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A dynamic estimation scheme of specific growth rates of bacteria for an anaerobic wastewater treatment process

S. Diop¹, J. P. Steyer² and I. Simeonov³

Abstract—The paper proposes an observability analysis and estimation schemes for specific growth rates for an anaerobic wastewater treatment process. A 2-stage model of 6 dynamic states is assumed, describing the acidogenesis and methanogenesis of two different populations of microorganisms (acidogenic and methanogenic), and the evaluation of the total carbon dioxide production including the soluble part. The main result is that the specific growth rates of the two populations of bacteria can be stability estimated only from easily measured quantities – the dilution rate and the flow rates of methane and carbon dioxide in the biogas.

I. INTRODUCTION

Before it may be discharged in natural water systems the chemical oxygen demand (COD: amount of oxygen needed to consume the organic and inorganic materials) of municipal or industrial wastewater often needs to be highly reduced. Otherwise, this COD amount of dissolved oxygen will be consumed by microorganisms leading to the mortality of aquatic organisms. Among the two usual processes used to reduce COD, aerobic and anaerobic wastewater treatments, the latter advantageously does not require the energy necessary for aeration, and yields methane as a by-product so as its energetic balance is rather positive. Anaerobic wastewater treatment is thus subject of many studies since decades, in particular, as a domain of application of system theory results. The dynamics of this process are the ones of standard anaerobic digestion, and depend on the type of organic matters contained in the wastewater. The specific model that is studied in this work was thoroughly developed in [3] for raw industrial wine distillery vinasses obtained from local wineries in the area of Narbonne, France. It is a 2-stage model of 6 dynamic states, describing the acidogenesis and methanogenesis of two different populations of microorganisms (acidogenic and methanogenic), and the evaluation of the total carbon dioxide production including the soluble part. It has been subject to many works, see for instance [1, 2, 7]. The model is based on mass balance arguments involving abstract quantities

named *specific growth rates* which are complex unknown functions of many other quantities and parameters influencing the dynamics of the process, and describe the kinetics of the process. Empirical modeling which are time consuming and difficult to identify and subject to change with the type of wastes are often invoked to express these specific growth rates. The contribution of the present work is to propose estimation schemes of specific growth rates from supposedly easily measured quantities such as the dilution rate and the flow rates of methane and carbon dioxide in the biogas. In [1, 2] estimation of substrate and bacteria concentrations has been considered, without having recourse to specific growth rates [2], and by treating specific growth rates as uncertainties with *known* bounds [1, 7]. The main point of the present work, compared to the previous ones, is to provide a systematic way to obtain the proposed estimation schemes. The method is part of a general approach of observation problems using tools from differential algebraic geometry [5].

The paper is organized as following. The next section is devoted to the description of the model of the specific anaerobic digestion process. Then the observability of the two specific growth rates is analyzed in the light of the differential algebraic approach. Finally estimation schemes are detailed for most of the quantities involved in the model. Illustrative simulations as well as confrontation to experimental data are postponed to future versions of this paper.

II. THE PROCESS MODEL

The following model of wastewater treatment of raw industrial wine distillery vinasses has been thoroughly developed in [3].

$$\dot{S}_1 = D S_{1\text{in}} - D S_1 - k_1 \mu_1 X_1$$

$$\dot{X}_1 = \mu_1 X_1 - \alpha D X_1,$$

$$\dot{S}_2 = D S_{2\text{in}} - D S_2 + k_2 \mu_1 X_1 - k_3 \mu_2 X_2,$$

$$\dot{X}_2 = \mu_2 X_2 - \alpha D X_2,$$

$$q_M = k_6 \mu_2 X_2,$$

$$q_C = k_L a (C + S_2 - Z - K_H P_C),$$

$$\dot{C} = D C_{\text{in}} - D C - q_C + k_4 \mu_1 X_1 + k_5 \mu_2 X_2,$$

$$\dot{Z} = D Z_{\text{in}} - D Z,$$

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with

$$\begin{aligned}
a_1 = & k_L a k_6 K_H P_T D q_M q_C + k_L a k_6 K_H P_T D q_C^2 \\
& + k_L a k_6 K_H P_T q_M \dot{q}_C - k_L a k_6 K_H P_T q_C \dot{q}_M \\
& + k_L a k_6 D Z_{in} q_M^2 + 2 k_L a k_6 D Z_{in} q_M q_C \\
& + k_L a k_6 D Z_{in} q_C^2 - k_L a k_6 D C_{in} q_M^2 \\
& - 2 k_L a k_6 D C_{in} q_M q_C - k_L a k_6 D C_{in} q_C^2 \\
& - k_L a k_6 D S_{2in} q_M^2 - 2 k_L a k_6 D S_{2in} q_M q_C \\
& - k_L a k_6 D S_{2in} q_C^2 + k_L a k_3 q_M^3 + 2 k_L a k_3 q_M^2 q_C \\
& + k_L a k_3 q_M q_C^2 - k_L a k_5 q_M^3 - 2 k_L a k_5 q_M^2 q_C \\
& - k_L a k_5 q_M q_C^2 + k_L a k_6 q_M^2 q_C + 2 k_L a k_6 q_M q_C^2 \\
& + k_L a k_6 q_C^3 + k_6 D q_M^2 q_C + 2 k_6 D q_M q_C^2 \\
& + k_6 D q_C^3 + k_6 q_M^2 \dot{q}_C + 2 k_6 q_M q_C \dot{q}_C + k_6 q_C^2 \dot{q}_C
\end{aligned}$$

and

$$d_1 = \alpha D - \frac{d}{dt} \ln \left((q_M + q_C)^3 \right).$$

This says that μ_1 is not observable (in the sense of [5]) with respect to D , Z_{in} , S_{1in} , S_{2in} , C_{in} , q_M , q_C and pH since it is introduced by a differential equation of order 1 and not 0.

But as previously explained in [4], dividing both sides of the previous equation by μ_1^2 , equation 2 becomes

$$\dot{z}_1 = -d_1 z_1 + Q_1 \quad (4)$$

with

$$z_1 = \frac{Q_1}{\mu_1}. \quad (5)$$

If d_1 could be proved to be of constant positive sign then equation 4 would lead to an estimation scheme of μ_1 with respect to D , Z_{in} , S_{1in} , S_{2in} , C_{in} , q_M , q_C and pH. The lack of clue on the positiveness of d_1 forces to look for a change of variable which is not as simple as in equation 5.

Elementary but tedious manipulations of the differential polynomial P_{μ_1} allows to see that, if

$$z_1 = \frac{q_1}{\mu_1} \quad (6)$$

with

$$q_1 = \frac{Q_1}{(q_M + q_C)^3} \quad (7)$$

then equation 2 may be rewritten as

$$\dot{z}_1 = -\alpha D z_1 + q_1 \quad (8)$$

which yields an estimation scheme for μ_1 :

$$\mu_1 = \frac{q_1}{z_1} \quad (9)$$

B. Observability of μ_2

It happens that the differential polynomial introducing μ_2 is much simpler than P_{μ_1} , and is as follows:

$$q_M \dot{\mu}_2 - \dot{q}_M \mu_2 - \alpha D q_M \mu_2 + q_M \mu_2^2 = 0 \quad (10)$$

yielding

$$\dot{z}_2 = -\alpha D z_2 + q_M \quad (11)$$

and

$$\mu_2 = \frac{q_M}{z_2}. \quad (12)$$

IV. DESIGN OF THE ESTIMATORS

Given their exponential stability (thanks to the constant positive sign of αD) the differential equations 8, and 11 are estimation schemes for μ_1 and μ_2 . The speed of convergence of these estimators cannot be changed by the user, they are fixed by the quantity αD .

In order to use equation 8 as an estimator for μ_1 it is necessary to properly evaluate the quantity q_1 in equation 7.

If the expression of q_1 taken from equations 7 and 3 were to be used as is in experimental data then difficulties would rise from the nonlinear dependency on measurements uncertainties through the time derivatives of q_M and q_C .

Therefore the challenge is to reduce this complex expression of q_1 to a form which is more favorable to online numerical differentiation.

Again, elementary but subtle calculations allow to see that q_1 may be written as

$$\begin{aligned}
q_1 = & k_L a k_6 K_H P_T \left(\frac{1}{1 + \frac{q_M}{q_C}} \right) + k_6 \dot{q}_C \\
& + k_L a (k_3 - k_5) q_M + k_6 (k_L a + D) q_C \\
& + k_L a k_6 D (Z_{in} - C_{in} - S_{2in}) \left(\frac{1 - \frac{q_M}{q_C}}{1 + \frac{q_M}{q_C}} \right)^2 \\
& + \frac{k_L a k_6 K_H P_T D}{1 + \frac{q_M}{q_C}}.
\end{aligned} \quad (13)$$

Assuming the inputs D , q_1 and q_M free of z_i the differential equations 8, and 11 are readily dynamic estimators of μ_1 and μ_2 :

$$\begin{cases} \hat{z}_i = -\alpha D \hat{z}_i + \hat{y}_i, \\ \hat{\mu}_i = \frac{\hat{y}_i}{\hat{z}_i}, \end{cases}$$

where

$$\hat{y}_1 = \hat{q}_1 \text{ and } \hat{y}_2 = \bar{q}_M.$$

The quantities \bar{q}_C , \bar{q}_M are the potentially noisy online measurements of q_C , q_M , respectively. There are two quantities which need to be numerically differentiated:

$$\bar{q}_C \quad \text{and} \quad \frac{1}{1 + \frac{\bar{q}_M}{\bar{q}_C}}.$$

The estimation error $\tilde{z}_i = z_i - \hat{z}_i$ evolves according to the following dynamics

$$\dot{\tilde{z}}_i = -\alpha D \tilde{z}_i + \tilde{y}_i \quad \text{with} \quad \tilde{y}_i = y_i - \hat{y}_i.$$

In every time interval $[r, s]$, where the quantity D is positive the estimation error decreases exponentially in norm as follows

$$\begin{aligned}\tilde{z}_i(t) &= \tilde{z}_i(r) \exp\left(-\int_r^t \alpha D(\sigma) d\sigma\right) \\ &+ \int_r^t \tilde{y}_i(\sigma) \exp\left(-\int_\sigma^t \alpha D(\tau) d\tau\right) d\sigma\end{aligned}$$

when t tends to s .

A. Estimation scheme for X_1 and S_1

The differential polynomial introducing X_1 reads as

$$k_L a k_6 (k_2 + k_4) (q_M + q_C)^2 \mu_1 X_1 = a_1 \quad (14)$$

which leads to the following estimation of X_1 :

$$\hat{X}_1 = \frac{\hat{z}_1}{k_L a (k_2 + k_4) k_6} \quad (15)$$

where z_1 is given by [equation 6](#).

The differential equation for S_1 in [equation 1](#) yields an estimator for this quantity:

$$\hat{S}_1 = -D \hat{S}_1 + D S_{1in} - \frac{k_1 \hat{q}_1}{k_L a (k_2 + k_4) k_6}.$$

B. Estimation scheme for X_2 and S_2

The quantity X_2 is readily seen as

$$\hat{X}_2 = \frac{\hat{z}_2}{k_6}.$$

In addition, S_2 turns out to be able to be estimated as

$$\hat{S}_2 = \hat{Z} - \frac{K_b K_H P_T}{\text{pHe}} \frac{1}{1 + \frac{\bar{q}_M}{\bar{q}_C}} - \frac{K_b \bar{q}_C}{k_L a \text{pHe}}, \quad (16)$$

where Z is given by

$$\hat{Z} = -D \hat{Z} + D Z_{in}.$$

V. CONCLUSION

It has been shown using the differential algebraic approach of observability and its accompanying differential algebraic decision methods (namely, characteristic set computations) that specific growth rates of the anaerobic wastewater of raw industrial wine distillery vinasses may be estimated from supposedly easily online measured data. This saves the time of empirical modeling and identification of specific growth rates, and allows the use of different kind of wastes without re-doing this empirical modeling. Moreover, it is believed that these estimates may serve as valuable tools in control and monitoring of highly unstable wastewater treatment processes.

APPENDIX

$$\begin{aligned}P_{\mu_1} &= (k_L a k_6 K_H P_T D q_M^2 q_C + 2 k_L a k_6 K_H P_T D q_M q_C^2 + \\ &k_L a k_6 K_H P_T D q_C^3 + k_L a k_6 K_H P_T q_M^2 \dot{q}_C - \\ &k_L a k_6 K_H P_T q_M q_C \dot{q}_M + k_L a k_6 K_H P_T q_M q_C \dot{q}_C - \\ &k_L a k_6 K_H P_T q_C^2 \dot{q}_M + k_L a k_6 D Z_{in} q_M^3 + \\ &3 k_L a k_6 D Z_{in} q_M^2 q_C + 3 k_L a k_6 D Z_{in} q_M q_C^2 + \\ &k_L a k_6 D Z_{in} q_C^3 - k_L a k_6 D C_{in} q_M^3 - 3 k_L a k_6 D C_{in} q_M^2 q_C - \\ &3 k_L a k_6 D C_{in} q_M q_C^2 - k_L a k_6 D C_{in} q_C^3 - k_L a k_6 D S_{2in} q_M^3 - \\ &3 k_L a k_6 D S_{2in} q_M^2 q_C - 3 k_L a k_6 D S_{2in} q_M q_C^2 - \\ &k_L a k_6 D S_{2in} q_C^3 + k_L a k_3 q_M^4 + 3 k_L a k_3 q_M^3 q_C + \\ &3 k_L a k_3 q_M^2 q_C^2 + k_L a k_3 q_M q_C^3 - k_L a k_5 q_M^4 - 3 k_L a k_5 q_M^3 q_C - \\ &3 k_L a k_5 q_M^2 q_C^2 + k_L a k_5 q_M q_C^3 + k_L a k_6 q_M^3 q_C + \\ &3 k_L a k_6 q_M^2 q_C^2 + 3 k_L a k_6 q_M q_C^3 + k_L a k_6 q_C^4 + \\ &k_6 D q_M^3 q_C + 3 k_6 D q_M^2 q_C^2 + 3 k_6 D q_M q_C^3 + k_6 D q_C^4 + \\ &k_6 q_M^3 \dot{q}_C + 3 k_6 q_M^2 q_C \dot{q}_C + 3 k_6 q_M q_C^2 \dot{q}_C + k_6 q_C^3 \dot{q}_C) \mu_1^2 + \\ &(-\alpha k_L a k_6 K_H P_T D^2 q_M^2 q_C - 2 \alpha k_L a k_6 K_H P_T D^2 q_M q_C^2 - \\ &\alpha k_L a k_6 K_H P_T D^2 q_C^3 - \alpha k_L a k_6 K_H P_T D q_M^2 \dot{q}_C + \\ &\alpha k_L a k_6 K_H P_T D q_M q_C \dot{q}_M - \alpha k_L a k_6 K_H P_T D q_M q_C \dot{q}_C + \\ &\alpha k_L a k_6 K_H P_T D q_C^2 \dot{q}_M - \alpha k_L a k_6 D^2 Z_{in} q_M^3 - \\ &3 \alpha k_L a k_6 D^2 Z_{in} q_M^2 q_C - 3 \alpha k_L a k_6 D^2 Z_{in} q_M q_C^2 - \\ &\alpha k_L a k_6 D^2 Z_{in} q_C^3 + \alpha k_L a k_6 D^2 C_{in} q_M^3 + \\ &3 \alpha k_L a k_6 D^2 C_{in} q_M^2 q_C + 3 \alpha k_L a k_6 D^2 C_{in} q_M q_C^2 + \\ &\alpha k_L a k_6 D^2 C_{in} q_C^3 + \alpha k_L a k_6 D^2 S_{2in} q_M^3 + \\ &3 \alpha k_L a k_6 D^2 S_{2in} q_M^2 q_C + 3 \alpha k_L a k_6 D^2 S_{2in} q_M q_C^2 + \\ &\alpha k_L a k_6 D^2 S_{2in} q_C^3 - \alpha k_L a k_3 D q_M^4 - 3 \alpha k_L a k_3 D q_M^3 q_C - \\ &3 \alpha k_L a k_3 D q_M^2 q_C^2 - \alpha k_L a k_3 D q_M q_C^3 + \alpha k_L a k_5 D q_M^4 + \\ &3 \alpha k_L a k_5 D q_M^3 q_C + 3 \alpha k_L a k_5 D q_M^2 q_C^2 + \\ &\alpha k_L a k_5 D q_M q_C^3 - \alpha k_L a k_6 D q_M^3 q_C - 3 \alpha k_L a k_6 D q_M^2 q_C^2 - \\ &3 \alpha k_L a k_6 D q_M q_C^3 - \alpha k_L a k_6 D q_C^4 - \alpha k_6 D^2 q_M^3 q_C - \\ &3 \alpha k_6 D^2 q_M^2 q_C^2 - 3 \alpha k_6 D^2 q_M q_C^3 - \alpha k_6 D^2 q_C^4 - \\ &k_L a k_6 K_H P_T D q_M^2 \dot{q}_C + k_L a k_6 K_H P_T D q_M q_C \dot{q}_M - \\ &k_L a k_6 K_H P_T D q_M q_C \dot{q}_C + k_L a k_6 K_H P_T D q_C^2 \dot{q}_M - \\ &k_L a k_6 K_H P_T \dot{D} q_M^2 q_C - 2 k_L a k_6 K_H P_T \dot{D} q_M q_C^2 - \\ &k_L a k_6 K_H P_T \dot{D} q_C^3 - \alpha k_6 D q_M^3 \dot{q}_C - 3 \alpha k_6 D q_M^2 q_C \dot{q}_C - \\ &3 \alpha k_6 D q_M q_C^2 \dot{q}_C - \alpha k_6 D q_C^3 \dot{q}_C - k_L a k_6 K_H P_T q_M^2 \ddot{q}_C + \\ &k_L a k_6 K_H P_T q_M q_C \ddot{q}_M - k_L a k_6 K_H P_T q_M q_C \ddot{q}_C + \\ &2 k_L a k_6 K_H P_T q_M \dot{q}_M \dot{q}_C + 2 k_L a k_6 K_H P_T q_M \dot{q}_C^2 + \\ &k_L a k_6 K_H P_T q_C^2 \ddot{q}_M - 2 k_L a k_6 K_H P_T q_C \dot{q}_M^2 - \\ &2 k_L a k_6 K_H P_T q_C \dot{q}_M \dot{q}_C - k_L a k_6 D \dot{Z}_{in} q_M^3 - \\ &3 k_L a k_6 D \dot{Z}_{in} q_M^2 q_C - 3 k_L a k_6 D \dot{Z}_{in} q_M q_C^2 - \\ &k_L a k_6 D \dot{Z}_{in} q_C^3 + k_L a k_6 D \dot{S}_{2in} q_M^3 + \\ &3 k_L a k_6 D \dot{S}_{2in} q_M^2 q_C + 3 k_L a k_6 D \dot{S}_{2in} q_M q_C^2 + \\ &k_L a k_6 D \dot{S}_{2in} q_C^3 - k_L a k_6 Z_{in} \dot{D} q_M^3 - 3 k_L a k_6 Z_{in} \dot{D} q_M^2 q_C - \\ &3 k_L a k_6 Z_{in} \dot{D} q_M q_C^2 - k_L a k_6 Z_{in} \dot{D} q_C^3 + \\ &k_L a k_6 C_{in} \dot{D} q_M^3 + 3 k_L a k_6 C_{in} \dot{D} q_M^2 q_C + \\ &3 k_L a k_6 C_{in} \dot{D} q_M q_C^2 + k_L a k_6 C_{in} \dot{D} q_C^3 + \\ &k_L a k_6 S_{2in} \dot{D} q_M^3 + 3 k_L a k_6 S_{2in} \dot{D} q_M^2 q_C + \\ &3 k_L a k_6 S_{2in} \dot{D} q_M q_C^2 + k_L a k_6 S_{2in} \dot{D} q_C^3 - \\ &k_L a k_3 q_M^3 \dot{q}_M - 3 k_L a k_3 q_M^2 q_C \dot{q}_M - 3 k_L a k_3 q_M q_C^2 \dot{q}_M - \\ &k_L a k_3 q_C^3 \dot{q}_M + k_L a k_5 q_M^3 \dot{q}_M + 3 k_L a k_5 q_M^2 q_C \dot{q}_M + \\ &3 k_L a k_5 q_M q_C^2 \dot{q}_M + k_L a k_5 q_C^3 \dot{q}_M + C_{in} k_L a k_6 D q_M^3 + \\ &3 C_{in} k_L a k_6 D q_M^2 q_C + 3 C_{in} k_L a k_6 D q_M q_C^2 + \\ &C_{in} k_L a k_6 D q_C^3 - k_L a k_6 q_M^3 \dot{q}_C - 3 k_L a k_6 q_M^2 q_C \dot{q}_C - \\ &3 k_L a k_6 q_M q_C^2 \dot{q}_C - k_L a k_6 q_C^3 \dot{q}_C - k_6 D q_M^3 \dot{q}_C - \\ &3 k_6 D q_M^2 q_C \dot{q}_C - 3 k_6 D q_M q_C^2 \dot{q}_C - k_6 D q_C^3 \dot{q}_C - \\ &k_6 \dot{D} q_M^3 q_C - 3 k_6 \dot{D} q_M^2 q_C^2 - 3 k_6 \dot{D} q_M q_C^3 - k_6 \dot{D} q_C^4 -\end{aligned}$$

$$\begin{aligned}
& k_6 q_M^3 \ddot{q}_C - 3 k_6 q_M^2 q_C \ddot{q}_C - 3 k_6 q_M q_C^2 \ddot{q}_C - k_6 q_C^3 \ddot{q}_C) \mu_1 + \\
& (k_L a k_6 K_H P_T D q_M^2 q_C + 2 k_L a k_6 K_H P_T D q_M q_C^2 + \\
& k_L a k_6 K_H P_T D q_C^3 + k_L a k_6 K_H P_T q_M^2 \dot{q}_C - \\
& k_L a k_6 K_H P_T q_M q_C \dot{q}_M + k_L a k_6 K_H P_T q_M q_C \dot{q}_C - \\
& k_L a k_6 K_H P_T q_C^2 \dot{q}_M + k_L a k_6 D Z_{in} q_M^3 + \\
& 3 k_L a k_6 D Z_{in} q_M^2 q_C + 3 k_L a k_6 D Z_{in} q_M q_C^2 + \\
& k_L a k_6 D Z_{in} q_C^3 - k_L a k_6 D C_{in} q_M^3 - 3 k_L a k_6 D C_{in} q_M^2 q_C - \\
& 3 k_L a k_6 D C_{in} q_M q_C^2 - k_L a k_6 D C_{in} q_C^3 - k_L a k_6 D S_{2in} q_M^3 - \\
& 3 k_L a k_6 D S_{2in} q_M^2 q_C - 3 k_L a k_6 D S_{2in} q_M q_C^2 - \\
& k_L a k_6 D S_{2in} q_C^3 + k_L a k_3 q_M^4 + 3 k_L a k_3 q_M^3 q_C + \\
& 3 k_L a k_3 q_M^2 q_C^2 + k_L a k_3 q_M q_C^3 - k_L a k_5 q_M^4 - 3 k_L a k_5 q_M^3 q_C - \\
& 3 k_L a k_5 q_M^2 q_C^2 - k_L a k_5 q_M q_C^3 + k_L a k_6 q_M^3 q_C + \\
& 3 k_L a k_6 q_M^2 q_C^2 + 3 k_L a k_6 q_M q_C^3 + k_L a k_6 q_C^4 + k_6 D q_M^3 q_C + \\
& 3 k_6 D q_M^2 q_C^2 + 3 k_6 D q_M q_C^3 + k_6 D q_C^4 + k_6 q_M^3 \dot{q}_C + \\
& 3 k_6 q_M^2 q_C \dot{q}_C + 3 k_6 q_M q_C^2 \dot{q}_C + k_6 q_C^3 \dot{q}_C) \mu_1
\end{aligned}$$

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