

Modelling and Reachability of Biological Sequencing Batch Reactor

Mazouni D.* — Harmand J.* — Rapaport A.** — Hammouri H.***

* Laboratoire de Biotechnologie de l'Environnement
INRA, Narbonne,
FRANCE

{mazouni,harmand,rapaport}@ensam.inra.fr

** Laboratoire d'Analyse des Systèmes et Biométrie
INRA, Montpellier

FRANCE

*** Laboratoire d'Automatique et Génie de Procédés
Université Claude Bernard, Lyon
FRANCE
hammouri@lagep.cpe.fr

ABSTRACT. In this paper, the dynamic behavior of biological sequencing batch reactor with carbon and nitrogen removal is studied. Our aim is to propose a reduced state space model to be used in the synthesis of an optimal time control strategy. The original state space model is described by ordinary differential equations. It has been simplified and converted into an algebraic-differential system. This new representation allows us to express the linear relationship existing between the state variables. Using this approach, the reachability is studied to determine the attainable set of the system.

RÉSUMÉ. Dans cet article, la dynamique d'un réacteur séquentiel traitant le carbone et l'azote est étudiée. L'objectif est de proposer un modèle d'état réduit pour la synthèse d'une commande optimale. Le modèle original décrit par des équations différentielles ordinaires est simplifié et réduit en un système algèbro-différentiel. La nouvelle représentation facilite l'étude d'atteignabilité et exprime les relations linéaires qui existent entre les variables d'états.

KEYWORDS : Modeling, SBR reactors, Nitrogen and Carbon removal, Reachability

MOTS-CLÉS : Modélisation, réacteur séquentiel, traitement d'azote et de carbone, atteignabilité

1. Introduction

The activated sludge bioreactors are more and more used for wastewater treatment, especially to remove organic carbon and nitrogen. Their basic principle is based on microbial growth reaction. The micro-organisms (biomass) grow by consuming the nutrients (substrate) rich in carbon and nitrogen. ([1]). There exists several kinds of biological reactors. The development and the use of mathematical models has attracted lots of attention and their performances are improved by the application of control and optimization strategies ([2], [3]). In this paper, a Sequencing Batch Reactors (SBR) is studied. In the first part, the modeling of an SBR treating both carbon and nitrogen is studied. The objective is to determine a model which is as complete as possible to take into account the principal biological phenomena and sufficiently simple to be used for the synthesis of optimal control laws. In the second part, a reduced model is derived and used to study the controllability of the process i.e. to determine the set of initial conditions and constraints that must be fulfilled to apply a time optimal control strategy. The SBR process is characterized by a series of process phases: fill, react, settle and draw. All of them taking place in the same tank. Initially, the reactor contains a volume V_0 and a quantity of biomass X_0 that remains from the last cycle. The cycle starts by introducing a volume $\Delta V = V_{max} - V_0$ into the reactor with a flow rate Q . The reaction phase can be divided in two sub-phases: aerated and non-aerated. These two steps allow nitrogen removal in aerobic and anoxic conditions. During these phases the reactor is assumed to be perfectly homogeneous. Once the reaction phase is completed, the mixing is stopped and the sludge starts coagulating and settling. The clean supernatant can then be separated from the sludge and withdrawn from the reactor. The reactor is then available to receive a new volume ΔV of wastewater. After few cycles, the biomass accumulates and it is necessary to waste some sludge ([5]).

The biological reactions take place between the fill and the end of mixing. We can distinguish two phenomena: biological (fill and react) and hydraulic (settle and draw). In this paper we consider only the biological reactions taking place during the reaction phase.

Three basic reactions are considered. The ammonium (S_2) is transformed into nitrogen gas in two steps: nitrification and denitrification ([4][6]). Nitrification is realized by Autotrophic bacteria (X_2) under aerobic conditions (reaction 2). Ammonium is converted into nitrates (S_3) with the growth rate $\varphi_2(\cdot)$. Denitrification is reducing nitrates into nitrogen gas. This reaction is done by Heterotrophic bacteria X_1 under anoxic conditions (presence of nitrates, absence of oxygen). This bacteria uses nitrites as electron acceptor when no oxygen is available. This reaction takes place only if organic carbon is available. In anoxic condition the heterotrophic growth rate is given by $\varphi_3(\cdot)$.

Carbon removal is realized by Heterotrophic bacteria ([6]). Carbon (S_1) can be eliminated either under anoxic conditions with nitrates in denitrification phase (reaction 3) or under aerobic conditions (Reaction 1). In the last case, the growth rate of Heterotrophic

is $\varphi_1(\cdot)$. In order to realize the three reactions in the same tank, we should have two sub-phases reactions: aerobic sub-phase to nitrify the nitrogen and anoxic sub-phase to denitrify it. The carbon is eliminated in both cases.

The reaction network is given by:



The realization of this process presents some problems. In aerobic phase, S3 is produced while S1 is consumed. In the anoxic phase, if there is not enough S1 to eliminate S3 produced during the aerobic phase, this last substrate cannot be eliminated and the nitrogen removal cannot be realized. Before any study of control law, we have to ensure that there exists a solution to this problem. The reachability analysis is necessary to characterize the reachable set and the initial condition from which a solution exists.

2. Modelling

2.1. Mass balance

In this section, a general state space model for the description of the SBR is proposed. The model is based on the mass balance in the reactor during the two phases of filling and reaction. Scientists have studied the bioreactors modeling for long time. They proposed a detailed Activated Sludge Model (ASM1) ([6]) which is very descriptive but too complicated for being used for control design. Other studies proposed reduced models with less state variables ([7]). In ([8]) authors propose a general method for modeling bioreactors from the reaction scheme. If we consider the reaction scheme (1) we can apply the mass balance principle to determine the state space model (2-7).

$$\dot{X}_1 = \mu_1(S_1, O_2)X_1 + \mu_3(S_1, S_3, O_2)X_1 - \frac{Q}{V}X_1 \quad [2]$$

$$\dot{X}_2 = \mu_2(S_2, O_2)X_2 - \frac{Q}{V}X_2 \quad [3]$$

$$\dot{S}_1 = -k_{11}\mu_1(S_1, O_2)X_1 - k_{11}\mu_3(S_1, S_3, O_2)X_1 + \frac{Q}{V}(S_{1in} - S_1) \quad [4]$$

$$\dot{S}_2 = -k_{22}\mu_2(S_2, O_2)X_2 + \frac{Q}{V}(S_{2in} - S_2) \quad [5]$$

$$\dot{S}_3 = k_{32}\mu_2(S_2, O_2)X_2 - k_{33}\mu_3(S_1, S_3, O_2)X_1 + \frac{Q}{V}(S_{3in} - S_3) \quad [6]$$

$$\dot{V} = Q \quad [7]$$

Now, let us introduce the following hypotheses:

– H1: The reactor is filled with the maximum available flow rate i.e. filling time is negligible compared to the reaction time. Reactions start immediately after filling and the reactor is operated in batch mode with a constant volume and a null flow.

– H2: During the aerobic phase, the dissolved oxygen is not limiting and denitrification cannot take place.

– H3: The switch between the aerobic and anoxic phase is instantaneous: reactions 1 and 2 begin immediately after the aeration has been activated and conversely stop immediately after the air has been turned out.

Thus one has : $\mu_1(S_1, O_2)|_{O_2 \neq 0} = \mu_1(S_1) > 0$, $\mu_1(S_1, O_2)|_{O_2 = 0} = 0$, $\mu_2(S_2, O_2)|_{O_2 \neq 0} = \mu_2(S_2) > 0$, $\mu_2(S_2, O_2)|_{O_2 = 0} = 0$, $\mu_3(S_1, S_3, O_2)|_{O_2 \neq 0} = 0$ and $\mu_3(S_1, S_3, O_2)|_{O_2 = 0} = \mu_3(S_1, S_3) > 0$.

Introducing now a control variable to represent the switch between aerobic and anoxic phases: $u = 1$ for aerobic mode and $u = 0$ for the anoxic mode. The following result is a direct consequence of hypotheses H_1 to H_3 :

- $Q = 0$,
- $V(t) = V(0) = V_{max}$
- the control variable u verifies $u \in \{0, 1\}$.

2.2. The aerobic sub-model

In aerobic phases, we have: $u = 1$ and $\mu_3 = 0$ (the third reaction is inhibited by the presence of dissolved oxygen), and we can write

$$S_1 + k_{11}X_1 = S_1(t_0) + k_{11}X_1(t_0) = M_1 \quad [8]$$

$$S_2 + k_{22}X_2 = S_2(t_0) + k_{22}X_2(t_0) = M_2 \quad [9]$$

$$S_3 - S_3(t_0) = -\frac{k_{32}}{k_{22}}(S_2 - S_2(t_0)) \quad [10]$$

$$\dot{S}_1 = \mu_1(S_1)(S_1 - M_1) = h_1^{ae}(S_1) \quad [11]$$

$$\dot{S}_2 = \mu_2(S_2)(S_2 - M_2) = h_2^{ae}(S_2) \quad [12]$$

$$\dot{S}_3 = -\frac{k_{32}}{k_{22}}\mu_2(S_2)(S_2 - M_2) = h_3^{ae}(S_2) \quad [13]$$

proof From equations (2) and (4) we get $\dot{S}_1 + k_{11}\dot{X}_1 = 0 \Rightarrow S_1 + k_{11}X_1 = S_1(t_0) + k_{11}X_1(t_0) = M_1$ which is equation (8). In a similar way, from equations (3) and (5) (resp. (5) and (6)) we get (9) (resp. (10)). To establish (11), we have to replace X_1 in (4)

with its expression obtained from (8). Thus we get $\dot{S}_1 = \mu_1(S_1)(S_1 - M_1)$, equation (11). We proceed in a similar way by replacing X_2 in equation (5) (resp. (6)) with its expression obtained from (9) to get (12) and (13). ■

2.3. The anoxic sub-model

In anoxic phase, $u = 0$. The first and the second reactions are then inhibited. This implies that $\mu_1(S_1) = \mu_2(S_2) = 0$ and we have :

$$S_1 + k_{11}X_1 = S_1(t_0) + k_{11}X_1(t_0) = M_1 \quad [14]$$

$$S_2 = S_2(t_0) \quad [15]$$

$$S_3 - S_3(t_0) = \frac{k_{33}}{k_{11}}(S_1 - S_1(t_0)) \quad [16]$$

$$\dot{S}_1 = \mu_3(S_1, S_3)(S_1 - M_1) = h_1^{an}(S_1, S_3) \quad [17]$$

$$\dot{S}_2 = 0 \quad [18]$$

$$\dot{S}_3 = \frac{k_{33}}{k_{11}}\mu_3(S_1, S_3)(S_1 - M_1) = h_3^{an}(S_1, S_3) \quad [19]$$

Proof From equations (2) and (4) we get $\dot{S}_1 + k_{11}\dot{X}_1 = 0 \Rightarrow S_1 + k_{11}X_1 = S_1(t_0) + k_{11}X_1(t_0) = M_1$ which is equation (14). To get (17) (resp. (19)), we have to replace X_1 in (4) (resp. (6)) with its expression obtained from (14). Equation (16) is obtained from equations (4) and (6). ■

REMARK. —

- The two states S_1 and S_2 are completely independent.
- In the aerobic mode, S_3 depends on S_2 but in the anoxic mode, S_3 depends on S_1
- If, at the initial time, no biomass is present in the reactor ($X_i(t_0) = 0$), then $M_i = S_i(t_0)$ and $\dot{S}_i = 0$ ($S_i(t) = S_i(t_0)$).
- In the aerobic as well as in anoxic mode, the biomass concentrations X_1 and X_2 can be respectively expressed as a function of S_1 and S_2 (referring to the algebraic equations (8)-(9) and (14)-(15)). Also, both in aerobic and anoxic phases, the nitrate concentration S_3 can be expressed as a function of S_1 or S_2 referring to the algebraic equations (10) and (16). Thus, whatever the operating mode, we can reduce the study of the global system (2-7) to a system with only three differentials equations and three algebraic equations. The existence of such an algebraic relationship between substrates and biomasses is due to conservation of the mass balance in the reactor. So the substrates consumed are proportional to the biomass formed.

In the following, in order to build a unique model, we combine the aerobic and the anoxic models to obtain one hybrid model linear in the control variable $u \in \{0, 1\}$.

$$\dot{S}_1 = h_1^{an}(S_1, S_3, t_0) + (h_1^{ae}(S_1, t_0) - h_1^{an}(S_1, S_3, t_0))u \quad [20]$$

$$\dot{S}_2 = h_1^{ae}(S_2, t_0)u \quad [21]$$

$$\dot{S}_3 = h_3^{an}(S_1, S_3, t_0) + (h_1^{ae}(S_2, S_3, t_0) - h_3^{an}(S_1, S_3, t_0))u \quad [22]$$

Equations of biomass evolution are given by the algebraic relations (8) and (9) when $u = 1$ (aerobic phase) and by the relations (14) and (15) when $u = 0$ (anoxic phase). The model (20)-(22) can be written as:

$$\dot{Z} = F(Z) + G(Z)u \quad [23]$$

with $Z^T = [S_1, S_2, S_3]$ is the space vector and u the control variable. Functions F and G are quickly identifiable from (20)-(22)

3. Reachability

Let C the target set to be defined as: $C = \{Z \in \mathfrak{R}^{3+} / S_1 < S_{1N}, S_2 < S_{2N}, S_3 < S_{3N}\}$ where S_{1N} , S_{2N} and S_{3N} are the normative constraints and the initial conditions $X_1(0) > 0$, $X_2(0) > 0$. The study of the reachability of system (23) consists in characterizing the set Ω of initial conditions for which there exists at least one admissible control sequence such that the final state lies, in a final time, the target C . We can say that the system (23) is reachable from Ω if and only if: $([10],[11]): \forall Z_0 \in \Omega, \exists u \in \{0, 1\}, \exists t_f \in [0, \infty[, \Rightarrow Z(t_f) \in C$.

Lets $\Psi(t, u, Z_0)$ the solution of (23) using an admissible control law u in a finite time t . The trajectory $Z = \Psi(t, u, Z_0)$ links a given initial point Z_0 to a point Z in \mathfrak{R}^{3+} . Therefore, Ω can be defined as $\Omega = \{Z / Z(t) = \Psi(-t, u, Z_{t0}), Z_{t0} \in C \text{ and } u \in \{0, 1\}\}$ In order to determine the reachable set we use a three dimensional geometric representation based on the linear relationships existing between the states space, (equations (8) to (10), (14) to (16) and the dynamic of system (23)).

– The set C is reachable from $\Omega_A \cup \Omega_B$:

$$\Omega_A = \left\{ S_2 < S_{2N}, S_3 < S_{3N} + \frac{k_{33}}{k_{13}} S_1 \right\} \quad [24]$$

$$\Omega_B = \left\{ S_{2N} \leq S_2 \leq S_{2N} + \frac{k_{32}}{k_{22}} S_{3N}, S_3 < S_{3N} + \frac{k_{33}}{k_{13}} S_1 - \frac{k_{32}}{k_{22}} (S_2 - S_{2N}) \right\} [25]$$

– The set C is reachable from Ω_C if and only if $T_2(X_2(0), Z_0) =$

$$\int_{S_2(t_0)}^{S_2^*} \frac{dS_2}{h_2^{ae}((S_2), X_2(0))} < \int_{S_1(t_0)}^{S_1^*} \frac{dS_1}{h_1^{ae}((S_1), X_1(0))} = T_1(X_1(0), Z_0)$$

where : $S_2^* = S_{2N} + \frac{k_{32}}{k_{22}} S_{3N}$ and $S_1^* = \frac{k_{11}}{k_{33}} \left(S_3(0) + \frac{k_{32}}{k_{22}} (S_2(0) - S_{2N}) - S_{3N} \right)$

$$\Omega_C = \left\{ S_2 > S_{2N} + \frac{k_{32}}{k_{22}} S_{3N}, S_3 < S_{3N} + \frac{k_{33}}{k_{13}} S_1 - \frac{k_{32}}{k_{22}} (S_2 - S_{2N}) \right\} [26]$$
 – The set C is not reachable from $R^{3+} - \{\Omega_A \cup \Omega_B \cup \Omega_C\}$

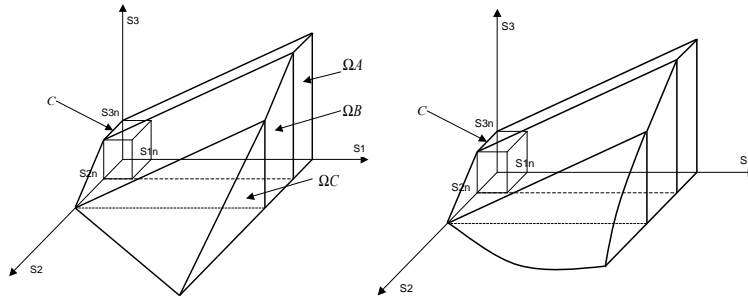


Figure 1. The set of reachability: In Left Ω_A , Ω_B and Ω_C , In Right the set Ω

We can deduce that $\Omega_A \cup \Omega_B \subset \Omega \subset \Omega_A \cup \Omega_B \cup \Omega_C$. The proof is not given here because of lack of space. For a detailed proof refer to ([12]). Ω is constructed by retrograde integration of system 23 from the target and using admissible control.

REMARK. — This result shows that in some cases of initial conditions, the final concentrations can not reach the target. In this case, the amount of ammonium and nitrogen is higher than the amount of carbon, there will not be enough carbon to be used by heterotrophic bacteria in the anoxic phase. In a such case, the totality of the nitrogen cannot be converted into nitrogen gas. One possible solution is to add some carbon in the reactor during the denitrification phase ([9]). In the case where the carbon amount is sufficient to realize nitrification and denitrification, there exists a switch scenario between anoxic and aerobic mode to reach the final target C in finite time.

4. Conclusion

In this paper, analytical analysis has been used to study the reachability properties of sequencing batch reactors with carbon and nitrogen removal. The original state space model (2-7) has two major properties:

- the mass balance conservation between biomass and substrates.
- relationships existing between the three substrates in the reactor due to mass balances the biological reactions (1)

Using these properties, the model was reduced and converted into an algebraic differential system. Then, with this new model, the reachability is studied. Using a three-dimensional geometric representation, the attainable set of the system was determined (i.e. the set of initial conditions for which there exists a sequence of control that allows system variables to reach the target set in a finite time). The reachability study shows that the attainable set does not depend on the growth rate functions $\mu_i(\cdot)$ in model (2-7), it only depends on the initial conditions (concentrations of substrates). This means that the attainability depends on the amount of substrates treated and not on system kinetics consumption. This result can be used to design the reactor. For a specific wastewater, the volume of the reactor and the wastewater volume treated per cycle can be computed so that the initial conditions satisfy the reachability constraints. A further work are investigated on the optimal time control based on the reduced model developed in this work and the reachability properties.

5. References

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