

On the Biomass Specific Growth Rates Estimation for Anaerobic Digestion using Differential Algebraic Techniques

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Abstract: *The paper deals with identifiability and observability of anaerobic digestion (AD) processes. In such kind of processes, generally carried out in continuously stirred tank bioreactors, the organic matter is depolluted by microorganisms into biogas and compost in the absence of oxygen. The biogas is an additional energy source, which can replace fossil fuel sources. The differential algebraic approach of general observation problems has been applied to investigate the identification and observation of a simple AD model. The major discovery is that the biomass specific growth rate can be stably estimated from easily measured quantities: the dilution rate and the biogas flow rate. Next if the yield coefficients are assumed known then, of course, the biomass concentration is observable. Unfortunately, even under the latter strongest assumption the substrate concentration is not observable. This concentration becomes observable if an additional model, say the Monod model, is assumed for the specific growth rate. Illustrative simulations are presented.*

Keywords: *Anaerobic digestion, Non-linear model, Observation, Differential algebraic approach.*

Introduction

Anaerobic digestion (AD) is a biotechnological process widely used in life processes and a promising method for solving some energy and ecological problems in agriculture and agro-industry. In such kind of processes, generally carried out in continuously stirred tank bioreactors, the organic matter is depolluted by microorganisms into biogas (methane and carbon dioxide) and compost in the absence of oxygen [1]. The biogas is an additional energy source which can replace fossil fuel sources. It therefore has a direct positive effect on greenhouse gas reduction. Unfortunately this process is very complex, may sometimes become very unstable and thus needs more investigations.

Many mathematical models of this process are known [2-4]. Generally they are very complex nonlinear sets of ordinary differential equations with a great number of unknown coefficients. The estimation of these coefficients is a very difficult task [2, 4]. Quite often one obtains only local solutions and it is impossible to validate the model in a large domain of experimental conditions.

In the present work we have recourse to the differential algebraic approach of general observation problems to investigate the identification and observation of anaerobic digestion processes.

The differential algebraic approach

The differential algebraic approach of observation problems dates back to late eighties and early nineties with works of [5-9]. See [10] for a recent survey. The main point of this approach, as first clarified in [8], is that a quantity, say z , of a system is observable with respect to some other one, say w (which is supposed to be available in some time interval), if each component of z is a solution of a (non differential) algebraic equation with coefficients eventually depending on w and finitely many of its time derivatives. The theory applies to models of systems in terms of *differential algebraic equations* only but which may be *implicit* in the variables to be observed.

It is a matter of fact that biotechnological process models are often described in terms of differential algebraic equations. The only non polynomial expressions that enter these models are often rational expressions. But, as argued in [10], the basic differential algebraic approach may handle such rational expressions. In summary, the differential algebraic approach to nonlinear observability can tackle the identifiability and observability questions which arise in biotechnological processes. The main limitations that may be encountered when following this approach are the availability of computation resources which are enough to carry over all the suggested calculations.

The differential algebraic approach is among the rare ones which provide *explicit* tests of observability. There are many such differential algebraic decision methods. The most attractive one uses notions of *characteristic set*. The reader is referred to [10] for details and references concerning characteristic sets. Here, it is enough to mention the fact that every differential algebraic model has a characteristic set which, *in principle*, may be computed in finitely many operations consisting of addition, multiplication and derivation of formal differential polynomials. Characteristic sets of systems of differential algebraic equations are defined relatively to *rankings*. And a ranking is merely a *total ordering* on the variables and their derivatives. In summary, the identifiability of a coefficient θ (or, more generally, the observability of a variable z) with respect to a supposedly measured variable w is verified by running characteristic set algorithms through the system equations relatively a ranking which orders w and all its derivatives before θ (or z) and all its derivatives, and any derivative of these two variables before any potentially remaining variable of the system.

Applying these theory and differential algebraic decision methods to the simple model (1) of AD process, a differential equation, which seems fundamental, was found. It provides a dynamic relation between the dilution rate, the biogas flow rate and the biomass specific growth rate. The fundamental character of this dynamic relation is thought as lying over the fact that *this relation does not depend on any model assumption for the biomass specific growth rate*. Rewriting this dynamic relation it was discovered that a simple rational function of the biomass specific growth rate is governed by a quite simple linear differential equation with coefficients depending only on measured quantities (dilution rate and biogas flow rate). This new dynamics appears to be *stable*. It is the latter property which allows a stable estimation procedure of the biomass specific growth rate.

Process model

We consider the following mathematical model of the continuous AD process [2]:

$$\begin{aligned} \frac{dX}{dt} &= \mu X - D X \\ \frac{dS}{dt} &= -K_1 \mu X + D(S_{in} - S) \\ Q &= K_2 \mu X \end{aligned} \quad (1)$$

In this mass-balance model, the first equation describes the growth and changes of the biomass X ($\text{g}\cdot\text{l}^{-1}$) consuming the appropriate substrate S ($\text{g}\cdot\text{l}^{-1}$). The first term in the right hand side reflects the growth of the bacteria and the second one reflects the effluent flow rate of liquid. The quantity μ (day^{-1}) is known as the specific growth rate of bacteria. The mass balance for the substrate is described by the second equation, where the first term reflects consumption by the bacteria, the second term reflects the influent flow rate of liquid with concentration of the inlet diluted organics S_{in} ($\text{g}\cdot\text{l}^{-1}$). The last equation in (1) describes the formation of biogas with flow rate Q [$\text{l gas}\cdot(\text{l liquid}^{-1}\cdot\text{day}^{-1})$]. In automatic control terms the dilution rate D (day^{-1}) is the control input, the output is the methane flow rate Q , and S_{in} is a disturbance.

A lot of well known nonlinear models of the specific growth rate of bacteria μ exist. The most frequently invoked ones are the following:

$$\begin{aligned} \mu &= \left(\frac{\mu_{\max} S}{(k_s + S)} - b \right) \\ \mu &= \left(\frac{\mu_{\max} S}{(k_m X + S)} - b \right) \\ \mu &= \left(\frac{\mu_{\max} S}{(k_s + S + S^2 / k_i)} - b \right) \end{aligned}$$

respectively known as Monod, Contois and Haldane models [2, 4]. In these models μ_{\max} , k_s , k_m , k_i and b are kinetics coefficients. The choice of such a model however usually is empirical and based upon an expert's knowledge [2].

That is why μ is preferably reconstructed from available measurements. State observers [4] already have been invoked.

This paper is an attempt to analyze the observability of μ with respect to potentially available measurements. This has not yet been done in the literature. Moreover, an interesting relation is found, and which leads to an alternative way for the estimation of μ .

Recall that the biological interpretation of X , S , Q , S_{in} , D , K_1 and K_2 implies the following consistency restrictions:

$$\begin{aligned} X &> 0, Q > 0, \\ K_1 &> 0, K_2 > 0, \\ 0 &< D < D_{\text{sup}}, 0 < S < S_{in} \end{aligned}$$

Signification as well as units and typical values of variables are summarized in Table 1.

Table 1

Symbol	Signification	Unit	Typical value
X	Concentration of bacteria	$\text{g}\cdot\text{l}^{-1}$	0.025 – 0.500
S	Concentration of soluble organics	$\text{g}\cdot\text{l}^{-1}$	0.025 – 0.125
μ	Specific growth rates of bacteria in the reactor	day^{-1}	0.020 – 0.140
D	Dilution rate	day^{-1}	0.025 – 0.125
S_{in}	Influent concentration of organic matter	$\text{g}\cdot\text{l}^{-1}$	0.300 – 3.000
Q	Biogas flow rate	$\text{l gas}\cdot(\text{l liquid}^{-1}\cdot\text{day}^{-1})$	0.020 – 0.700
K_1	Yield coefficient	-	6.70
K_2	Yield coefficient	$\text{l gas}\cdot\text{g}^{-1}$	16.78

Observability and identifiability of the process variables

As announced the identifiability and observability of the process variables is approached here by means of the differential algebraic theory of nonlinear observability.

On the differential algebraic approach

The reader is referred to [10] for details and references on this approach. Here are the main lines of the application of this theory to our biotechnological processes. First note that the theory applies to systems which are described by differential polynomials with coefficients which are meromorphic functions of the time. The theory may be extended to include descriptions involving differential rational fractions. Then one needs to consider differential equations and inequations (the sign \neq). In summary, in order to check the observability of a latent variable z with respect to, say u and y , of a system

$$P_i(u, \frac{du}{dt}, \frac{d^2u}{dt^2}, \dots, y, \frac{dy}{dt}, \frac{d^2y}{dt^2}, \dots, z, \frac{dz}{dt}, \frac{d^2z}{dt^2}, \dots, \xi, \frac{d\xi}{dt}, \frac{d^2\xi}{dt^2}, \dots) = 0 \quad (i = 1, 2, \dots,)$$

one computes the characteristic set of the previous set of differential polynomials with respect to a ranking $\{\{u, y\}, \{z\}, \{\xi\}\}$.

This notation of rankings is very intuitive. It says that all derivatives of u and y are lower than z , and all derivatives of z are lower than ξ . The characteristic set is merely a set A of differential polynomials each one being *led* by one (and only one) of the variables (at some derivative order). The testing device then reads as: z is observable with respect to u and y if, and only if, each component of z *leads* (i.e., is the highest variable derivative according to the ranking which appears in A) one differential polynomial in A .

The characteristic set computations mentioned in this communication all have been carried out by means of a *REDUCE* package called *astb* written more than ten years ago and which is based upon Kolchin's revisit of Ritt's characteristic set algorithm. The reader who is familiar with differential algebraic decision methods knows that a practical and complete effective algorithm is still lacking. The package *astb* will fail to yield a characteristic set of systems in

many circumstances due to factorization issues for instance. But when *astb* exhibits a differential polynomial then of course the latter is a consequence of the system's equations.

Observability of the specific growth rate of bacteria

The observability of the biomass specific growth rate is tested by calculating the characteristic set of the following set of differential polynomials

$$\begin{aligned}
 \frac{dX}{dt} &= \mu X - DX \\
 \frac{dS}{dt} &= -K_1 \mu X + D(S_{in} - S) \\
 Q &= K_2 \mu X \\
 \frac{dK_1}{dt} &= 0 \\
 \frac{dK_2}{dt} &= 0
 \end{aligned} \tag{2}$$

with respect to the ranking

$$\{\{D, Q, S_{in}, K_1, K_2\}, \{\mu\}, \{X, S\}\}$$

The result is the following

$$\begin{aligned}
 \frac{dK_1}{dt} &= 0 \\
 \frac{dK_2}{dt} &= 0 \\
 Q \frac{d\mu}{dt} + Q \mu^2 - \mu \frac{dQ}{dt} - DQ \mu - K_2 \mu X + Q \\
 K_2 \frac{dS}{dt} + K_2 D (S - S_{in}) + K_1 Q
 \end{aligned} \tag{3}$$

It indicates that

Lemma 1: μ is not observable with respect to D, Q, S_{in}, K_1 and K_2 since the differential polynomial which introduces μ (the third line of (3)) is of order 1 (and not 0) in μ . Moreover, neither K_1 nor K_2 is identifiable with respect to D, Q, S_{in} and μ due to the presence of the first two differential polynomials in (3).

Next, the differential polynomial introducing μ is examined

$$Q \frac{d\mu}{dt} + Q \mu^2 - \frac{dQ}{dt} \mu - DQ \mu = 0.$$

Rewriting this equation as follows

$$\frac{dQ}{dt}\mu - Q\frac{d\mu}{dt} = -DQ\mu + Q\mu^2$$

then in time intervals where μ is not identically zero, the two members of the previous equation may be divided by μ^2 to yield

$$\frac{d}{dt}\left(\frac{Q}{\mu}\right) = -D\left(\frac{Q}{\mu}\right) + Q \quad (4)$$

Given the constant sign of D and Q the quantity

$$z = Q/\mu$$

thus can be estimated thanks to the exponential stability of the previous dynamic equation. Of course, the previous linear dynamics is exponentially stable only in time intervals where none of D and Q is identically zero. Since these singular cases are easily handled in practice, it follows that

Lemma 2: μ may generically be estimated. Moreover, the estimation of μ does not involve neither yield coefficients nor the inlet diluted organics concentration S_{in} .

When Eq. (4) is directly used to estimate μ the user should bear in mind the following matters of fact:

Remark 3: In time intervals where D and Q do not identically vanish the estimate $\hat{\mu}$ of μ taken from Eq. (4) will converge no matter how $\hat{\mu}$ is initialized (provided that obvious consistency conditions are satisfied). In addition, the higher D is the faster $\hat{\mu}$ converges to μ .

The specific growth rate μ being estimated through equation (4), μ is then considered as an additional measurement.

Lemma 1 does not answer the following question: are the variables X and S observable with respect to D , Q , S_{in} and μ ? The answer to this question is provided by the characteristic set of equations (2) with respect to a ranking such as

$$\{\{D, Q, S_{in}, \mu\}, \{X, S\}, \{K_1, K_2\}\}$$

that is

$$Q\frac{d\mu}{dt} + Q\mu^2 - \frac{dQ}{dt}\mu - DQ\mu,$$

$$\frac{dX}{dt} - \mu X + DX,$$

$$Q\frac{d^2S}{dt^2} - \frac{dQ}{dt}\frac{dS}{dt} + DQ\frac{dS}{dt} - D\frac{dQ}{dt}S + \frac{dD}{dt}QS + D\frac{dQ}{dt}S_{in} - DQ\frac{dS_{in}}{dt} - Q\frac{dD}{dt}S_{in}$$

$$K_1\mu X + \frac{dS}{dt} + D(S - S_{in}),$$

$$K_2\mu X - Q,$$

in other words

Lemma 4: None of X and S is observable with respect to D , Q , S_{in} and μ since the differential polynomials introducing X and S are of orders 1 and 2 in X and S , respectively (and not of order 0).

The negative answers to the above two questions implies that for X and S to be observable with respect to (D, Q, S_{in}, μ) additional information is required. This is usually introduced in the literature in the form of Monod, Contois or Haldane models for μ .

Simulation results

The dynamic evolution of the process (1) is simulated with a Monod model for the bacteria specific growth rate. The parameters K_1 and K_2 were given values as in Table 1, $\mu_{max} = 0.35 \text{ day}^{-1}$ and $k_s = 2.3 \text{ g}\cdot\text{l}^{-1}$. The dilution rate time history is as in Fig. 1. The initial conditions are given by $X(t_0) = 0.1$, $S(t_0) = 34.0$.

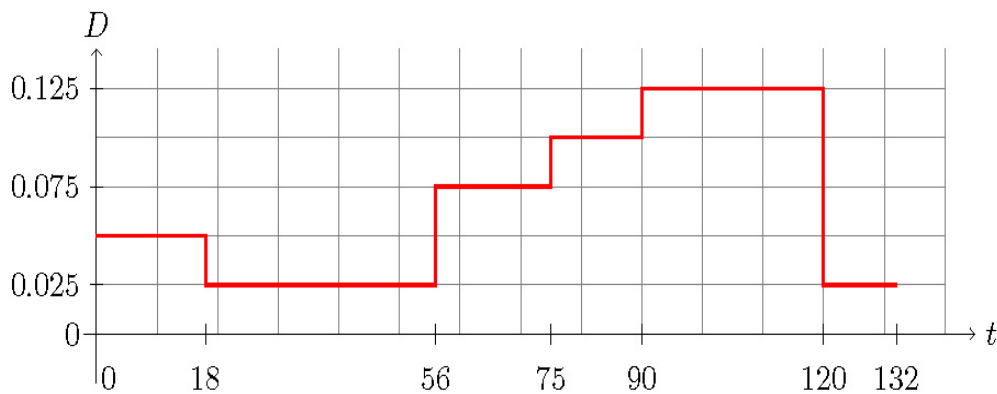


Fig. 1 Time history of D : t is in days and D is in day^{-1}

The biomass specific growth rate is estimated by means of the exponential stable dynamics (4):

$$\frac{dz}{dt} = -Dz + Q \tag{5}$$

$$\hat{\mu} = \frac{Q}{z}$$

which is better initialized with $z(t_0) = z_0 = Q(t_0)/D(t_0)$.

The estimated specific growth rate $\hat{\mu}$ with data from Fig. 2 using Eq. (5) is shown on Fig. 3. The estimated biomass concentration \hat{X} with data from Fig. 2 using the expression $\hat{X} = z/K_2$ is shown on Fig. 4.

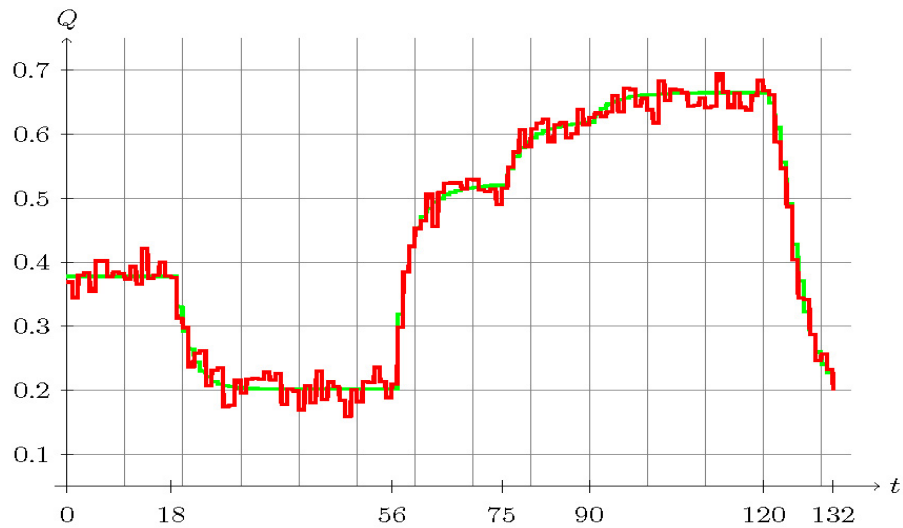


Fig. 2 Simulated data for Q with 5% relative measurement noise for step changes of D presented in Fig. 1. t is in days and Q is in $\text{l gas} \cdot (\text{l liquid} \cdot \text{day})^{-1}$

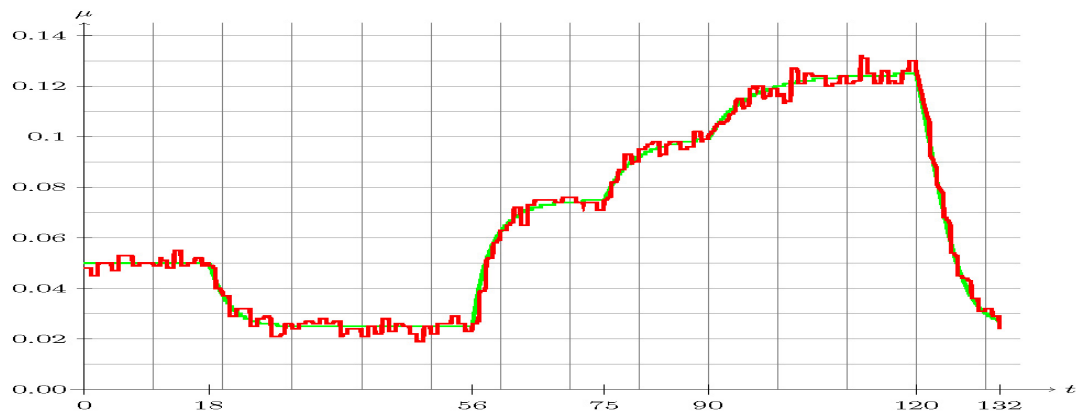


Fig. 3 The estimated specific growth rate

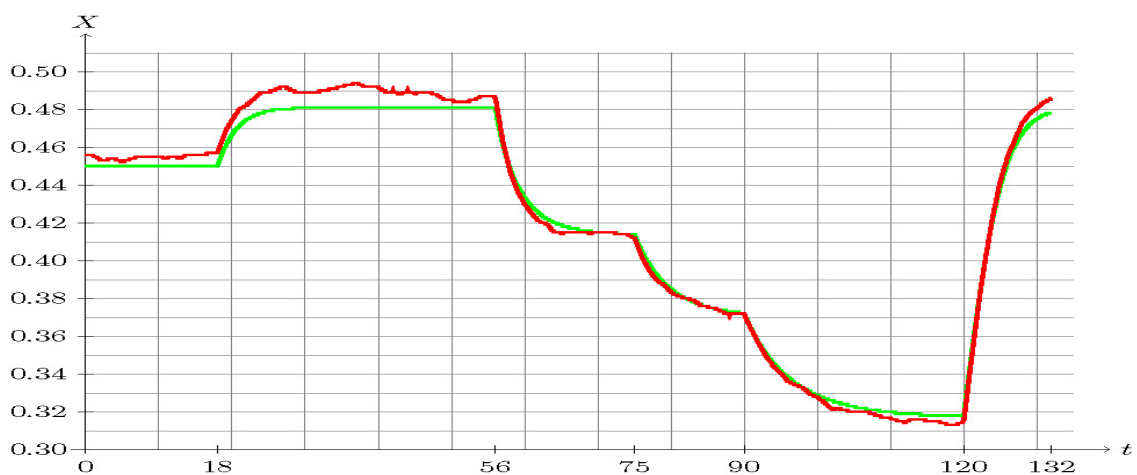


Fig. 4 The estimated biomass concentration

Concluding remarks

In this work some new insights have been obtained concerning the identifiability and observability of methane fermentation processes. A major discovery was that the biomass specific growth rate can be stably estimated from easily measured quantities, the dilution rate D and the biogas flow rate Q . If that estimate of biomass specific growth rate is next considered as an additional measurement then, of course, the biomass concentration becomes observable if the yield coefficient K_2 is known, and the biomass concentration is not observable if K_2 is not known. The experimental validation which is under investigation will allow us to extend these conclusions to more complex and more realistic models.

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