SIMULTANEOUS ESTIMATION OF NITRIFICATION/DENITRIFICATION KINETICS AND INFLUENT NITROGEN LOAD USING ORP AND DO DYNAMICS

Isabelle Queinnec*, **Mathieu Spérandio**†

* LAAS-CNRS, 7 avenue du Colonel Roche, 31077 Toulouse cedex 04, France - email: queinnec@laas.fr
† Laboratoire d'Ingénierie des Procédés de l'Environnement (LIPE), DGPI-INSA, 135 Avenue de Rangueil, 31077 Toulouse cedex 04, France - email: sperandi@insa-tlse.fr

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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 (ORP) and dissolved oxygen (DO) 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 on experimental data.

1 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. These disturbances and variations can put additional load onto the treatment process. There is a need to manage the process to avoid disturbances of the nutrient removal performance of the overall wastewater treatment process.

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 active biomass concentration, nitrogenous removal rate are not measurable online. 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 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 ASM initially proposed by the IWA task group [4].

[13] have proposed an algorithm for eliminating state variables from a model based on variables affection over the process depending of the time scales dynamics of interest ; oxygen dynamics were not taken into account. [15] have proposed a reduced order model describing only the nitrogen dynamics (ammonia and nitrate concentrations) of the alternating sludge process. [5] has used a more complex model with five variables : heterotrophic and autotrophic biomasses, biodegradable organic substrate, ammonia nitrogen and nitrate. Dissolved oxygen concentration was regulated to $2mg/l$, and not considered in that model. [6] proposed a simplification of the ASM which leaded to two sub-models (one for anoxic conditions and one for aerobic conditions) based on nitrogen related concentrations (ammonium and nitrate) and dissolved oxygen 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 [3].

Because 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 [7], [11]. Stoechiometric and kinetic parameters of nitrification have been determined by several authors by means of model fitting on respirometric signal or DO response [2], [10], [14]. 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, 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], [8], [9].

Here a simplified system is proposed for simultaneously characterising activated sludge process and wastewater nitrifiable nitrogen evolutions. It is based on the ORP and DO measurement in a continuously fed reactor in which dynamic response are due to intermittent aeration. An observer allows to estimate the following parameters: nitrifiable nitrogen concentration in wastewater ($S^{in}_{NH_4^+}$), nitrification rate (r_n), denitrification rate (r_{dn}) and/or COD available for denitrification.

2 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.

The reduced model proposed in this paper is derived from the model originally presented in [3]. In that model, the four dynamics described by this reduced non linear model were the readily biodegradable concentration S_s, the nitrate concentration $S_{NO_3^+}$, the ammonia nitrogen concentration $S^{in}_{NH_4^+}$ and the dissolved oxygen concentration 0_2. Further simplifications have been done on this basis, under the hypothesis of non-limiting presence of carboneous substrate for denitification conditions. The influence of the readily biodegradable substrate on the denitrification was then hided 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 dissolved oxygen was expressed through model kinetics.

The model is given as follows:

$$
\begin{aligned}
\frac{dS_{NH_4^+}}{dt} &= \frac{Q_{ww}}{V} S^{in}_{NH_4^+} - \frac{Q_{ww}+Q_x}{V} S_{NH_4^+} \\
&\quad - r_n \frac{S_{NH_4^+}}{K_{NH_4^+}+S_{NH_4^+}} \frac{O_2}{K_{O_2A}+O_2} \\
\frac{dS_{NO_3^-}}{dt} &= \frac{Q_x}{V} S^x_{NO_3^-} - \frac{Q_{ww}+Q_x}{V} S_{NO_3^-} \\
&\quad + K_1 r_n \frac{S_{NH_4^+}}{K_{NH_4^+}+S_{NH_4^+}} \frac{O_2}{K_{O_2A}+O_2} \\
&\quad - r_{dn} \frac{S_{N0_3^-}}{K_{NO_3^-}+S_{NO_3^-}} \frac{K_{O_2dn}}{K_{O_2dn}+O_2} \\
\frac{dO_2}{dt} &= K_La(O_2^* - O_2) - OUR_0 \frac{O_2}{K_{O_2H}+O_2} \\
&\quad - K r_n \frac{S_{NH_4^+}}{K_{NH_4^+}+S_{NH_4^+}} \frac{O_2}{K_{O_2A}+O_2}
\end{aligned} \tag{1}
$$

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:

$$Q_{ww},\ Q_x,\ V,\ O_2^*$$

- 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:

$$r_n,\ r_{dn},\ K_La,\ OUR_0,\ S^{in}_{NH_4^+},\ S^x_{NO_3^-}$$

Remark 1 *We consider in the following that sludge are free from nitrate, then* $S^x_{NO_3^-} = 0$.

K	4.24
K_1	0.9
$K_{NH_4^+}\ (gN/m^3)$	0.2
$K_{NO_3^-}\ (gN/m^3)$	0.2
$K_{O_2A}\ (gO_2/m^3)$	0.1
$K_{O_2dn}\ (gO_2/m^3)$	0.2
$K_{O_2H}\ (gO_2/m^3)$	0.2

Table 1: Default values of parameters

The estimation procedure is based on the error between an experimental cycle and a simulated cycle. Then in plus of 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 dissolved oxygen 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 Δt^{prev}_{an}. It is then directly related to the influent ammonia nitrogen concentration:

$$S_{NH_4^+}(0) = \frac{S^{in}_{NH_4^+} Q_{ww} \Delta t^{prev}_{an}}{V} \tag{2}$$

Moreover, parameters related to the dissolved oxygen 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:

$$K_La = \frac{p_1 - p_2}{O_2^* - O_2^{max}} \tag{3}$$

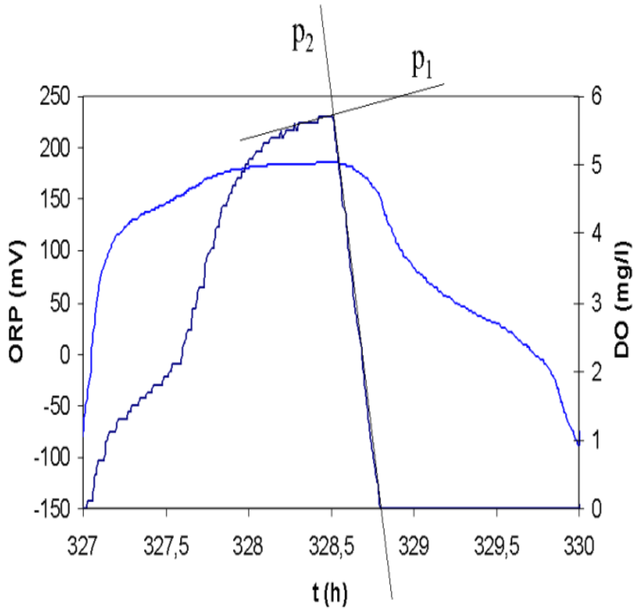

Figure 1: Standard evolution of the dissolved oxygen concentration and ORP signal

where the slopes p_1 and p_2 are illustrated in Figure 1. O_2^{max} represents the maximum value of dissolved oxygen concentration. This approximation is particularly true when the slope p_1 tends towards 0.

The endogenous and heterotroph activity OUR_0 may be estimated from the influent ammonia nitrogen concentration when $S_{NH_4^+}$ becomes equal to 0, i.e. $\frac{S_{NH_4^+}}{dt} = \frac{O_2}{dt} = 0$. Under the hypothesis that $\frac{O_2^{max}}{K_{O_2H}+O_2^{max}}$ approximately equals to 1, one obtains:

$$OUR_0 = K_La(O_2^* - O_2^{max}) - \frac{S_{NH_4^+}^{in} Q_{ww} K}{V} \qquad (4)$$

Inspired by these observations, the identification problem then consists to determine the three remaining parameters r_n, r_{dn}, $S_{NH_4^+}^{in}$, by using the data collected on one alternated cycle.

3 Observation procedure

Parameter identification has been carried out by using a Simplex procedure. 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 $t_{\alpha O_2}$ and $t_{\chi ORP}$, respectively. The cost function was then given by the weighted addition of:

- the error between the simulated oxygen profile and measurements

$$\sum_{t=t_{0ae}}^{t_{0an}} (O_2^{mes}(t) - O_2(t))^2$$

- 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

$$t_{\alpha O_2} - t(S_{NH_4^+} \leq K_{NH_4^+})$$

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

$$S_{NH_4^+}(t_{\alpha O_2}) - K_{NH_4^+}$$

- 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

$$t_{\chi ORP} - t(S_{NO_3^-} \leq K_{NO_3^-})$$

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

$$S_{NO_3^-}(t_{\chi ORP}) - K_{NO_3^-}$$

Moreover, the Simplex procedure is particularly robust as the number of parameter to identify is decreased. In the current case, the influent ammonia concentration and nitrification rate mainly affect the aerobic period of the cycle although 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 $S_{NH_4^+}^{in}$ only use information about the aerobic period, and identification of r_{dn} is related to the anoxic period.

4 Validation on experimental data

Experiments were performed at 15^{o}C with a 40-litre 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 2. Chemical Oxygen Demand (COD), nitrate, nitrite and ammonia were analysed using Standard Methods (1995).

Experimental data used for parameter estimation are shown on Figure 2. An example of four successive cycles are shown. Knee points are clearly visible on DO and ORP signals (decreasing) during aerobic phase, which characterises

Q_{ww} (m^3/day)	Q_x (m^3/day)	V (m^3)	O_2^* (gO_2/m^3)
0.0374	0.0432	0.04	10

Table 2: Process operation - Experimental conditions

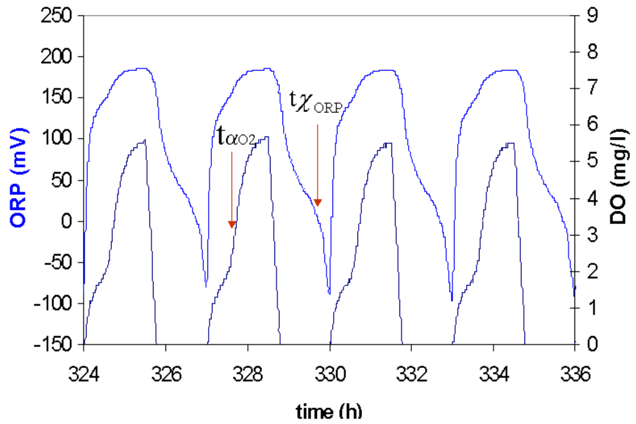

Figure 2: Experimental data used for model calibration. Oxygen and ORP profiles during four aerobic-anoxic cycles

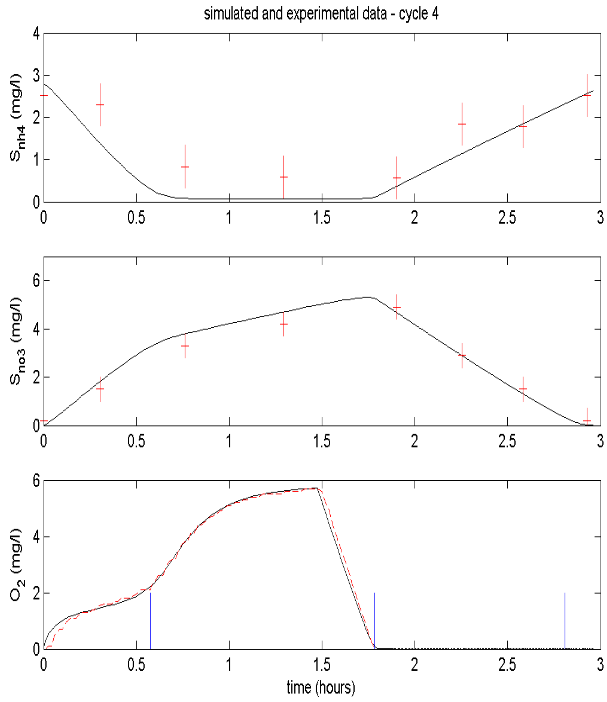

Figure 3: Experimental (+ or dashed line) and estimated (solid line) time-evolution of process variables

depletion of ammonia. Before the end of the anoxic period, an acceleration appeared on the ORP signal due to nitrate depletion.

The estimation procedure is checked on the cycle 4, for which off-line analysis of the influent ammonia concentration and reaction rates have been done. Figure 3 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 3.

First of all, the modelled dissolved oxygen profile fits very well with the measured one. 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 reactor can be calculated with the final set of parameters. Ammonia and nitrate concentration have been measured by discrete sampling at different time and are compared to the calculated ones in the Figure 3. Modelled and experimental nitrate concentration are in good accordance. Concerning ammonia, calculated values are lower than measured one, although the shape of the evolution are the same. This systematic underestimation can be explained by the fact that only nitrifiable ammonia is estimated by the model, i.e., the ammonia assimilated by growth is not considered. For the same reason, estimated influent nitrifiable ammonia is slightly lower than measured value.

	estimated	measured
$S_{NH_4^+}^{in}(mg/l)$	58.5 (nitrified)	60.9 (NTK)
$r_n(mg/l/h)$	215	–
$r_{dn}(mg/l/h)$	117	119
$COD_{dn}(mgDCO/h)$	1065	1124

Table 3: Results of parameter estimation for experimental conditions

The experimental denitrification rate has been deduced from nitrate concentration measurement in the reactor. The value obtained (119 $mg/l/day$) is closed 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:

$$COD_{dn} = \frac{2.86}{1 - Y_{hd}} V r_{dn}$$

with

$$Y_{hd} = 0.5 gCOD/gCOD \text{(measured by [12])}$$

It is compared in the last column of table 3 with the measured inlet COD flux, which is the product of measured COD concentration of wastewater and the influent flow rate. 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, commonly 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 plus of 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 parameter. 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 $S^{in}_{NH_4^+}$. Results are plotted on Figure 4. 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 $S^{in}_{NH_4^+}$. Moreover, it must be noted that if the identification of r_n and $S^{in}_{NH_4^+}$ 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.

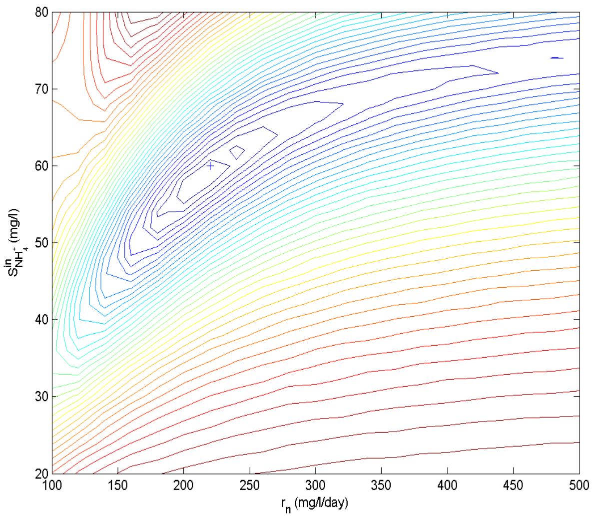

Figure 4: Cost function with respect to parameter values. The cross represents the optimal solution given by the Simplex procedure

5 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.

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 other tests on various simulations done with GPSX software have confirmed that the procedure gives good predictions of kinetics rates, influent ammonium and state variables profiles.

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