Simultaneous estimation of sludge biological activity and influent nitrogen load using ORP and DO dynamics

Abstract This paper proposes a new optimization strategy to estimate nitrifiable nitrogen concentration in wastewater, nitrification rate, denitrification rate and/or COD available for denitrification of an activated sludge process submitted to intermittent aeration. The approach uses the oxydo-reduction potential and dissolved oxygen measurements only. The parameter identification is based on a Simplex optimization of a cost function related to the error between an experimental cycle (an aerobic period followed by an anoxic one) and a simulation of a reduced model derived from ASM1. Results show very good prediction of experimental oxygen, ammonium and nitrate profiles. The estimation of nitrifiable nitrogen and removal rates has been validated both on simulated data obtained from COST action 624 benchmark and on experimental data.

Keywords Activated sludge · Wastewater treatment · Unknown input · Modelling · Estimation

Introduction

Nitrogen removal is commonly performed in wastewater treatment plant by biological processes, i.e. nitrification and denitrification in activated sludge process, which are susceptible to disturbances. These disturbances to the process can be due to changes in influent flow, concentration and composition from the influent itself or from concentrated return streams. The main challenge to manage the process is then to avoid or at least reduce disturbances of the nutrient removal performance of the overall wastewater treatment process. Depending on the configuration of the process (pre-denitrification, alternated aeration, post-denitrification), different control strategies can be employed to help the process cope with dynamic variations that are inherent in the nature of the wastewater treatment process. By means of varying the volume of nitrification and denitrification, by an equalizing zone, by changing aeration power or aeration time internal and recycled flows or by the addition of external carbon source, ammonium and inorganic nitrogen concentration in the effluent of the biological process can be controlled.

To apply advanced control strategies to the activated sludge process the state of the process needs to be observed using process variables. Internal process variables like the active biomass concentration or the nitrogen removal rate are not measurable on-line. Therefore, indirect methods have been proposed for estimating relevant variables. Such state and input observation as parameter estimation approaches require a model of the process. This model has to be, on the one hand the most accurate as possible such as to mimic the main characteristics and dynamics of the process and, on the other hand, simple enough to be used for model-based control and observation. This compromise has been exhibited in several strategies proposed in previous works, which all intended to propose a simplified version of the highly complex and non-linear state-of-the-art Activated sludge Model N°1 (ASM1) initially proposed by the IWA task group [5].

As on-line monitoring of ammonia and nitrate in the mixed liquor are still costly and impractical due to the maintenance requirements, respiration rate (the rate at which activated sludge consumes oxygen) can be used as an indicator of the process state and its use has generated much interest in nitrogen removal control [8, 13]. Stoichiometric and kinetic parameters of nitrification have been determined by several authors by means of model fitting on respirometric signal or DO response [3, 12, 16]. The nitrifiable nitrogen also may be estimated
by means of respirometry. The approach typically involves the model-based interpretation of the OUR profile. The amount of nitrogen that is nitrified is calculated from the oxygen consumption or from a titrimetric sensor. In anoxic conditions, oxydo-reduction potential (ORP) can be used as a control parameter. The main ORP time feature used for control is the 'nitrate knee', observed when denitrification is complete and nitrate is depleted. Several authors have used the bending point method to evaluate the process state using DO, ORP and pH profiles [1, 10, 11].

Here, a simplified system is proposed for simultaneously characterizing the activated sludge process and wastewater nitrifiable nitrogen evolutions. It is based on the ORP and DO measurements in a continuously fed reactor in which dynamic responses are due to intermittent aeration. An observer allows to estimate the following parameters: nitrifiable nitrogen concentration in wastewater \( S_{\text{in} \ \text{NH}_4} \), nitrification rate \( r_n \), denitrification rate \( r_{dn} \) and/or COD available for denitrification. The paper is organized as follows. The activated sludge model and process operation conditions are stated. The observation procedure is presented and discussed. It is then validated on simulated data issued from the COST action 624 benchmark and on experimental data. A conclusion ends the paper.

**Activated sludge process modelling**

The observation approach is based on DO and ORP profiles interpretation of a reactor with alternated aeration. The reactor is continuously fed both with wastewater and sludge. Alternance of aerobic and anoxic conditions is controlled to guarantee ammonia and nitrate depletion. The reactor may be an independent vessel, or the activated sludge reactor itself. The sludge is brought from the recirculated activated sludge of a parallel wastewater treatment plant in the first configuration or may be provided directly by recirculation from the clarifier of the process in the second case (Fig. 1).

As said in the introduction, the modelling of the process must enable the compromise between the precision required to simulate the process and the objective of the modelling. In this context, Steffens et al. [15] have proposed an algorithm for eliminating state variables from a model based on variables affection over the process depending on the time scales dynamics of interest; oxygen dynamics were not taken into account. Zhao et al. [17] have proposed a reduced order model describing only the nitrogen dynamics (ammonia and nitrate concentrations) of the alternating sludge process. Jeppson [6] has used a more complex model with five variables: heterotrophic and autotrophic biomasses, biodegradable organic substrate, ammonia nitrogen and nitrate. Dissolved oxygen (DO) concentration was regulated to 2 mg/l, and not considered in that model. Julien et al. [7] proposed a simplification of the ASM which led to two submodels (one for anoxic conditions and one for aerobic conditions) based on nitrogen-related concentrations (ammonium and nitrate) and DO concentration. However, the modified model was still complex and highly non-linear and to further simplify it, an unique model for both phases has been proposed and model parameters have been grouped to reduce the number of unknown parameters [4].

The reduced model proposed in this paper is derived from the model originally presented in [4]. The four dynamics described by this reduced non-linear model were the readily biodegradable concentration \( S_{s} \), the nitrate concentration \( S_{\text{NO}_3} \), the ammonia nitrogen concentration \( S_{\text{in} \ \text{NH}_4} \) and the DO concentration \( O_2 \). Further simplifications have been done on this basis, under the hypothesis of non-limiting pres-

<table>
<thead>
<tr>
<th>( K )</th>
<th>( K_1 )</th>
<th>( K_{\text{NH}_4} )</th>
<th>( K_{\text{NO}_3} )</th>
<th>( K_{O_2} )</th>
<th>( K_{O_2dn} )</th>
<th>( K_{O_2H} )</th>
</tr>
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<tbody>
<tr>
<td>4.24</td>
<td>0.9</td>
<td>0.2</td>
<td>0.1</td>
<td>0.2</td>
<td>0.2</td>
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</table>
ence of carbonaceous substrate for denitrification conditions. The influence of the readily biodegradable substrate on the denitrification was then hidden inside the maximum denitrification rate $r_{dn}$, while the limiting nitrate concentration was described through Monod kinetics. The limitation of the nitrification rate with respect to availability of ammonia nitrogen and DO was expressed through Monod kinetics. The model is given as follows:

$$\frac{dS_{NH_4}^+}{dt} = \frac{Q_{ww}}{V} S_{in}^{NH_4^+} - \frac{Q_{ww} + Q_x}{V} S_{NH_4^+}^t - r_n \frac{S_{NH_4^+}}{K_{NH_4^+} + S_{NH_4^+}} O_2 - r_{dn} \frac{S_{NH_4^+}}{K_{NH_4^+} + S_{NH_4^+}} K_{O_2A} + O_2$$

$$\frac{dS_{NO_3^-}}{dt} = \frac{Q_x}{V} S_{NO_3^-}^t - \frac{Q_{ww} + Q_x}{V} S_{NO_3^-} - K_{1} r_n \frac{S_{NH_4^+}}{K_{NH_4^+} + S_{NH_4^+}} K_{O_2A} + O_2 - r_{dn} \frac{S_{NO_3^-}}{K_{NO_3^-} + S_{NO_3^-}} K_{O_{2dn}} + O_2$$

$$\frac{dO_2}{dt} = K_{La}(O_2^t - O_2) - OUR_0 \frac{O_2}{K_{O_2A}} + O_2 - K_{rn} \frac{S_{NH_4^+}}{K_{NH_4^+} + S_{NH_4^+}} K_{O_2A} + O_2$$

This model was complemented by numerical values of the parameters. Key parameters had to be identified through the observer while the other parameters were set to default or measured experimental values. Three different classes of parameters were then considered:

- experimental data related to the process operation and typically measured: $Q_{ww}, Q_x, V, O_2^t$
- standard values of kinetics parameters: $K, K_1, K_{NH_4^+}, K_{NO_3^-}, K_{O_2A}, K_{O_{2dn}}, K_{O_2H}$ given in Table 1;
- parameters to be identified: $r_n, r_{dn}, K_{La}, OUR_0, S_{in}^{NH_4^+}, S_{NO_3^-}^{x}$

The estimation procedure is based on the error between an experimental cycle and a simulated cycle. Then, in addition to the model parameters, the initial condition of the cycle has to be known. A cycle is defined as an aerobic period followed by an anoxic period. The DO concentration is initialized to 0 (and measured). According to the hypothesis for the cell operation of optimized conditions, we assume total removal of ammonia nitrogen and nitrate during aerobic and anoxic periods. Then, the initial nitrate concentration is equal to 0. On the other hand the initial ammonia nitrogen is given by the accumulation of ammonia nitrogen during the anoxic phase of the previous cycle $\Delta_{an}^{prev}$. It is then directly related to the influent ammonia nitrogen concentration:

$$S_{NH_4^+}(0) = \frac{S_{in}^{NH_4^+} Q_{ww} \Delta_{an}^{prev}}{V}$$

Moreover, parameters related to the DO time-evolution are directly related to some characteristic point and slope of its evolution. The oxygen transfer is deduced from the variation of slopes of oxygen consumption at the end of the aerobic phase, when the aeration is stopped:

$$K_{La} = \frac{p_1 - p_2}{O_2^2 - O_2^{max}}$$

where the slopes $p_1$ and $p_2$ are illustrated in Fig. 2. $O_2^{max}$ represents the maximum value of DO concentration. This approximation is particularly true when the slope $p_1$ tends towards 0.

\footnote{We consider in the following that the return sludge is free from nitrate, then $S_{x(NO_3^-)}^{x} = 0$}
The endogenous and heterotrophic activity OUR\(_0\) may be estimated from the influent ammonia nitrogen concentration when \(S_{\text{NH}_4}^r\) tends towards 0, i.e. \((dS_{\text{NH}_4}^i)/dt \simeq dO_2/\tau \simeq 0\). Under the hypothesis that \((O_{2,\text{max}}^\text{sim}/(K_{O_2,\text{f}} + O_{2}^\text{max}))\) approximately equals to 1, one obtains:

\[
\text{OUR}_0 = K_{\text{La}}(O_2^\text{sim} - O_{2}^\text{max}) - \frac{S_{\text{NH}_4}^\text{in} Q_{\text{ww}} K}{V}
\]  

In order to validate the strategy, the observer was first applied on simulated data. A simulation system was built using the software GPS-X (see Fig. 1a), based on the ASM1 model [5]. The sensor was simulated as a completely mixed reactor with the operation conditions given in Table 2.

Moreover, the Simplex procedure is particularly robust as the number of parameters to be identified is decreased. In the current case, the influent ammonia concentration and nitrification rate mainly affect the aerobic period of the cycle while the denitrification rate mainly affects the anoxic period. The iterative identification procedure is then decomposed into two successive steps, such that identification of \(r_n\) and \(S_{\text{NH}_4}^\text{in}\) only use information from the aerobic period, and identification of \(r_{dn}\) is related to the anoxic period.

**Observation procedure**

Parameter identification has been carried out using Nelder-Mead Simplex procedure [9]. The cost function was formed of five terms involving both continuous-time and discrete-time information. Continuous-time information was furnished by the oxygen concentration profile during the aerobic period. Discrete-time information was related to inflexion points of oxygen and ORP profiles, denoted \(t_{O_2}\) and \(t_{\text{ORP}}\), respectively. The cost function was then given by the weighted addition of:

- the error between the simulated oxygen profile and measurements

\[
\sum_{t=\text{last}}^{t_{\text{last}}} (O_{2}^\text{mes}(t) - O_{2}(t))^2
\]

- the error in determination of the ammonia depletion (accumulated during the previous anoxic period). This error represents both an error between the simulated time of ammonia depletion and the inflexion point of the experimental oxygen profile

\[
t_{O_2} - t(S_{\text{NH}_4}^i \leq K_{\text{NH}_4})
\]

and an error between the simulated ammonia concentration value at the experimental inflexion point on the oxygen profile and the theoretical value

\[
S_{\text{NH}_4}^i(t_{O_2}) = K_{\text{NH}_4}
\]

- the error in determination of the nitrate depletion (accumulated during the previous aerobic period). This error represents both an error between the simulated time of nitrate depletion and the inflexion point of the experimental ORP profile

\[
t_{\text{ORP}} - t(S_{\text{NO}_3}^i \leq K_{\text{NO}_3})
\]

and an error between the simulated nitrate concentration value at the experimental inflexion point on the ORP profile and the theoretical value

\[
S_{\text{NO}_3}^i(t_{\text{ORP}}) = K_{\text{NO}_3}
\]

- the error between the simulated nitrate concentration value at the experimental inflexion point on the ORP profile and the theoretical value

\[
S_{\text{NO}_3}^i(t_{\text{ORP}}) = K_{\text{NO}_3}
\]

In order to validate the strategy, the observer was first applied on simulated data. A simulation system was built using the software GPS-X (see Fig. 1a), based on the ASM1 model [5]. The sensor was simulated as a completely mixed reactor with the operation conditions given in Table 2.

The standard simulation Benchmark wastewater treatment plant was used to generate mixed liquor. For the stoichiometric and kinetic parameters default values at 15°C were used [5]. The sensor was operated as an alternating aeration system by adjusting the oxygen mass transfer coefficient, \(K_{\text{La}}\). The outputs from the simulations were \(DO\), \(\text{NH}_4\) and \(\text{NO}_X\) concentrations. For estimation only \(DO\) and time of nitrate depletion were supposed to be known via \(DO\) and ORP measurement. Cycle time refers to the time to achieve a complete nitrification–denitrification cycle. The aerobic cycle time and the anoxic cycle time were automatically adapted in order to be long enough to clearly observe the bending points and the minimum required to achieve complete nitrification and denitrification.

Reproducibility of estimation results has been checked for a test case. The test case is based on a numerical simulation model [2] which was designed by an European expert group within the COST 682, then 624, framework as a benchmark. Typical diurnal evolution was simulated followed by a rain event during half a day. The simulated set used for parameter estimation is given in Fig. 3. Note that since ORP is not available in GPS-X software, the information related to the inflexion point used in the estimation procedure is equivalently given by nitrate depletion. As shown in Fig. 3, simulated \(DO\) is fitted very accurately to the data from GPS-X. Nitrate profiles which are recalculated by the sensor are in good accordance with original data. Estimated nitrifiable nitrogen in the reactor shows an evolution close to the ammonia concentration of

<table>
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<th>(Q_{\text{ww}}) (m³/day)</th>
<th>(Q_x) (m³/day)</th>
<th>(V) (m³)</th>
<th>(O_2) (gO₂/m³)</th>
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<tr>
<td>10000</td>
<td>10000</td>
<td>6000</td>
<td>10</td>
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Indeed assimilation of nitrogen consumes organic nitrogen made available to biomass by hydrolysis and ammonification. It leads to the conclusion that the observer is able to estimate the internal concentration of nitrate and nitrifiable nitrogen, the sum of which is close to the ammonia level in these data. From these, the nitrifiable nitrogen concentration in the wastewater feeding of the system was estimated. It is
compared in Figs. 4 and 5 with the ammonia and total nitrogen (TN) set in GPS-X. A new estimation of nitrifiable nitrogen is obtained for each aerobic-anoxic cycle, and the result is a mean value over this period.

Nitrifiable nitrogen estimation remains close to the ammonia nitrogen during most of the dry period. This result is not surprising as in the reactor organic nitrogen is converted into ammonia but only a part of it is nitrified, i.e. a fraction is assimilated by biomass for protein synthesis. In normal conditions, depending on the COD to N ratio of the influent, about 20–25% of total nitrogen is assimilated by biomass. Therefore nitrified (or nitrifiable) nitrogen is about 75–80% of total nitrogen and thus near to influent ammonia concentration. During the rainy period (from time 11 to 11.5 days), the nitrifiable nitrogen estimated value decreases rapidly but is higher than ammonia and similar to total nitrogen. During this period, COD (i.e. organic matter) is less usable for heterotrophic growth and hence the assimilation of nitrogen is lower. This could explain why the major part of total nitrogen is nitrified and hence the estimated $S_{\text{NH}_4}^{\text{in}}$ is nearer to the total nitrogen in this period.

Validation on experimental data

The observation strategy has also been evaluated on experimental data. Experiments were performed at 15°C with a 40-l aerated reactor continuously stirred, in which oxygen concentration and ORP were measured and monitored. Pumps controlled by the software fed the reactor with concentrated sludge and wastewater. The operation conditions are given in Table 3. COD, nitrate, nitrite and ammonia were analysed using Standard Methods (1995).

Experimental data used for parameter estimation are shown in Fig. 6. An example of four successive cycles is shown. Knee points are clearly visible on DO and ORP signals (decreasing) during aerobic phase, which characterizes depletion of ammonia. Before the end of the anoxic period, a rapid decrease appeared on the ORP signal due to nitrate depletion.

The estimation procedure is checked on cycle 4, for which off-line analysis of the influent ammonia concentration and reaction rates have been done. Figure 7 shows in solid line the time-evolution of the reduced process model with estimated values of the influent ammonia nitrogen concentration and reaction rates given in Table 4.

First of all, the modelled DO profile fits the measured one very well. It shows that the reduced model describes accurately biological oxygen consumption as well as gas–liquid transfer, and in addition that the mathematical fitting procedure is successful. At the end of this procedure, ammonia and nitrate concentrations in the

<table>
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<th>Table 3 Process operation—experimental conditions</th>
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<tr>
<td>$Q_{\text{ww}}$ (m$^3$/day)</td>
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<td>0.0374</td>
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</table>
The reactor can be calculated with the final set of parameters. Ammonia and nitrate concentration have been measured by discrete sampling at different times and are compared to the calculated ones in Fig. 7. Modelled and experimental nitrate concentration are in good accordance. As expected from the discussion of the previous section, calculated values of ammonia concentration are lower than the measured one, although the shapes of the evolution are the same.

The experimental denitrification rate has been deduced from nitrate concentration measurement in the reactor. The value obtained (119 mg/l/day) is close to the estimated one (117 mg/l/day). From this estimated denitrification rate, the influent COD used for denitrification entering the cell per unit of time can be calculated:

\[ \text{COD}_{dn} = \frac{2.86}{1 - Y_{hd}} r_{dn} \]

with (measured by [14])

\[ Y_{hd} = 0.5 \text{ gCOD/gCOD} \]

It is compared in the last column of Table 4 with the measured inlet COD flux, which is the product of measured COD concentration of wastewater and the influent
flow rate divided by reactor volume. Values are in the same order of magnitude, estimated COD being 5% higher than the COD entering with wastewater. As only a part of the wastewater COD is biodegradable, generally 70 to 90%, it would be logical that the estimated denitrifiable COD was lower than the wastewater COD. Therefore the estimated denitrifiable COD seems to be overestimated in our result. It may be due to endogenous denitrification which was not taken into account in the formula.

In addition to direct analysis of estimated data with respect to measured or expected values, one main point of interest is to evaluate confidence of estimated data, that is, to evaluate the quality of the observation procedure by examination of the cost function with respect to the parameters. A multi-start procedure (optimization initialized from several random initial conditions) has confirmed the solution. The cost function during the aerobic phase does not depend on the denitrification rate \( r_{dn} \). It may then be determined for several values of nitrification rate \( r_n \) and nitrifiable nitrogen concentration in wastewater \( S_{NH_4}^{in} \). Results are plotted in Fig. 8. Although the multi-start procedure exhibits some robustness of the parameter estimation, the form of the valley of the cost function shows that there is some dependency between the nitrification rate and the influent nitrifiable nitrogen. It is then preferable to initialize the optimization procedure at low values of \( r_n \) and \( S_{NH_4}^{in} \). Moreover, it must be noted that if the identification of \( r_n \) and \( S_{NH_4}^{in} \) has converged to erroneous values, then the accumulation of nitrate during the aerobic phase will be under or overestimated, and so the denitrification rate will be badly estimated during the anoxic phase.

### Conclusion

The proposed sensor, based on DO and ORP measurements, allows to estimate and monitor nitrifiable nitrogen as well as nitrification and denitrification rates. By a model identification technique, these variables are determined for each successive aerobic-anoxic cycle, in a continuously fed reactor submitted to intermittent aeration. Periodicity of estimation will depend on duration of aerobic and anoxic cycle which can be optimized by on-line adaptation of these phases. The alternance and duration of anoxic and aerobic periods may be controlled by a time table or through feedback control based on the detection of the bending points related to the ammonia nitrogen and nitrate depletion [11].

Experiments show that the sensor gives a correct estimation of the denitrification rate and indirectly an estimation of wastewater denitrification capacity, i.e. biodegradable COD available for denitrification. Some

<table>
<thead>
<tr>
<th>( S_{NH_4}^{in} ) (mg/l)</th>
<th>( r_n ) (mg/l/day)</th>
<th>( r_{dn} ) (mg/l/day)</th>
<th>COD(_{dn} ) (gDCO/l/day)</th>
</tr>
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<tbody>
<tr>
<td>Estimated 58.5 (nitrified)</td>
<td>215</td>
<td>117</td>
<td>0.672</td>
</tr>
<tr>
<td>Measured 60.9 (NTK)</td>
<td>–</td>
<td>119</td>
<td>0.639</td>
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Fig. 8 Cost function with respect to parameter values. The cross represents the optimal solution given by the Simplex procedure.
other tests on various simulations done with GPS-X software have confirmed that the procedure gives good predictions of kinetics rates, influent ammonium and state variables profiles.

References