

DYNAMICAL ANALYSIS OF GLOBAL OBSERVABILITY PROPERTIES FOR A CLASS OF BIOLOGICAL REACTORS

Alexander Schaum* Jaime A. Moreno*

* *Instituto de Ingeniería, Universidad Nacional Autónoma
de México (UNAM), México D.F., MEXICO,
{ASchaum, JMorenoP}@ii.unam.mx*

Abstract: The observability properties of a 3-D aerobic biological reactor are analyzed in a general global sense. Using basic definitions of indistinguishability, observability and detectability a recently developed method is used to determine a dynamical representation of all possible indistinguishable trajectories of the model for the reactor class. This dynamics is analyzed for the representative case of a non-monotonic Haldane-type kinetics law. It is shown that the reactor model is not observable. Nevertheless, using the theory of asymptotic autonomous systems it is shown that the system is detectable under practically reasonable conditions.
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Keywords: Aerobic Biological Processes, Non-monotonic kinetics, Global Observability and Detectability, Asymptotic autonomous systems

1. INTRODUCTION

The analysis of the observability properties of dynamical systems is an important task, necessary for the assurance of observer convergence. Observability is equivalent to the possibility of dynamically distinguishing the system's internal trajectories using information of the input and output signals only. This intrinsic property is of immense importance in general systems theory. Further, it has direct implications on the possibilities of estimating the actual unmeasured system states. There are some (classical) criteria that imply the observability of a dynamical system in the nonlinear case, at least in a local sense. These are in principle: (i) the application of the Kalman observability matrix rank condition and (ii) the analysis of the invertibility of the observability

map, consisting of successive time derivatives of the output signal along the system trajectories. Nevertheless, both methods are only sufficient. Recently a method using a natural direct implications of the fundamental definitions of indistinguishability / observability has been introduced and applied to several dynamical systems of practical importance, illustrating the great advantages in comparison with the mentioned (classical) methods (Ibarra Rojas *et al.* (2004), Moreno and Dochain (2005)). A great advantage is that the method yields directly a dynamical representation of all *indistinguishable trajectories* as well as the corresponding *bad inputs* and thus enables a deep analysis of the natural system properties, eventually improving or obstructing the design of observers as has been shown e.g. in (Schaum and Moreno (2006)). The purpose of the work presented here is the global analysis of the observability properties of an aerobic biological reactor applying this method. The used model finds ap-

¹ This work has been supported by DGAPA-UNAM project IN112207-3 and CONACyT Grant 51244. A.Schaum thanks DGEP-UNAM for financial support.

plication e.g. in the control of a biological reactor used in the treatment of industrial wastewater (Moreno *et al.* (2006)). For this process there has been tried to design several (classical) observers for control purposes. All of them have failed, in principle, at least for non monotonic kinetics (see Vargas (1999); Schaum (2006)). This has been in some sense surprising and motivated further investigations in the intrinsic dynamical nature of the general model, especially in the inherent properties influencing the design of observers. Classical analysis methods do not yield sufficient information to allow a discussion of the problem. For example, with the Kalman rank condition the lack of observability of the linearization around the point of maximum growth for non-monotonic kinetics is obtained, but no global analysis is possible. The observability map, on the other hand is not conclusive, since it is only a sufficient condition, i.e. the fact, that the observability map loses rank for all states except the point of maximum growth does not imply that the system is not observable. This motivates the application of the above mentioned method, using a basic dynamical interpretation of the underlying concepts. The main results of this investigation are presented here.

The paper is organized as follows: Section 2 presents some preliminaries of the work. Section 3 is dedicated to the analysis of the models for a representative non-monotonic (Haldane-type) kinetics. It further includes some illustrative simulations. Some conclusions finish the paper.

2. PRELIMINARIES

2.1 Model Description

This subsection is dedicated to the presentation of the mathematical model of the biological processes to be analyzed. The model equations read

$$\Sigma \begin{cases} \dot{X} = (\mu(S) - D - K_d)X \\ \dot{S} = -C_1\mu(S)X + D(S_{in} - S) \\ \dot{O} = -[C_2\mu(S) + b]X + D(O_{in} - O) \\ \quad + K_1a(O_s - O) \\ y = O \end{cases}, \quad (1)$$

with biomass $X \in \mathbb{R}_+$, substrate $S \in \mathbb{R}_+$ and dissolved oxygen $O \in \mathbb{R}_+$ concentrations in the reactor. $\mu : \mathbb{R} \rightarrow \mathbb{R}$, is the reaction rate, $D \in \mathbb{R}_+$ is the dilution rate, $K_d \geq 0$ is the mortality rate, $b > 0$ the respiration rate and C_1, C_2 are yield coefficients. The inflow concentrations of the substrate $S_{in} > 0$, the dissolved oxygen $O_{in} > 0$, the transfer coefficient $K_1a > 0$ and the saturation concentration of the dissolved oxygen $O_s > 0$ are assumed constant and known. The given reactor model is used e.g. in a process for the treatment of industrial wastewater (see e.g. Moreno *et al.* (2006)). For the observability analysis it will be

assumed that the model parameters and the input D are known, and that the only state available for measurement is O . The nonlinearity of the process is given by the kinetics $\mu(S)$, representing the specific growth rate, that, in general, can be of two different types: monotonic (as e.g. Monod) or non-monotonic (as e.g. Haldane). Since the observability properties for the monotonic case can be completely studied using the observability map, in this paper we will concentrate mainly on the non-monotonic case, for which the observability map criterion is not applicable and many observer design methods fail (Schaum (2006)) (e.g. High-Gain and Reduced Order Observers). For the parts of the analysis not valid in general a Haldane type kinetics will be used, i.e.

$$\mu(S) = \frac{\mu_0 K_i S}{S^2 + K_i S + K_s K_i},$$

with positive and constant kinetic parameters μ_0 , K_i and K_s which are assumed to be known. The graph of this kinetics is illustrated in Figure 1. The maximum value $\mu^* = \mu(S^*)$ is reached at the point $S^* = \sqrt{K_s K_i}$.

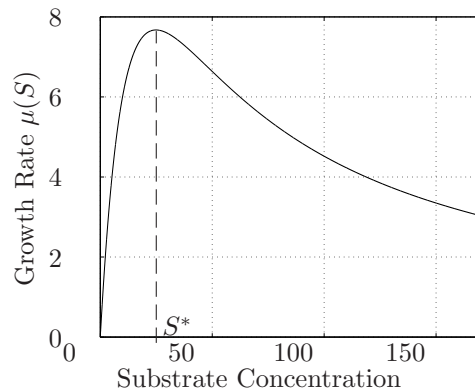


Fig. 1. Essential dependence of the Haldane kinetics on the substrate concentration.

2.2 Dynamical Interpretation of Observability

In this subsection the dynamical concept of observability is discussed. *Observability* represents in principle the property of an open dynamical system to permit a dynamic distinction of all system trajectories by information about the system's input and output signals only. The basic condition that has to be fulfilled therefore is the *distinguishability* of all trajectories under the influence of all possible input signals, i.e. trajectories having different initial conditions and the same input produce a different output. But for many systems there exist distinct trajectories that cannot be distinguished from the input/output behavior. Such trajectories are called *indistinguishable*. The indistinguishability thus eventually permits identical outputs for not necessarily identical trajectories.

Nevertheless if it is ensured that such not identical trajectories converge to the same trajectory, then they are called *detectable* (or determinable). These considerations are interpreted in the following Gedanken-experiment:

Consider two identical reactors Σ^1 and Σ^2 , driven by the same input signal D , guiding the internal trajectories $z^1 \triangleq [X^1, S^1, O^1]^T$ of Σ^1 and $z^2 \triangleq [X^2, S^2, O^2]^T$ of Σ^2 . The trajectories z^1 and z^2 yield the two output signals $y^1 = O^1$ and $y^2 = O^2$, respectively. In order to analyze the observability of the reactor, one has to determine for which initial values of the two plants, and for which input signals D , the output signals O^1 and O^2 are identical. Is it possible that different initial values, i.e. $[X_0^1, S_0^1, O_0^1]^T \neq [X_0^2, S_0^2, O_0^2]^T$, guided by the same input signal (in the following denoted as D^*), produce identical measurements in both reactors, then the system is not observable. The input signal D^* corresponding to this situation is then called *bad input*. In order to analyze the observability (or distinguishability) properties, note that the condition on the initial values can be expressed in terms of the incremental error $\epsilon \triangleq [X^2 - X^1, S^2 - S^1, O^2 - O^1]^T$ between the states. Detectability in this framework means the asymptotic stability of $\epsilon = 0$. It is important to note that the incremental error is not independent on the system state, and an analysis based on the consideration of ϵ thus has to be carried out for an extended system, given by the six dimensional dynamics of $[X^1, S^1, O^1, \epsilon_1, \epsilon_2, \epsilon_3]^T$.

3. DYNAMICAL ANALYSIS OF OBSERVABILITY PROPERTIES

3.1 A pathologic situation

To motivate the following analysis consider the special case that the initial condition of the biomass vanishes, i.e. $X_0 = 0$. As can be directly seen from (1) the complete biomass concentration remains zero for all time. This causes a decoupling of the oxygen concentration from the substrate concentration. The evolution of the oxygen O in fact becomes absolutely independent of S or more explicitly $\dot{O} = K_l a(O_s - O) + D(O_{in} - O)$ and it becomes impossible to get any information about the substrate concentration from measuring the oxygen concentration. Thus for $X_0 = 0$ the system is unobservable for all inputs and further initial states and, therefore, it is impossible to reconstruct the substrate concentration in this case. This consideration shows the following direct result, valid for an arbitrary kinetics

Proposition 1. The biological reactor model (1) is neither observable nor detectable.

In practical terms this case represents a reactor that does not work effectively and is thus pathologic. Nevertheless, it shows that the process has unobservable trajectories. Thus it seems quite interesting to analyze in detail the possibilities for trajectories to be indistinguishable following the Gedanken-experiment from the previous section.

This analysis is realized in the following. For this purpose the complete *indistinguishable dynamics* (ID) of (1) is derived. It represents all possible indistinguishable trajectories of the system. Analysis of the ID shows that there are other indistinguishable trajectories, apart from the pathologic situation $X_0 \neq 0$. However, surprisingly, if the set of pathologic trajectories and the ones converging asymptotically to a pathologic one are excluded, the system turns out to be *detectable*!

3.2 The indistinguishable dynamics

In the sequel set $[X^1, S^1, O^1]^T = [X, S, O]^T$.

Lemma 1. The ID for (1) is given by the following DA (Differential Algebraic) system:

$$\Sigma_{\mathcal{I}} \begin{cases} \dot{X} = \mu(S)X - (D^* + K_d)X \\ \dot{S} = -C_1\mu(S)X + D^*(S_{in} - S) \\ \dot{O} = -[C_2\mu(S) + b]X + D(O_{in} - O) + K_l a(O_s - O) \\ \dot{\epsilon}_1 = -(bC_2^{-1} + K_d + D^*)\epsilon_1 \\ \dot{\epsilon}_2 = bC_1C_2^{-1}\epsilon_1 - D^*\epsilon_2 \\ \Delta \equiv -bC_2^{-1}\epsilon_1 \\ 0 \leq \{X, S, O, X + \epsilon_1, S + \epsilon_2, D^*\}, \end{cases} \quad (2)$$

where $\Delta \triangleq \mu(S + \epsilon_2)(X + \epsilon_1) - \mu(S)X$, and D^* is given by (5).

To prove this result following the argumentation of the previous subsection, the complete six dimensional dynamics of the incremental error system is determined:

$$\Sigma_e \begin{cases} \dot{X} = \mu(S)X - (D + K_d)X \\ \dot{S} = -C_1\mu(S)X + D(S_{in} - S) \\ \dot{O} = -[C_2\mu(S) + b]X + D(O_{in} - O) + K_l a(O_s - O) \\ \dot{\epsilon}_1 = \Delta - (K_d + D)\epsilon_1 \\ \dot{\epsilon}_2 = -C_1\Delta - D\epsilon_2 \\ \dot{\epsilon}_3 = -C_2\Delta - b\epsilon_1 - (K_l a + D)\epsilon_3, \end{cases} \quad (3)$$

For indistinguishable trajectories the restriction $\epsilon_3 \equiv 0$ is satisfied, which represents the identity of the measurements. This condition implies that all time derivatives of ϵ_3 vanish too. Setting to zero the first time derivative of ϵ_3 in (3) one obtains with $\epsilon_3 = 0$ the algebraic restriction

$$\Delta \equiv -bC_2^{-1}\epsilon_1. \quad (4)$$

This condition has to be fulfilled for all indistinguishable motions and thus represents a restriction on the initial values. Calculating the second

time derivative of ϵ_3 the input function D appears in the corresponding condition so that one can deduce a correspondence for the *bad input* function D^* . In effect, from

$$\ddot{\epsilon}_3 = \frac{d}{dt} \{-C_2\Delta - b\epsilon_1\} \equiv 0$$

it follows, after some calculations, that

$$D^* = \frac{C_1\mu(\mu' - \hat{\mu}')X^2 + \epsilon_1 \left[C_1\hat{\mu}'(bC_2^{-1}\hat{X} - \dots \right.}{(S_{in} - S)\mu'X - \dots} \frac{\dots - \mu X) - (\hat{\mu} + bC_2^{-1})(\mu + bC_2^{-1})}{\dots - (S_{in} - (S + \epsilon_2))\hat{\mu}'(X + \epsilon_1)} \quad (5)$$

where $\hat{X} \triangleq X + \epsilon_1$, $\hat{\mu} \triangleq \mu(S + \epsilon_2)$, $\hat{\mu}' \triangleq \mu'(S + \epsilon_2)$ and the prime stands for the derivative with respect to S . The restriction $D^* \geq 0$ in (2) represents the fact, that only those indistinguishable trajectories are considered that are caused by feasible (i.e. in this case positive) bad input functions. Furthermore note that both processes considered, i.e. $z^1 = [X, S, O]^T$ and $z^2 = [X + \epsilon_1, S + \epsilon_2, O + \epsilon_3]^T$ are supposed to be physically realistic, so that the considered concentrations in z^1 and z^2 are all positive. This yields the given restrictions on $X, S, O, X + \epsilon_1, S + \epsilon_2$. These considerations show that the dynamical properties of all physically realistic indistinguishable trajectories are determined by the DA system given in Lemma 1.

Summarizing, the ID of the bioreactor is represented by a five dimensional DA system with one algebraic constraint, i.e. a system evolving on a four dimensional submanifold of \mathbb{R}^5 . Since in (2) the oxygen concentration does not influence the incremental error dynamics it can be excluded from the ID for the following analysis, and so the analysis of the ID (2) reduces to an autonomous three dimensional system (a four dimensional DA system). However, note that from the dynamics of ϵ_1 in (2) and the positivity of all system parameters as well as of D^* , it follows immediately that $\epsilon_1 \rightarrow 0$ exponentially as $t \rightarrow \infty$. This fact allows to write (2) as a *non autonomous* DA system:

$$\Sigma_{\mathcal{I}} \begin{cases} \dot{X} = \mu(S)X - (D^* + K_d)X \\ \dot{S} = -C_1\mu(S)X + D^*(S_{in} - S) \\ \dot{\epsilon}_2 = \epsilon_{10}e^{-\gamma(t)} - D^*\epsilon_2 \\ \Delta \equiv -bC_2^{-1}\epsilon_{10}e^{-\gamma(t)}, \end{cases} \quad (6)$$

where $\gamma(t) \triangleq (bC_2^{-1} + K_d)t + \int_0^t D^*d\tau \rightarrow \infty$. This shows that the behavior of the ID converges asymptotically to the *autonomous limit system* obtained from (2) when $\epsilon_1 = 0$. The study of the ID for non pathologic situations reduces to the analysis of a limit system (Thieme (1994a)), since the asymptotic behavior of the non autonomous system (6) coincides with that of the limit system determined in the following subsection.

3.3 The autonomous limit system

In the following the set of pathologic trajectories of the plant (1), i.e. for which $X(t) = 0$, and the ones that converge asymptotically to them, i.e. $\lim_{t \rightarrow \infty} X(t) = 0$ will be excluded. Note that if $K_d > \mu^*$ then $\lim_{t \rightarrow \infty} X(t) = 0$.

Lemma 2. If the biomass X does not converge to zero, then the autonomous limit system of (2) is given by the system in the plane

$$\Sigma_{\text{lim}} \begin{cases} \dot{X} = (\mu(S) - \tilde{D}^* - K_d)X \\ \dot{\epsilon}_2 = -\tilde{D}^*\epsilon_2 \\ S = \frac{1}{2} \left(-\epsilon_2 + \sqrt{\epsilon_2^2 + 4K_sK_i} \right) \\ 0 \leq \{X, S, S + \epsilon_2, \tilde{D}^*\}. \end{cases} \quad (7)$$

This result follows from the fact that (4) can also be written as

$$\epsilon_1 = X \frac{\mu(S) - \mu(S + \epsilon_2)}{\mu(S + \epsilon_2) + bC_2^{-1}}. \quad (8)$$

According to this constraint, in the limit $\epsilon_1 = 0$ either $X = 0$ or $\mu(S + \epsilon_2) - \mu(S) = 0$ holds. The first case is excluded as mentioned above. The second possibility for the limit corresponds to $\mu(S) = \mu(S + \epsilon_2)$. Due to the positivity of S , this condition can be rewritten (for the Haldane growth rate) as

$$S = \frac{1}{2} \left(-\epsilon_2 + \sqrt{\epsilon_2^2 + 4K_sK_i} \right). \quad (9)$$

The bad input signal (5) converges with $\epsilon_1 \rightarrow 0$ and $\mu(S) \rightarrow \mu(S + \epsilon_2)$ to the (formally) simpler form

$$\tilde{D}^* = \frac{C_1\mu X(2S + \epsilon_2)}{S_{in} \left[2S + \epsilon_2 - 2\frac{K_sK_i}{S_{in}} \right]}, \quad (10)$$

where μ denotes here $\mu(S)$. The positivity of $X, S, S + \epsilon_2$ and \tilde{D}^* is a physical requirement.

Further take note of the following result

Lemma 3. If $S_{in} > S^*$ then $\tilde{D}^* > 0$ holds.

This is shown as follows. From the physical restrictions it follows that the numerator in (10) is positive. The denominator on the other hand can be rewritten, taking into account (9) as

$$S_{in} \left[\sqrt{\epsilon_2^2 + 4S^{*2}} - 2\frac{S^{*2}}{S_{in}} \right],$$

with $S^{*2} = \sqrt{K_sK_i}$ as defined above. So the input signal \tilde{D}^* is positive if it holds

$$\epsilon_2^2(t) > 4S^{*2} \left(\frac{S^{*2}}{S_{in}^2} - 1 \right).$$

It turns out that the only possibility to ensure this condition for all initial values of ϵ_2 is that the term in parenthesis remains negative, i.e.

$$S^* < S_{in} = \text{const.} \quad (11)$$

The condition on S_{in} is natural considering that condition $\mu(S) = \mu(S + \epsilon_2)$ signifies that for $\epsilon_2 \neq 0$ the trajectories of the two substrate concentrations $S^1 = S$ and $S^2 = S + \epsilon_2$ are moving in inverse directions in such a way that the growth rates keep identical in opponent branches, what is possible only if S_{in} is greater than the maximum growth rate, as it holds $S \leq S_{in}$ (see 1).

3.4 Analysis of the limit system

This subsection aims to illustrate the following

Lemma 4. If $S^* < S_{in}$ and $K_d < \mu(S^*)$, then the trajectories of (7) converge either to $X = 0$, $\epsilon_2 \in \mathbb{R}$ or to $X = \frac{\mu(S^*) - K_d}{C_1 \mu(S^*)} (S_{in} - S^*)$ and $\epsilon_2 = 0$.

To prove this Lemma, remember that (7) is autonomous and planar. So its stability behavior can be analyzed using the theorem of Poincaré-Bendixson. Therefore note, that the only equilibria are $X = 0$, $\epsilon_2 \in \mathbb{R}$ and the isolated equilibrium $X = \frac{\mu(S^*) - K_d}{C_1 \mu(S^*)} (S_{in} - S^*)$, $\epsilon_2 = 0$. The positivity of the second equilibrium for the biomass X under the condition $S_{in} > S^*$ is ensured by the constraint on the mortality rate $K_d < \mu(S^*)$. Effectively, this equilibrium disappears if this condition does not hold anymore, an interesting and typical nonlinear phenomenon. Note that if X is unbounded then $\bar{D}^* \rightarrow \infty$ because of (10) and thus $\epsilon_2 \rightarrow 0$. On the other hand a cyclic motion can not occur as ϵ_2 is non increasing, due to the – physically motivated and by $S^* > S_{in}$ formally assured – positivity of \bar{D}^* . Thus the trajectories converge to an equilibrium point.

Note that the autonomous limit system corresponds to the case when the biomass concentration is measured, a particular case studied in detail in other works (Schaum (2006); Schaum and Moreno (2006)). The previous result shows that in this case the bioreactor is detectable (i.e. $\epsilon_2 \rightarrow 0$), if the (asymptotically) pathologic trajectories are excluded.

It is important to point out, that this result does not permit the "a priori" conclusion that the dynamics including the (exponentially vanishing) biomass concentration (2) is detectable too, as this depends on the properties of the four dimensional DA system (6) with solutions in a three dimensional submanifold of the \mathbb{R}^4 . The clarification of this problem is attacked in the following subsection.

3.5 Analysis of the asymptotic autonomous system

This subsection aims to clarify the question of which dynamical observability properties of the reactor model (1) can be concluded based on the analysis of the autonomous limit system (7). The pathologic case as well as situations converging to it remain excluded. The result is presented in the following

Proposition 2. If $S_{in} > S^*$ as well as $K_d < \mu(S^*)$, then $\epsilon_1 \rightarrow 0$ as well as $\epsilon_2 \rightarrow 0$, i.e. system (1) is detectable if all (asymptotically) pathologic trajectories are excluded. Further it follows that $S \rightarrow S^*$, i.e. the indistinguishable trajectories converge to the maximum of the biomass growth rate.

To prove this a result of Thieme (1992) can be applied, which relates the asymptotic behavior of trajectories of asymptotic autonomous systems (as it is Σ_I (2)) to the dynamical characteristics of the autonomous limit system Σ_{lim} (7). The result of Thieme states the following:

Let ω be the ω -limit set of a forward bounded solution of Σ_I (2). If there exists a neighborhood of ω which contains at most finitely many equilibria of Σ_{lim} (7), then the following Poincaré-Bendixson type trichotomy holds (see the Appendix for a general version):

- (i) $\omega(\cdot)$ consists of an equilibrium of Σ_{lim} , or
- (ii) ω is the union of periodic orbits of Σ_{lim} and possibly of centers of Σ_{lim} that are surrounded by periodic orbits of Σ_{lim} lying in ω , or
- (iii) ω contains equilibria of Σ_{lim} that are cyclically chained to each other in ω by orbits of Σ_{lim} .

Note that this theorem considers only separated trajectories (corresponding to the classical Poincaré-Bendixson result). Note that the equilibrium corresponding to $X = 0$ is not isolated as it represents a whole family of equilibria. Thus Thieme's Theorem can not be applied to trajectories moving toward $X = 0$. Nevertheless the second equilibrium point corresponding to $\epsilon_2 = 0$ is isolated and thus if there exists a trajectory which is bounded and not moving toward $X = 0$, then the Theorem can be applied. It follows that there is only the possibility of convergent or cyclical motion. But as has been seen above, the dynamics (7) can not exhibit cyclic motions due the non increasing character of ϵ_2 . Thus the only remaining possibility is $\epsilon_2 \rightarrow 0$. Finally note that $\epsilon_2 \rightarrow 0$ itself implies that $S \rightarrow S^* = \sqrt{K_s K_i}$, i.e. the two substrate concentrations $S^1 = S$ and $S^2 = S + \epsilon_2$ move toward each other in such a way that $\mu(S^1) = \mu(S^2)$ holds and they converge

finally in the maximum argument in S of the growth rate $\mu(S)$.

3.6 Illustrative Simulation

The obtained results are illustrated in a simulation. The bad input signal D^* , the measured output signal, i.e. the dissolved oxygen concentration evolution over time $O(\cdot)$, as well as two indistinguishable different evolutions of the biomass and substrate concentrations, $X(\cdot)$ and $S(\cdot)$, respectively, are illustrated. The Figure shows the

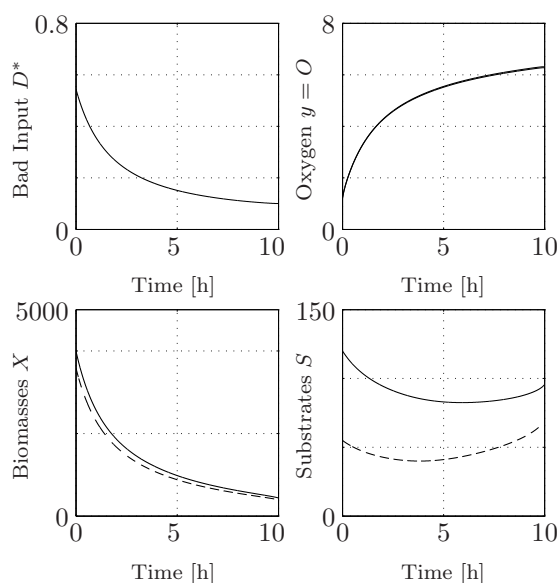


Fig. 2. Simulation results for initial values: $[4000, 120, 1.2]^T$ and $[3588.6486, 55, 1.2]^T$.

behavior of distinct indistinguishable trajectories of (1) for initial conditions $[4000, 120, 1.2]^T$ and $[3588.6486, 55, 1.2]$. It displays the existence of the corresponding bad input with physical meaning. The fact that there are distinct concentrations of X and S while input and output signals are identical illustrates the impossibility of obtaining a direct estimation of not identical indistinguishable trajectories using output error injection in an observer. The severeness and importance of this intrinsic dynamical property thus becomes clear.

4. CONCLUSIONS

The mathematical model of a class of aerobic biological processes is analyzed with respect to its dynamical properties of observability, i.e. global observability and detectability. Using a recently developed method for the dynamical analysis of global observability properties of general nonlinear systems, based on basic definitions of indistinguishability, it is shown that for any kinetics

the system is not globally observable. Further the system's detectability, i.e. the convergence of all pairs of indistinguishable trajectories to the same trajectory, is analyzed. It turns out, that for practically reasonable conditions the system is detectable.

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