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. First it introduces the sequential process and reviews the DO dynamics discussing all its important components and how to deal with sensor response delay. Subsequently it presents a formal discrete event system (DES) model for the traditional SBR process as well as a modification that introduces new states and enables our monitoring methodology. The presented approach will allow the online identification of the oxygen transfer parameter $K_L a$ in an aggregated state, enabling tendency monitoring, as well as apart from it, the online monitoring of the respiration rate during the reaction phase. 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.

Keywords: Safeprocess, Monitoring, Sequential Batch Process, Dissolved Oxygen

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 -linearity, multi-variable aspects and suffers from measurement uncertainties. In other words, this 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 pa-
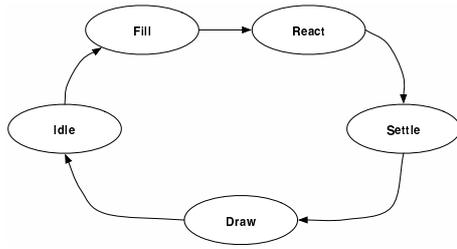
Figure 1. Sequential Process Scheme

rameters 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 and Balle, 1997) we elaborated a scheme for monitoring the 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 sound review of the generic DO dynamics for activated sludge processes. Section 3 introduces a formal discrete event system (DES) model for the SBR process. Section 4 presents our proposal for monitoring the sequential process, exploiting the separation of phases and an extension of the formerly presented formal DES model of the process. Finally some conclusions are drawn and possible future work is outlined.

2. DISSOLVED OXYGEN DYNAMICS

The oxygen dynamics are included in all generic activated sludge process models in form of a mass balance equation. This balance can be described in simple qualitative terms, revealing the rate components it is composed of:

$$\frac{dO(t)}{dt} = oxygen\ transfer - respiration$$
$$\pm dilution \qquad (1)$$

where $O(t)$ is the dissolved oxygen concentration in the bulk liquid.

2.1 Rate Components

Oxygen Transfer

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:

$$OTR = \tilde{K}_L a\left(O_{sat} - O(t)\right) \qquad (2)$$

where $\tilde{K}_L a = K_L a$ when aeration is on, and $\tilde{K}_L a = 0$ otherwise. 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 $K_L a$, 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 oxigen 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:

- An approximation of the partial pressure at a given sea level (x) based on the partial oxygen pressure at sea level.
- A linear interpolation of Henry's constant at a given temperature H_T.
- And Henry's law.

Respiration

The consumption of the oxygen by microorganisms is described by the respiration rate $r(t)$. 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 sythesize complex organic substances from other more simple ones (anbolic metabolism).
(2) Processes and phenomena of auto-regulation that intent to maintain the composition and properties of the organism in equilibrium (Homeostasis).
(3) And Activities like for example cell movement.

The models for the respiration are usually based on two elements (Henze *et al.*, 1987; Henze *et al.*, 1995; Gujer *et al.*, 1995):

(1) A relationship between the consumption of substrate and the growth rate.
(2) And the Respiration under absence of substrate.

We will focus on recuperation of the respiration rate $r(t)$ without establishing a specific microscopic model for oxygen usage, other than a qualitative description of the behaviour in absence of substrates that can be described as $r(t)$ is constant (Marsili-Libelli, 1990; Henze *et al.*, 1987; Henze *et al.*, 1995; Gujer *et al.*, 1995).

Dilution

The dilution rate term describes the concentration change caused by mixing liquids with different DO concentration, where an inflow at rate Q_{in} and with the concentration O_{in} dilutes the liquid in the tank of volume $V(t)$ with a concentration of $O(t)$ and therefore can be described by:

$$Dilution = \frac{Q_{in}}{V(t)}(O_{in} - O(t)) \qquad (3)$$

2.2 Generic Activated Sludge Model

The mass balance presented as eqn. (1) has been formally described by (Spanjers *et al.*, 1996) for aerobic activated sludge treatment processes, giving

$$\frac{dV(t)O(t)}{dt} = Q_{in}O_{in} - Q_{out}O(t) + V(t)$$
$$K_{La}\left(O_{sat} - O(t)\right) - V(t)\,r(t) \quad (4)$$

where Q_{out} corresponds to an outflow rate from the tank. Given also that $\frac{dV(t)}{dt} = Q_{in} - Q_{out}$, eqn. (4) can be reduced to

$$\frac{dO(t)}{dt} = K_{La}(O_{sat} - O(t)) - r(t) +$$
$$\frac{Q_{in}}{V(t)}(O_{in} - O(t)) \qquad (5)$$

The key for monitoring the process from a practical point of view, is the DO measurement in the bulk liquid phase.

Dissolved Oxygen Measurement

Economic sensors for the measurement of the DO concentration $O(t)$ are available on the market today. However, 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, we have implemented a filter based on the design procedure proposed by (Lindberg and Carlson, 1996) that is based on (Ahlén and M.Sternad, 1989) and compared it with a stable inverse of the DO sensor model (see Fig. 2). Since the stable inverse filter (SIF) could be obtained and provides better recuperation for a noise filtered DO signal, the data in our case is filtered with the SIF.
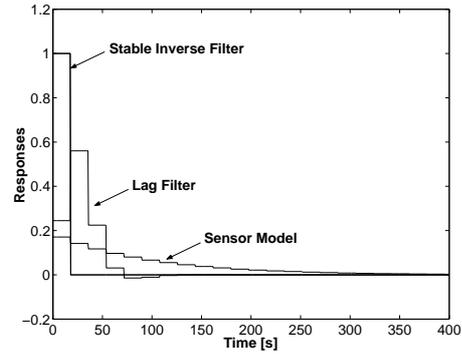
Figure 2. Impulse Responses of Sensor and Filters
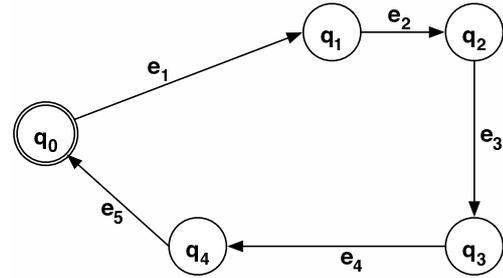
Figure 3. SBR Process State Automaton

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. 3) can be defined as the five-tuple (E, X, Γ, f, x_0):

$$E = \{e_1, e_2, e_3, e_4, e_5\}$$
$$X = \{q_0, q_1, q_2, q_3, q_4\}$$
$$\Gamma = \Gamma(q_0) = \{e_1\}, \Gamma(q_1) = \{e_2\}, \Gamma(q_2) = \{e_3\},$$
$$\Gamma(q_3) = \{e_4\}, \Gamma(q_4) = \{e_5\}$$
$$f = f(q_0, e_1) = q_1, f(q_1, e_2) = q_2, f(q_2, e_3) = q_3,$$
$$f(q_3, e_4) = q_4, f(q_4, e_5) = q_0,$$
$$x_0 = q_0 \qquad (6)$$

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 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. The temporally separated process phases demand that the following elements can be controlled:

- Inflow
- Outflow
- Aeration

This property of the sequential process has an influence on the structure of the generic DO balance given as eqn. (5). As a consequence of switching on or off the above mentioned items in specific process phases, certain terms of eqn. (5) will dissappear, a fact that can be exploited for implementing a monitoring scheme and presents the main contribution of this paper.

4. MONITORING OF THE SEQUENTIAL PROCESS

We propose to implement a monitoring scheme that operates with three main tasks:

(1) Online Identification of the Oxygen Mass Transfer Parameter $K_L a$
(2) Observation of the respiration rate $r(t)$ during the reaction phase
(3) Test of substrate presence

The first two tasks allow the identification of the $K_L a$ apart from the observation of the respiration rate, as compared to formerly presented concurrent methods for continous AS processes (Marsili-Libelli, 1990; Lindberg and Carlson, 1996). This separation is based on the fact that the parameter $K_L a$ changes only slowly when the air flow rate is constant (Lindberg and Carlson, 1996).

The test of the substrate presence allows us to verify if the biomass has successfully degraded the substrates during the reaction phase, which might be of special interest when treating organic toxic substances.

To accomplish these tasks, we have aggregated two special phases to the traditional process scheme and as a consequence the formerly presented DES model (see Fig. 4) is extended to

$$
\begin{aligned}
E_e &= E \cup \{e_6, e_7, e_8, e_9, e_{10}\} \\
X_e &= X \cup \{q_5, q_6\} \\
\Gamma_e &= \Gamma \cup \Gamma(q_0) = \{e_6\}, \Gamma(q_5) = \{e_7\}, \\
&\quad \Gamma(q_2) = \{e_8\}, \Gamma(q_6) = \{e_9, e_{10}\} \\
f_e &= f \cup f(q_0, e_6) = q_5, f(q_5, e_7) = q_1, \\
&\quad f(q_2, e_8) = q_6, f(q_6, e_9) = q_2, \\
&\quad f(q_6, e_{10}) = q_3
\end{aligned}
\tag{7}
$$

where $q_5 =$ Re-Aerate and $q_6 =$ Test-Respiration.

The aggregation of the special process phases enables us to exploit the structure of the DO mass balance equation (5), exactly for the purpose of identifying the oxygen transfer parameter when the process is in state q_5 and testing substrate presence when it is in state q_6.
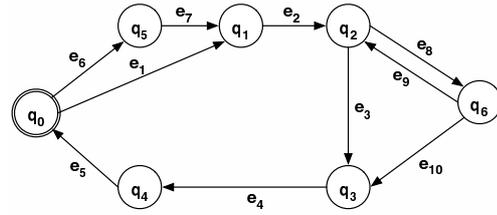
Figure 4. Extended State Automaton

In all phases except *Fill* and *Draw*, there is no inflow or outflow from the reactor. Thus, $\frac{dV}{dt} = 0$ and we can obtain a simple discrete model from eqn. (5) using a Zero-Order-Hold (ZOH) as described by (Åström and Wittenmark, 1984):

$$
\begin{aligned}
O(k+1) = e^{-K_L a\, h}\, O(k) &+ \frac{(1 - e^{-K_L a\, h})}{K_L a} \\
&(-r(k) + K_L a\, O_{sat}(k))
\end{aligned}
\tag{8}
$$

when the aeration is on, and

$$
O(k+1) = O(k) - h\, r(k)
\tag{9}
$$

otherwise, where h represents the sampling time and k the normalized step.

4.1 Online Identification of $K_L a$

The state q_6 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 hold:

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

Therefore the discrete model from eqn. (8) can be reduced to

$$
\Delta O(k) = \theta\, \Delta O(k-1)
\tag{10}
$$

which represents the difference between two subsequent samples (i.e. at time k and $k-1$) and describes the behaviour of the DO curve, where $\Delta O(k-i) = O(k-i) - O(k-(i+1))$ and $\theta = e^{-K_L a\, h}$. Note that eqn. (10) does no longer depend on the O_{sat} and the respiration rate $r(t)$.

Based on eqn. (10) we have implemented two identification algorithms for the parameter $K_L a$.

(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) [2].

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[2] The advantage of the Kalman algorithm over a Recursive Least Squares algorithm is the fact that literature suggests
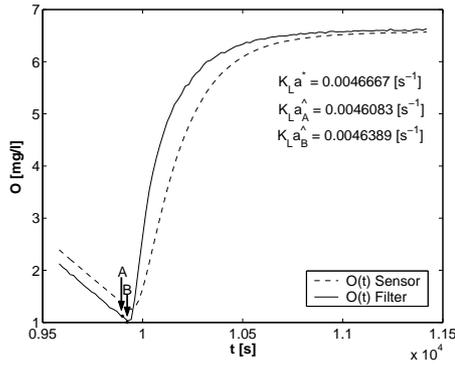
Figure 5. Parameter Identification in state q_5

Both implementations have been successfully verified in simulation and with data from EOLI model identification experiments. Fig. 5 presents an example identification using online measurement data. $\hat{K}_L a = 0.0046083[s^{-1}]$ is the result of the Kalman filter algorithm when started from the point in time when aeration is switched on (A; with initial covariance $P(0) = 100$ and $\theta(0) = 0$), $\hat{K}_L a = 0.0046389[s^{-1}]$ is the result when the algorithm starts after we can assume that the aeration system has achieved steady state (B). 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 $\hat{K}_L a^* = 0.0046667[s^{-1}]$ reported by (Betancour et al., 2004) for the same data.

The implementation of the online identification of the oxygen transfer parameter $K_L a$ over consecutive cycles principally allows to enhance the result using the estimated $\hat{K}_L a$ 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.

4.2 Respiration Monitoring in the Reaction Phase

Since the transfer parameter $K_L a$ is identified during the state q_5 of every cycle of the automaton, one can use its estimation $\hat{K}_L a$ as a known fix value in the subsequent state q_2 and the respiration rate $r(t)$ can be monitored during this state using eqn. (8). Considering that $O(t)$ changes faster than the $r(t)$, one can propose for its model

$$r(k + t) = r(k) + n(k) \quad for \ 0 < t < 1 \qquad (11)$$

with $n(k)$ a white noise. Now from eqns. (8) and (11) one obtains the observable augmented model

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

values for the initial values of the parameter $\hat{\theta}(0)$ and the filter parameter $P(0)$ and R_1
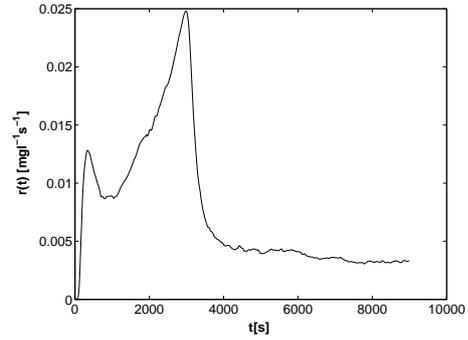
Figure 6. Respiration rate in state q_2

where

$$A = \begin{bmatrix} a & -\dfrac{1-a}{\hat{K}_L a} \\ 0 & 1 \end{bmatrix}, \ B = \begin{bmatrix} 1-a \\ 0 \end{bmatrix}$$

with constant $a = e^{-\hat{K}_L a \, h}$ 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, we use the structure

$$\hat{x}(k\backslash k) = (I - KC)(A\hat{x}(k-1\backslash k-1) + BO_{sat}(k-1)) + Ky(k) \qquad (12)$$

with $C = [1 \ 0]$ and K chosen such that the eqn. (12) is asymptotically stable (Åström and Wittenmark, 1984).

Fig. 6 shows the recuperated r(t) from an EOLI model identification experiment. The location and interpretation of patterns in the respiration rate for process fault diagnosis is subject of future work.

4.3 Test of Substrate Presence

Additionally we can exploit the qualitative behaviour of respiration under absence of substrate ($r(t)$ is constant), applying simple model based fault detection. During a short respiration test phase (state q_6) without aeration but with mixing, the model describing the DO behaviour is eqn. (9) and one can derive the following parity equation:

$$2\,O(k-1) - O(k) - O(k-2) = 0 \qquad (13)$$

A deviation from this parity equation exceeding a certain permissible error 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. 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 (the test phase should be very small in comparison to the cycle time). It is possible and anticipated, that the test is only performed when the respiration rate $r(t)$ exhibits abnormal patterns during the reaction phase.

5. CONCLUSIONS

This paper presented the development of a monitoring scheme for the aerobic SBR process utilizing the DO measurement and two special aggregated process phases. It introduces a formal model for the process and extends it with the aggregated phases, to accomplish three main monitoring tasks

(1) The online identification of the the oxygen transfer parameter $K_L a$ that allows to monitor its tendencies in continous reactor operation and can be exploited to simplify the second task.
(2) The observation of the respiration rate $r(t)$ during the reaction phase, which is a key indicator for biomass activity.
(3) And a test for verifying substrate presence, that can be specially useful when treating organic toxic compounds to prevent environmental and human impact.

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 location, recognition and interpretation of respiration patterns during the reaction phase could further enhance this approach, a fact our current investigation is concerned with.

6. ACKNOWLEDGEMENTS

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