Observability analysis of a nonlinear tubular bioreactor

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Abstract

In this paper an observability analysis is performed for an axial dispersion tubular bioreactor that involves one nonlinear growth reaction. The process is described by a semilinear parabolic Partial Differential Equation (PDE). More precisely, the analysis is performed on a tangent linearized model, that is described by a linear PDE with a spatial-dependent coefficient. It is reported that the associated linear infinite-dimensional operator is a Riesz-spectral operator and generates a C_0-semigroup. Then it is shown that a finite number of dominant modes of the system are observable when the substrate concentration is measured at the reactor output by an appropriate sensor. This result is confirmed by a numerical simulation.

1 Introduction

State observation is certainly a fundamental problem in bioprocess monitoring and control, even more in distributed parameter bioreactors. Beside the question of designing efficient state estimators, the information contents of on-line measurements is crucial.

Observability studies may be carried out through finite-dimensional models by the use of dicretization methods (Galerkin, orthogonal collocation...). However infinite dimensional system theory allows one to take explicitely into account the distributed nature of tubular reactor models. Linear C_0-semigroup theory is a particularly powerful tool for the study of distributed parameter systems, e.g. linear tubular reactor models [1].

In this paper an observability analysis is performed for a tubular bioreactor model that involves one growth reaction. The dynamics of the process are described by a nonlinear Partial Differential Equation (PDE). More precisely, the observability analysis is performed on a linearized tangent model of the process obtained via linearization around a steady state profile of the process. A crucial difficulty in the analysis derives from the explicit dependence of a parameter of the linearized model with respect to the spatial variable.

2 Basic dynamical model

Let us consider an anaerobic digestion process (used for wastewater treatment) operated in a fixed bed reactor (described in [2]). We consider that methanisation is the limiting step. Then the process kinetics can be characterized by the following reaction scheme :

$$S \longrightarrow X + gas \tag{1}$$

where S and X represent the substrate (organic matter to be degraded) and the biomass, respectively. In a first approximation and in line with the physical evidence, we consider that the biomass varies very slowly in comparison to S, and remains almost constant. Furthermore we assume that the kinetics follow the Monod law (see e.g. [3]). Therefore we can write the process dynamics in dimensionless form by the following parabolic equation (diffusion-convection-reaction model) [4] :

$$\frac{\partial \tilde{s}}{\partial \tau} = \frac{1}{P_e}\frac{\partial^2 \tilde{s}}{\partial \zeta^2} - \frac{\partial \tilde{s}}{\partial \zeta} - k_0 \frac{\tilde{s}}{\tilde{s}+1} \tag{2}$$

with the Danckwerts' boundary conditions :

$$\frac{1}{P_e}\frac{\partial \tilde{s}}{\partial \zeta}(0,\tau) - \tilde{s}(0,\tau) = -\tilde{s}_{in}(\tau) \tag{3}$$

$$\frac{1}{P_e}\frac{\partial \tilde{s}}{\partial \zeta}(1,\tau) = 0 \tag{4}$$

where P_e is the (dimensionless) Peclet number ($P_e = vL/D_a$), and $\tilde{s}$, $\tilde{s}_{in}$, τ and ζ are dimensionless variables defined as follows :

$$\tilde{s} = \frac{S}{K_S},\ \tilde{s}_{in} = \frac{S_{in}}{K_S},\ \tau = \frac{tv}{L},\ \zeta = \frac{z}{L} \tag{5}$$

with v, L, D_a, S, K_S, S_{in}, t and z, the fluid superficial velocity, the reactor length, the axial diffusion coefficient, the substrate concentration, the saturation constant, the inlet substrate concentration, the time and the spatial variable, respectively. The parameter k_0 is given by :

$$k_0 = \frac{\mu_{max} L X}{K_S v Y} \tag{6}$$

where X, μ_{max} and Y are the assumed constant biomass, the maximum specific growth rate and the yield coefficient, respectively.

In order to use linear C_0-semigroup theory for the observability analysis, a linearized system description is considered. It is derived by considering the linearized tangent model around a steady-state profile of the substrate concentration, i.e. $\bar{s}(\zeta)$.

$\bar{s}(\zeta)$ is typically determined as a steady-state of the system (2-4) for a time-constant value of the input $\tilde{s}_{in}(\tau)$. The existence of this equilibrium profile $\bar{s}(\zeta)$ was proved in [5] by considering upper and lower solutions theory. (See [6] for a survey on this approach.)

Then we obtain the following linearized model :

$$\dot{s}(\tau) = As(\tau) \tag{7}$$

where $s \in L^2(0,1)$ is defined by $\forall \tau, s(\tau) = \tilde{s}(\tau) - \bar{s}$, and A is a linear operator on $L^2(0,1)$ defined as follows :

$$(Af)(\zeta) = \frac{1}{P_e}\frac{d^2 f}{d\zeta^2} - \frac{df}{d\zeta} - k_0 \frac{1}{(1+\bar{s}(\zeta))^2} f \tag{8}$$

on its domain $D(A)$ given by :

$$\begin{aligned} D(A) \quad = \quad & \{s \in L^2(0,1) \mid s,\ \frac{ds}{d\zeta} \ \in L^2(0,1) \textit{ are absolutely continuous}, \\ & \frac{ds^2}{d\zeta^2} \in L^2(0,1),\ \frac{1}{P_e}\frac{ds}{d\zeta}(0) - s(0) = 0,\ \frac{ds}{d\zeta}(1) = 0\} \end{aligned} \tag{9}$$

Note that the above linearized tangent model explicitly depends on the spatial variable ζ, and that the inlet substrate concentration is neglected for the observability analysis.

3 Observability Analysis

First let us define a measurement vector $y(\tau)$ by :

$$y(\tau) = Cs(\zeta, \tau),$$

where $C : L^2(0,1) \rightarrow R^m$ is a bounded linear operator in this framework.

In the following analysis, we consider the *approximate observability* defined in [7, def. 4.1.17].

Our analysis consists of using C_0-semigroup theory in the Hilbert space $L^2(0,1)$ endowed with the usual inner product $< \cdot, \cdot >_2$, in particular the observability properties of *Riesz-spectral operators*. (See e.g. [7, section 2.3].)

The following theoretical results are reported :

Lemma 1 *Let A be the linear operator on $L^2(0,1)$ defined by :*

$$\forall f \in D(A),\ (Af)(\zeta) = \frac{1}{P_e}\frac{d^2\, f}{d\zeta^2} - \frac{d\, f}{d\zeta} - k(\zeta)\, f, \tag{10}$$

where $k(\zeta)$ is a continuous real function, and the domain $D(A)$ of A is given by (9). Then

1. *A is a Riesz-spectral operator.*

2. *A is the infinitesimal generator of a C_0-semigroup of bounded linear operators.*

Note that this previous results holds for any continuous real function $k(\zeta)$, and, in particular, for the linear operator A defined by (8).

Theorem 1 *Let us consider a system (C, A), where A is the linear operator defined by (10) on its domain $D(A)$ given by (9), let $(\phi_n)_{n\geq 1}$ be its Riesz basis of eigenvectors. Moreover let us define the measurement $y(\tau)$ by :*

$$y(\tau) = Cs(\zeta, \tau),$$

where $C : L^2(0,1) \rightarrow R^m$ is a bounded linear operator in this framework..
Then the system (C, A) is (approximately) observable if and only if, for all $n \geq 1$

$$rank(C\phi_n) = 1 \tag{11}$$

The proof of Theorem 1 is based on Lemma 1 and on [7, Theorem 4.2.3].
Note that Theorem 1 is a powerful tool for the observability analysis of any axial-dispersion reactor defined by a continuous coefficient $k(z)$ and Danckwerts' boundary conditions.
Theorem 1 justifies the concept of *modal observability* for Riesz spectral operators :

Definition 1 (see [1, definition 5.1].) *Let A be a Riesz spectral operator. The nth mode of A is (λ_n, ϕ_n), where λ_n is the nth eigenvalue of A, and ϕ_n its corresponding eigenvector. Moreover, let $C : L^2(0,1) \rightarrow R^m$ be a bounded linear observation operator. Then the nth mode of A is said to be $(C-)$observable whenever the condition 11 holds.*

Now let us locate the measurement $y(\tau)$ at the bioreactor *output*. This point measurement is defined by the following bounded operator :

$$y(\tau) = (C_\varepsilon s)(\tau) = \frac{1}{\varepsilon}\int_{1-\varepsilon}^{1} s(\zeta, \tau) d\zeta, \tag{12}$$

where $\varepsilon > 0$ is very small.

Then according to Definition 1, the nth mode (λ_n, ϕ_n) of the linearized system (C_ε, A) is observable if and only if the following condition holds :

$$\frac{1}{\varepsilon}\int_{1-\varepsilon}^{1} \phi_n(\zeta) d\zeta \neq 0.$$

Since every ϕ_n is continuous, the following proposition holds.

Proposition 1 *Let us consider the system (C_ε, A) where A is defined by (8),(9) and C_ε is given by (12). Then its nth mode (λ_n, ϕ_n) is C_ε-observable if the following condition holds :*

$$\forall \zeta \in [1-\varepsilon, 1], \;\; \phi_n(\zeta) \neq 0. \tag{13}$$

Let us study the zeros of the functions $(\phi_n(\zeta))_{n\geq 1}$. Since the eigenequation

$$A\phi = \lambda\phi,\ \phi \in D(A) \tag{14}$$

cannot be solved analytically in general, the following theoretical results are then required.

Lemma 2 *Let $(\phi_n)_{n\geq 1}$ be the Riesz basis of eigenvectors of A, which is given by (8) and defined on $D(A)$ (9). Then*

1. *$\forall n \geq 1$, ϕ_n has a finite number of zeros in $[0,1]$.*
2. *Moreover,*
$$\forall n \geq 1,\ \phi_n(1) \neq 0. \tag{15}$$

Hence

$$\forall N \geq 1,\ \exists \delta > 0,\ \forall \zeta \in [1-\delta,\ 1],\ \phi_N(\zeta) \neq 0. \tag{16}$$

Proof. 1. This result holds in any Sturm-Liouville problem (see e.g. [8, Theorem V.4]).

2. Let n be any positive integer. According to Sagan, each zero of ϕ_n is simple ([8, Theorem V.1]). Moreover $\phi_n'(1) = 0$ – since $\phi_n \in D(A)$ – then $\phi_n(1) \neq 0$. As ϕ_n is continuous, (16) follows.

Theorem 2 *For any positive integer N, there exists $\varepsilon > 0$ (in Equation (12)) such that the modes $(\lambda_n,\ \phi_n)$ of A are C_ε-observable for any $n \leq N$.*

Proof. This theorem follows from Lemma 2.

Remarks.

1. We cannot conclude that any mode above N is unobservable, even if it admits some zeros in $[1-\varepsilon, 1]$.
2. It is worth reminding that in a parabolic PDE, the lower modes are dominant.

4 Numerical Results.

The numerical analysis is performed with numerical values given by [2].

Eigenequation (14) is solvable neither analytically – since it has no analytical solution, – nor numerically – since λ and ϕ are both unknown. Therefore A is approximated by the operator $\tilde{A}$ defined as follows :

$$\forall f \in D(\tilde{A}),\ (\tilde{A}f)(\zeta) = \frac{1}{P_e}\frac{\partial^2 f}{\partial \zeta^2} - \frac{\partial f}{\partial \zeta} - (a + b_1 e^{c\zeta} - b_2 e^{2c\zeta})f \tag{17}$$

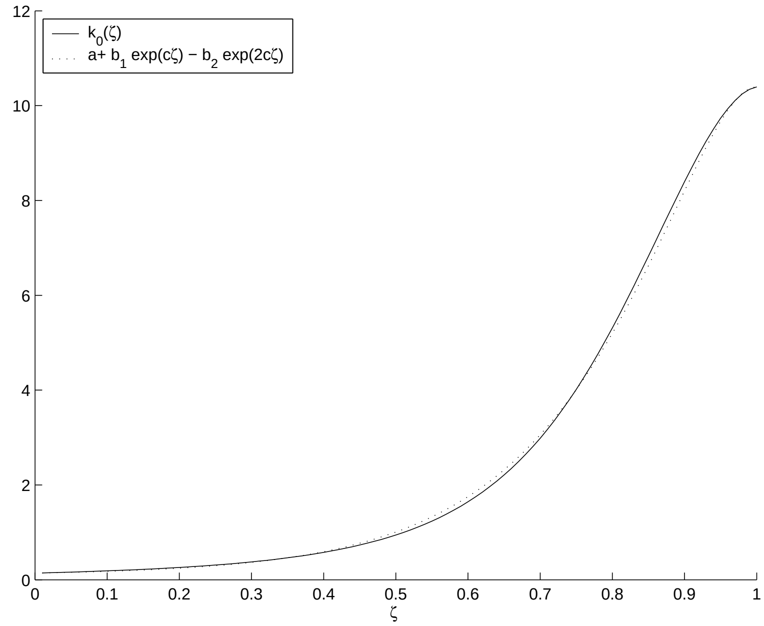

Figure 1: Approximation of $k_0(\zeta)$ by a double exponential function

where a, b_1, b_2, c are real constants, and $D(\tilde{A}) = D(A)$ is the domain of $\tilde{A}$. We use this approximation since equation $\tilde{A}\phi = \lambda\phi$ is solvable and since both ζ-dependent coefficients $(a + b_1 e^{c\zeta} - b_2 e^{2c\zeta})$ and $k_0 \frac{1}{(1+\bar{s}(\zeta))^2}$ have a similar form on $[0, 1]$ (Cf. Fig. 1). Note that the theoretical results of the previous section hold for $\tilde{A}$ as well as for A.

Solving the differential equation $\tilde{A}\phi = \lambda\phi$ where $\phi \in D(A)$ (e.g. by considering Murphy's approach [9]) leads to :

1. a resolvent equation involving λ. Although the set of solutions $(\lambda_n)_{n\geq 1}$ cannot be analytically expressed, the λ_n can be computed one by one numerically using a zero finding software.

2. ϕ is expressed as a linear combination of Whittaker functions (see [10, chap. 13] for definitions) depending on λ and of course ζ. Then, for all $n \geq 1$, $\phi_n(\zeta)$ is numerically deduced from the value of λ_n.

The modes (λ_n, ϕ_n) are computed for $n = 1, 2, ..., 10$. It is then observed on Fig. 2 that each $\phi_n(\zeta)$ confirms the theoretical results, in particular Lemma 2 : for each n, there exists $\delta > 0$ such than $\phi_n(\zeta) \neq 0$ for all $\zeta \in [1 - \delta, 1]$. Moreover δ decreases as n gets larger, i.e. the largest zero of $\phi_n(\zeta)$ is closer to 1 as n gets larger.

Hence Theorem 2 is confirmed in this example.

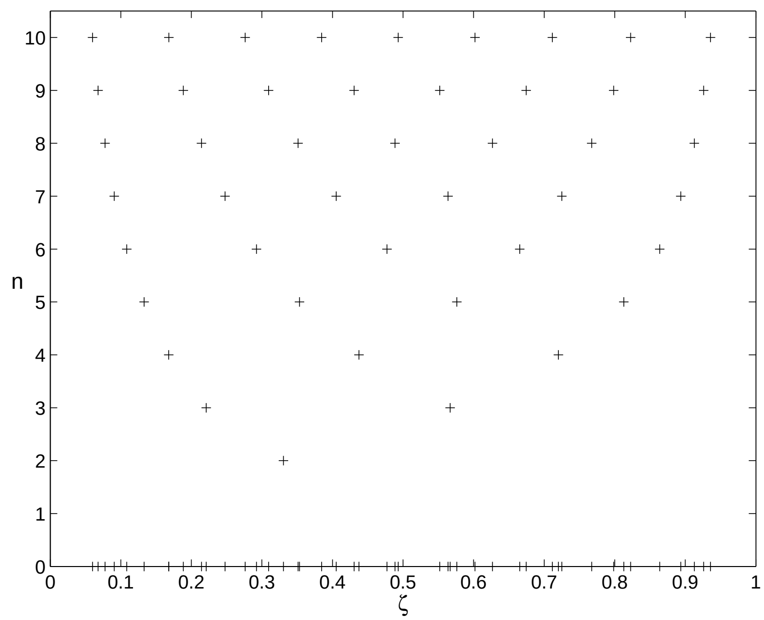

Figure 2: Location of the zeros of the eigenfunctions $\phi_n(\zeta)$

Remarks.

1. It may be observed than $\phi_n(\zeta)$ has one more zero than $\phi_{n-1}(\zeta)$. This confirms the theoretical result of [8, theorem V.8].

2. We notice that the more n increases (i.e. the larger $-\lambda_n$ gets), the more ϕ_n looks like a sum of two complex exponentials. This confirms the intuitive idea that the eigenfunctions $\phi_n(\zeta)$ satisfying equation $\tilde{A}\phi = \lambda\phi$ tend to the solutions of

$$\frac{1}{P_e}\frac{d^2\phi}{d\zeta^2} - \frac{d\phi}{d\zeta} - \lambda\phi = 0 \tag{18}$$

when λ become much larger than $(a + b_1 e^{c\zeta} - b2e^{2c\zeta})$.

5 Conclusions and perspectives

In this paper we have discussed the observability of a nonlinear tubular reactor. As it is a distributed parameter system (modelled by a PDE), the analysis is based on C_0-semigroup theory. First the linearized model operator A is reported to be a Riesz-spectral operator, and the infinitesimal generator of a linear C_0-semigroup. Then it is shown that a finite number of dominant modes of the process is observable when the substrate concentration is measured at the reactor output by an appropriate sensor. Finally these results are confirmed by a numerical simulation.

It shall be noted that these results are consistent with the study [1] of a bioreactor involving linear reaction kinetics. However, both studies are based on a "yes-or-no" observability criterion. In finite dimensional approximation analyzes, some numerical functions "measure" the system observability (see e.g. [11]), so that the process is shown to be more or less observable. Therefore it could be interesting to use such observability measure for infinite-dimensional system. A further work could also study a more complete bioreactor involving several biochemical reactions, or on a more complex one. As first step we could consider the reaction $S \longrightarrow X + P$, now described by two PDEs. Another perspective for this study is a comparison with the results of a finite-dimensional approach (Galerkin, finite-difference, orthogonal collocation ...). Finally a further study could consider the actual nonlinear system, without preliminary linearization.

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