ONLINE MONITORING OF AN AEROBIC SBR PROCESS BASED ON DISSOLVED OXYGEN MEASUREMENT

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Abstract: This paper presents results that enable monitoring of an aerobic sequencing batch wastewater treatment (WWT) process based on online dissolved oxygen (DO) concentration measurement. It introduces the sequential process and the DO dynamics, presents a formal discrete event system (DES) model for the traditional SBR process and a modification that enables online monitoring of the respiration rate during the reaction phase and of the oxygen transfer parameter K_{La} over process cycles. Finally a test method for verifying the presence of substrate in the reactor is introduced. Parts of the results have been validated with experimental data from the EOLI project. *Copyright © 2005 IFAC*

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1. INTRODUCTION

Biotechnological processes are often characterized by a high level of uncertainty. This is especially evident in the case of wastewater treatment (WWT), when residual waters vary considerably in composition and flow. The Sequencing Batch Reactor (SBR) and its traditional process scheme is based on the fill-and-draw principle (EPA, 1999), which consists of 5 process phases (see Fig. 1):

(1) *Idle*: The reactor is not in use.
(2) *Fill*: The reactor is filled with residual waters.
(3) *React*: The microorganisms in suspension (activated sludge) within the reactor utilize organic and nitrogen compounds for metabolic activity.
(4) *Settle*: The activated sludge sediments to the bottom of the tank.
(5) *Draw*: The treated water is removed from the reactor (effluent). Note that only a specific part of the utilizable tank volume will be interchanged in each cycle.

While this approach offers greater flexibility for transitory flows, it still exposes weakness in experiment reproducibility, non-stationarity and non-linearity, multi-variable aspects and suffers from measurement uncertainties. In other words, these processes represent unique systems, where a mathematical model often cannot capture all required information to describe the process variables, its different phases, parameter drifts and unexpected disturbances (e.g. concentration shocks, inhibition). Given the characteristics of the process and the fact that many of the parameters cannot be measured economically online, control often fails or does not provide a sufficient level of confidence, performance and reliability. Following the terminology described by Isermann
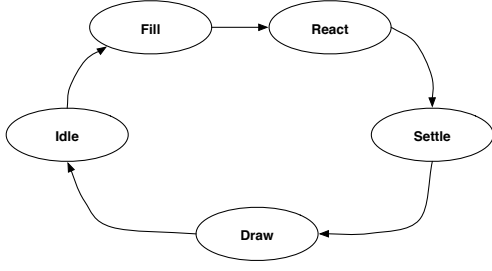
Figure 1. Sequential Process Scheme

and Ballé (1997) the authors have elaborated a scheme for monitoringthe aerobic sequential process using online measurements of the DO concentration and aggregated process phases. This approach can improve the operation of the SBR process under abnormal conditions and prevent economical and environmental impact.

The paper is organized as follows: Section 2 presents a review of the DO dynamics as applicable for the activated sludge process. Section 3 introduces a formal discrete event system (DES) model for the SBR process. Section 4 presents our proposal for monitoring the sequential process based on an extension of the traditional process schema that allows to exploit the DO dynamics. Finally some conclusions are drawn and possible future work is outlined.

2. DISSOLVED OXYGEN DYNAMICS

The DO dynamics for a biological reactor can be described in form of a mass balance equation as used for chemical reactors and presented as eqn. (1) (Rawlings and Ekerdt, 2002).

$$\frac{d}{dt}\int_V O\,dV = Q_{in}O_{in} - Q_{out}O +$$
$$\int_V OTR\,dV - \int_V OUR\,dV \quad (1)$$

where V is the reactor volume, Q_{in} the inflow rate, Q_{out} the outflow rate, O the oxygen in the reactor, O_{in} the oxygen in the inflow medium, OTR the oxygen transfer rate and OUR the oxygen uptake rate.

Given that one has a well stirred batch reactor with $Q_{in}, Q_{out} = 0, V = const.$, one can

(1) assume that there are no concentration gradients and thus it is natural to take the complete reactor volume as volume element
(2) use the concentrations and component mass equivalently

and thus reduce eqn. (1) to eqn. (2).

$$\frac{dO}{dt} = OTR - OUR \quad (2)$$

2.1 Oxygen Transfer Rate, OTR

The transfer of O_2 molecules from the gas phase to the liquid phase is limited by the movement of the molecules through the boundary layer of the air bubbles (difusion). In the boundary layer the saturation concentration of oxygen is assumed and the oxygen transfer term can be described as:

$$OTR = \tilde{K}_L a\,(O_{sat} - O) \quad (3)$$

where $\tilde{K}_L a = K_L a$ when aeration is on, and $\tilde{K}_L a = 0$ when aeration is off. The oxygen transfer coefficient K_L and the interfacial area a between gas and liquid phase per unit volume are usually unified into a single parameter K_{La}, as a is impossible to measure and very difficult to estimate. The O_{sat} is the maximum concentration in the liquid phase, which is equal to the oxygen solubility in aqueous solutions. It is function of the temperature, partial oxygen pressure and salinity of the solution. In WWT it is common practice to assume it constant and obtain it only once from tabular oxygen solubility data, although the temperature influence has been studied and verified (Vogelaar *et al.*, 1996). However, convenient models for the oxygen solubility in aqueous solutions exist (Tromans, 1999) and can be approximated very well using three steps: *(a)* an approximation of the partial pressure at a given level based on the partial oxygen pressure at sea level, *(b)* a linear interpolation of Henry's constant at a given temperature H_T and *(c)* Henry's law.

2.2 Oxygen Uptake Rate, OUR

The consumption of the oxygen by microorganisms is described by the oxygen uptake rate that is also called respiration rate, which will be denoted as $r(t)$ subsequently. Organisms use the O_2 molecules as an electron receptor in the catabolic metabolism to produce energy (usually stored in chemical form) that is subsequently used for:

(1) Processes that synthesize complex organic substances from other more simple ones (anabolic metabolism).
(2) Processes and phenomena of auto-regulation that intent to maintain the composition and properties of the organism in equilibrium (Homeostasis) and
(3) other processes and activities like for example cell movement.

The models for the respiration are usually based on two elements (Henze *et al.*, 2000): *(a)* a relationship between the consumption of substrate and the growth rate and *(b)* the respiration under absence of substrate, that can be assumed unchanging (Marsili-Libelli, 1990; Henze *et al.*, 2000) and thus can be replaced by a constant that will

successively be denoted as r_e.

Later this paper will focus on recuperation of the respiration rate $r(t)$, as it obviously represents a key indicator for biological activity.

2.3 Dissolved Oxygen Measurement

From eqn. (2) and (3) one obtains:

$$\frac{dO}{dt} = \tilde{K}_{La}\left(O_{sat} - O(t)\right) - r(t) \qquad (4)$$

as the description of the DO dynamics, taking advantage of the available measurement of DO in the bulk liquid phase. Although economic sensors are available on the market today, an important factor in utilizing the measurement can be the dynamics of the sensor itself. If it is comparable to the process dynamics that one wants to observe, it is required to deal with the delay in the sensor response (Lindberg and Carlson, 1996). In our particular case (DO probe COS4 from Endress + Hauser), to reduce the response delay, one can implement a lag-smoothing filter (LSF) based on the design procedure proposed by Lindberg and Carlson (1996) that is based on Ahlén and Sternad (1989) and compared it with a stable inverse of the DO sensor model. Since a stable inverse filter (SIF) could be obtained and provides better recuperation for a noise filtered DO signal, the data used in our case is filtered with the SIF.

3. FORMAL MODEL OF THE SEQUENTIAL PROCESS

To introduce a monitoring system, a formal model of the whole process needs to be established. The formerly presented sequence of process phases (Fig. 1) can be directly translated into a simple discrete event system (DES) model, a modified state automaton as described by Cassandras (1993, p. 82). The resulting state automaton (see Fig. 2) can be defined as the five-tuple (E, X, Γ, f, x_0):

$$E = \{e_1, e_2, e_3, e_4, e_5\}$$
$$X = \{q_0, q_1, q_2, q_3, q_4\}$$
$$\Gamma = \Gamma(q_0) = \{e_1\}, \Gamma(q_1) = \{e_2\}, \Gamma(q_2) = \{e_3\},$$
$$\quad \Gamma(q_3) = \{e_4\}, \Gamma(q_4) = \{e_5\}$$
$$f = f(q_0, e_1) = q_1, f(q_1, e_2) = q_2, f(q_2, e_3) = q_3,$$
$$\quad f(q_3, e_4) = q_4, f(q_4, e_5) = q_0,$$
$$x_0 = q_0 \qquad (5)$$

where E is the set of events, X the set of states, Γ the active events for each state, f the set of transition functions and x_0 the initial state respectively. The set X is given by a state for
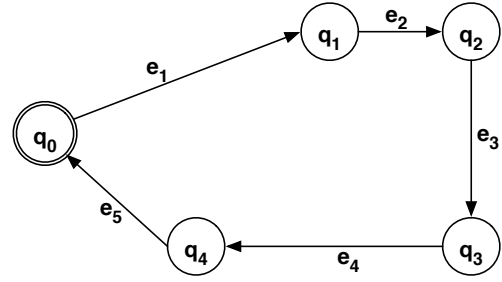

Figure 2. SBR Process State Automaton

each traditional SBR process phase from Fig. 1: $q_0 = Idle$, $q_1 = Fill$, $q_2 = React$, $q_3 = Settle$, $q_4 = Draw$. The events in set E will be generated by a control system, using for example a simple scheme with fixed times, according to the process description presented in the introduction.

4. MONITORING OF THE SEQUENTIAL PROCESS

Within the previously established DES model, the eqn. (4) is actually only validly applicable in state q_2. However, with the given process limitations it is not possible to observe the respiration rate with formerly presented concurrent methods for continuous activated sludge processes (Marsili-Libelli, 1990; Lindberg and Carlson, 1996). Thus the authors propose to extend the traditional process schema with two special phases that allow us to validly apply and exploit eqn. (4) and thus enable DO based monitoring of the process, in particular via

(1) the online identification of the oxygen transfer parameter K_{La} apart from the observation of the respiration rate $r(t)$ as well as
(2) a test of substrate presence that might be of special interest when treating influents with organic toxic substances

As a consequence the previously presented DES model (see Fig. 3) is extended to

$$E_e = E \cup \{e_6, e_7, e_8, e_9, e_{10}\}$$
$$X_e = X \cup \{q_5, q_6\}$$
$$\Gamma_e = \Gamma \cup \Gamma(q_0) = \{e_6\}, \Gamma(q_5) = \{e_7\},$$
$$\quad \Gamma(q_2) = \{e_8\}, \Gamma(q_6) = \{e_9, e_{10}\}$$
$$f_e = f \cup f(q_0, e_6) = q_5, f(q_5, e_7) = q_1,$$
$$\quad f(q_2, e_8) = q_6, f(q_6, e_9) = q_2,$$
$$\quad f(q_6, e_{10}) = q_3 \qquad (6)$$

where $q_5 = Re\text{-}Aerate$ and $q_6 = Test\text{-}Respiration$.

State q_5, Re-Aerate Represents a phase of the process where the bulk liquid remaining in the reactor is re-aerated until $\frac{dO}{dt} \cong 0$. During this phase, following assumptions have to hold:
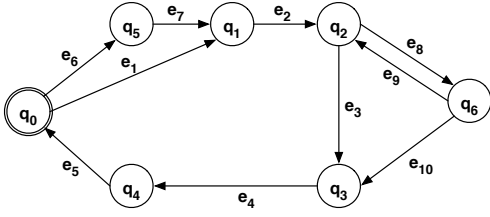
Figure 3. Extended State Automaton

(1) $\frac{dV}{dt} = 0$, $V = const.$
(2) $O_{sat} = const.$
(3) $r(t) = r_e = const.$

State $q_6, Test - Respiration$ Represents a short phase where the aeration is turned off (mixing required), to make the OTR term disappear from eqn. 4. The time required to perform this test has to be selected by the operator, taking into account the sampling time, the expected respiration rate and the total cycle time since the test phase should be very small in comparison to the cycle time.

Discrete Model From eqn. (4) one obtains a simple discrete model using a Zero-Order-Hold (ZOH) as described by Åström and Wittenmark (1984):

$$O(k+1) = e^{-K_{La} h} O(k) + \frac{(1 - e^{-K_{La} h})}{K_{La}}$$
$$(-r(k) + K_{La} O_{sat}(k)) \qquad (7)$$

when the aeration is on, and

$$O(k+1) = O(k) - h \, r(k) \qquad (8)$$

when the aeration is off, where h represents the sampling time and k the normalized step.

4.1 Online Identification of K_{La}

Assuming that (*a*) the parameter K_{La} changes only slowly when the air flow rate is constant (Lindberg and Carlson, 1996) and (*b*) that respiration behavior is invariable, state q_5 can be exploited for it's online identification and use the obtained estimate in the subsequent batch cycle for the estimation of $r(t)$. Based on the assumptions, one can reduce the discrete model from eqn. (7) to:

$$\Delta O(k) = \theta \, \Delta O(k-1) \qquad (9)$$

which represents the difference between two subsequent samples (i.e. at time k and $k-1$) and describes the behavior of the DO curve in an incremental form (Åström and Wittenmark, 1984, p. 181), where $\Delta O(k-i) = O(k-i) - O(k-(i+1))$ and $\theta = e^{-K_{La} h}$. Note that eqn. (9) does no longer depend on the O_{sat} and the respiration rate r_e.

Using eqn. (9) the authors have implemented two identification algorithms for the parameter K_{La}. Both can be applied if re-aeration starts from an initial condition value $O(0) << O_{sat} - r_e$ and ends near steady state conditions ($\frac{dO}{dt} \cong 0$, or $O \cong O_{sat} - r_e$).

(1) *A Linear Regression (Least Squares Estimate)*, using all samples obtained during the Re-Aeration period, a standard offline parameter identification method as described in Söderström and Stoica (1989, Sec. 4.1).
(2) *A Kalman Filter for Parameter Identification*, an online parameter identification method as described in Söderström and Stoica (1989, p. 325).

The advantage of the Kalman algorithm over a Recursive Least Squares algorithm is the fact that literature suggests values for the initial values of the parameter $\hat{\theta}(0)$ and the filter parameter $P(0)$ and R_1. Both implementations have been successfully verified in simulation and with data from EOLI model identification experiments. Fig. 4 presents an example for identification using online measurement data. $\hat{K}_{La,A} = 0.00461[s^{-1}]$ is the result of the Kalman filter algorithm when started from the point in time when aeration is switched on (with initial covariance $P(0) = 100$ and $\theta(0) = 0$), $\hat{K}_{La,B} = 0.00464[s^{-1}]$ is the result when the algorithm starts after one can assume that the aeration system has achieved steady state. The latter is slightly better, as the starting point and the first part of the re-aeration curve is the most critical part for the identification and is influenced by the delay of the aeration mechanism in aerating the reactor. These results are comparable to $K_{La}^* = 0.00467[s^{-1}]$ reported by Betancour *et al.* (2004) for the same data.

The implementation of the online identification of the oxygen transfer parameter K_{La} over consecutive cycles allows to enhance the result using the estimated $\hat{K}_{La}$ as initial value $\theta(0)$ for the algorithm in the subsequent cycle. However, it also enables monitoring of the oxygen transfer, through the detection of deviations from acceptable/usual/standard condition using methods as described in Basseville and Nikiforov (1993).

4.2 Observation of the Respiration Rate

Since the transfer parameter K_{La} is identified during the state q_5 of every batch cycle, one can use its estimation $\hat{K}_{L}a$ as a known constant value in the subsequent cycle's state q_2 (reaction phase) and the respiration rate $r(t)$ can be monitored during this state using eqn. (7). Considering that $O(t)$ changes faster than the $r(t)$, one can propose for its model

$$r(k+t) = r(k) + n(k) \quad for \; 0 < t < 1 \qquad (10)$$

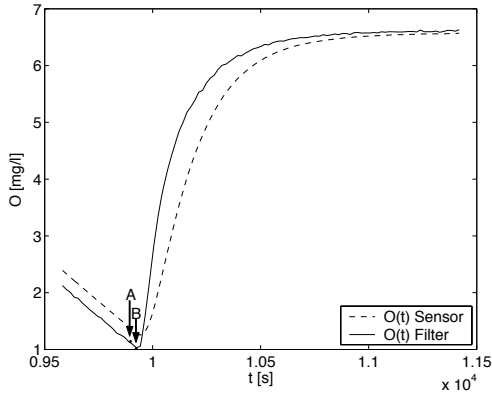Figure 4. Parameter Identification in state q_5

Figure 5. Respiration Rate Patterns

with $n(k)$ a white noise. Now from eqns. (7) and (10) one obtains the observable augmented model

$$\begin{bmatrix} O(k+1) \\ r(k+1) \end{bmatrix} = A \begin{bmatrix} O(k) \\ r(k) \end{bmatrix} + BO_{sat}(k) + \begin{bmatrix} 0 \\ 1 \end{bmatrix} n(k)$$

where

$$A = \begin{bmatrix} \alpha & -\dfrac{1-\alpha}{\hat{K}_{La}} \\ 0 & 1 \end{bmatrix}, \ B = \begin{bmatrix} 1-\alpha \\ 0 \end{bmatrix}$$

with constant $\alpha = e^{-\hat{K}_{La} h}$ and output $y(k) = O(k)$. This model can be used to monitor $r(k)$ using a full or reduced order observer. For this task, one can use the structure

$$\hat{x}(k\backslash k) = (I - KC)(A\hat{x}(k-1\backslash k-1) +$$
$$BO_{sat}(k-1)) + Ky(k) \qquad (11)$$

with $C = [1 \ 0]$ and K chosen such that the eqn. (11) is asymptotically stable (Åström and Wittenmark, 1984).

Example for $r(t)$ Based Monitoring The EOLI project involves batch processes for the purpose of combined carbon and nitrogen removal. Nitrate (NO_2) is an intermediate product formed during the reaction phase of these processes, that is subject of strict emission limits. Therefore, the excessive outflow of NO_2 has been defined as process fault.

In various identification experiments this fault has been detected by measurements of component concentrations in the effluent. The fact that this occurred in all experiments with reduced (compared to the standard condition) carbon to nitrogen content ratio (COD/N) in the influent, establishes a causal link between the COD/N ratio of the influent as cause and the process fault as effect. Fig. 5 presents the respiration rate profile for three selected identification experiments: *(a)* Standard Conditions (SC), $COD/N \cong 8$, *(b)* 20% reduced COD/N ratio in the influent and *(c)* 50% reduced COD/N ratio in the influent, obtained
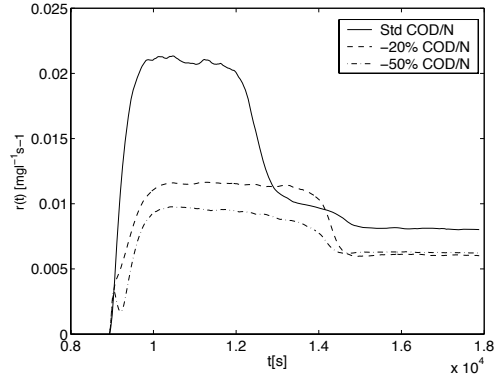
using eqn. (11). The latter two are faulty experiments and exhibit a visually perceptible pattern, different from the SC experiment. This implies that by means of respiration rate observation, another causal link between the respiration rate profile and the COD/N ratio of the influent could be found, that temporally precedes the formerly established one and thus can be exploited for monitoring purposes: detect and inform the process operator of unfavorable COD/N ratios in the influent and forewarn that under such conditions excessive NO_2 outflow is likely to occur.

The algorithmic recognition and interpretation of these patterns in the respiration rate for monitoring and process fault diagnosis is subject of current investigation.

4.3 Test of Substrate Presence

The behavior of the respiration in continual absence of substrate, $r(t) = r_e = const.$) can be exploited applying simple model based fault detection. During the test phase (state q_6) the model describing the DO behavior is eqn. (8) from which one can derive the following parity equation:

$$2\,O(k-1) - O(k) - O(k-2) = 0 \qquad (12)$$

A deviation from this parity equation exceeding a certain threshold is a symptom for the undesired presence of respirable substrates in the reactor. Its detection allows to take appropriate actions (e.g. prolonged reaction phase; e_9 causing a transition back to state q_2; see Fig. 3). It is possible and anticipated, that the test is only performed when the profile of the respiration rate $r(t)$ exhibits abnormal patterns during the reaction phase.

5. CONCLUSIONS

This paper presents the development of a monitoring schema for the aerobic SBR process utilizing only the DO measurement and aggregated process phases. It introduces a formal model for the process and extends it with two special phases that enable:

(1) The online identification of the the oxygen transfer parameter K_{La} that gives the opportunity to detect parameter variation during continuous reactor operation and can be exploited for an observation of $r(t)$ during the reaction phase. The evaluation of the K_{La} would otherwise require a special experiment that cannot be and is not performed for every batch cycle.

(2) The continuous observation of the respiration rate $r(t)$ during the reaction phase, which is a key indicator for biomass activity. The presented method is different from that described in Yoong *et al.* (2000), which provides an in-situ measurement but does not provide a continuous respiration rate profile. It is also disimilar from respirograms obtained by a respirometer that are not in-situ and require additional hardware.

(3) A test for verifying substrate presence, that can be specially useful when treating organic toxic compounds to prevent environmental and human impact. This would otherwise demand taking a sample for offline lab analysis, which is time consuming and does as well require additional equipment.

The developed and presented corresponding algorithms have been verified with simulations and experimental data from the EOLI project. As an online monitoring approach, the results can improve the operation of the SBR process under abnormal conditions and prevent economical and environmental impact, despite the uncertain character of the biological WWT process. Nonetheless, the algorithmic recognition and interpretation of respiration patterns during the reaction phase could further enhance this approach, a fact our current investigation is concerned with.

6. ACKNOWLEDGMENTS

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