUSIONS

The results of a tracer test on an industrial WWTP consisting of three bioreactors in parallel revealed that there is an improper mixing of the incoming wastewater with the recycle sludge. This results in different sludge concentrations and thus different volumetric loading rates in the three reactors. The hydraulic pattern was modelled with an ideally mixed tanks in series model. A non-linear parameter estimation routine calculated the optimal number of tanks in series and the active volume of each reactor. With another approach (Battaglia *et al.*, 1993) the single pass RTD was derived from the experimental data. Simulation of the single pass RTD gave the same estimate for the number of tanks in series and comparable estimates for the active volume of each reactor.

Respirometric batch experiments were carried out off-line to determine a model structure to describe the influent characteristics and kinetics of the sludge. It was found that the same model structure could be applied to all influent samples under study and that the kinetic parameters were comparable. Moreover, all wastewaters could be fractionated into three fractions albeit in different amounts, and one of the fractions was acetate-like. However the ratio between the substrates varied significantly over the 10 month period studied. The model structure was also applied on the DO profiles collected on-line for automatic parameter estimation. It was found that the wastewater composition and kinetics of the sludge did not change significantly over a short-term period of 40 hours. This implies that the proposed procedure for on-line interpretation of the respirometric data is feasible, and that the model parameters can therefore be updated periodically since the ratio between the three substrate fractions varies slowly.

ACKNOWLEDGEMENT

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