

Exponential Regulation of Alkalinity and VFA in Continuous Anaerobic Digestion Processes under Uncertain Operational Conditions

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Abstract: - In this paper we propose a multivariable robust feedback control for regulating the alkalinity and the volatile fatty acid concentration in continuous anaerobic digestion processes used in wastewater treatment. The system exhibits a large lack of knowledge on kinetic parameters. Furthermore, key state variables, which cannot be measured, are estimated by using a Luemberger observer. Thus, even under this highly uncertain scenario, the proposed control law uses this partial information for regulating exponentially the control variables. The control objectives are firstly established upon physicochemical criteria based on normal operational conditions and then formally stated in terms of the concerned state variables. The resulting control law is tested experimentally in a 1 m³ pilot plant for the treatment of red wine vinasses under several uncertain situations in which the multivariable control law is able to recover the system stability around the pre-specified set points showing a very high performance and usefulness for this kind of processes.

Key-Words: - Alkalinity, Anaerobic Digestion, Interval Observers, Robust Regulation, Wastewater Treatment, Stability

1 Introduction

Anaerobic digestion is a very complex multi-biomass and multi-substrate process commonly used in wastewater treatment in which the organic matter expressed as chemical oxygen demand (COD) is decomposed firstly into volatile fatty acids (VFA) and then converted into biogas, (a mixture mainly composed of CO₂ and CH₄), microbial biomass and residual organic matter.

Even when anaerobic digestion has been largely studied, its operational stability, mainly concerning the methanogenic phase is still an intense field of research. For instance, it is well known that serious problems in industrial applications are produced because the variations on the process inputs that can lead the process to substrate inhibition conditions. This problem is produced by VFA accumulation in the reactor and must be solved rapidly in order to avoid the acidification of the reactor [1].

Closely related with VFA acidification troubles, the problems in the regulation of pH are accentuated when the process inputs are not buffer solutions or their buffer capacity is weak. Then, under these unstable conditions the VFA production is higher than its consumption. If this instability takes a long time, the buffer capacity inside the bioreactor becomes insufficient, and then, the VFA accumulation may lead the bioreactor to a pH drop and the inhibition of methanogenic bacteria. In fact, regulation of VFA only for any apparently correct pH value or *vice versa* is not enough to guaranty operational stability.

Thus, the regulation of both, VFA concentration and alkalinity concentration have taken importance for maintaining the operational stability in anaerobic bioreactors [2], [3]. However, only a few recent works have studied the simultaneous regulation of both, VFA and alkalinity in order to guarantee the bioreactor stability. In [4] an

approach based in geometric control for the regulation of VFA and the strong ions concentration (which is related to alkalinity) was proposed. Nevertheless, in that work, neither TA nor the relationship IA/TA was used directly as stability criterions. The absence of works in which the alkalinity is directly regulated, rises surely from the fact that this variable is a function of the pH and it involves all the physicochemical equilibrium in the system. Therefore, it is not an easy task to represent the dynamics of alkalinity as a state variable.

In this work a robust Multiple-Input, Multiple-Output (MIMO) approach is proposed for the regulation of VFA and alkalinity, which is based on the operational criteria suggested in [5], that guarantees the stability within the bioreactor. Criteria on the alkalinity references are rigorously adapted in function of true state variables and then expressed directly as control objectives upon these variables [6]. In order to deal with important uncertainties on kinetic parameters and process inputs, the proposed control law is based upon the basis of adaptive approaches [7], [8], [9]. Moreover, concerning non measured state variables, and kinetic uncertainties, this control law uses a Luemberger observer [4].

The paper is organized as follows: First, the particular system in which the MIMO control approach is applied as well as the control objectives proposed in this work are shown in section 2, i.e., the Problem Formulation. Then the Problem Solution, i.e., the robust feedback regulation as well as the experimental implementation, are depicted in section 3. Finally, conclusions are addressed in section 4.

2 Problem Formulation

2.1 Dynamical Model

The following time-varying nonlinear system for continuous stirred tank reactors is considered:

$$\dot{x}(t) = Cf(x(t), t) + A(D(t), t)x(t) + b(t) \quad (1)$$

where $x(t) \in \mathfrak{R}_+^n$ represents the state vector, $f(x(t), t) \in \mathfrak{R}_+^r$ is a positive vector that lumps the process kinetic terms, matrix $C \in \mathfrak{R}^{n \times r}$ is a coefficients matrix (i.e., yield coefficients). $A(t) \in \mathfrak{R}^{n \times n}$ denotes the state matrix of the linear

part of the system. In this paper, it is considered that the input flow rate can be split in several streams which will be used as manipulated variables in the form of dilution rates. They are gathered in the vector $D(t) \in \mathfrak{R}_+^l$. Finally $b(t) \in \mathfrak{R}^n$ is a vector that gathers the process inputs (i.e. the mass feeding rate vector) and other functions possibly time-varying (e.g. the gaseous outflow rate vector, if any).

Now, let us consider that m states are measured on-line and l from them are the states to be regulated ($l \leq m$). Then the state space can be split in such a way that (1) can be rewritten in measurable and non-measurable state variables as follows:

$$\begin{aligned} \dot{x}_1(t) &= C_1 f(x(t), t) + A_{11}(t)x_1(t) + A_{12}(t)x_2(t) + b_1(t) \\ \dot{x}_2(t) &= C_2 f(x(t), t) + A_{21}(t)x_1(t) + A_{22}(t)x_2(t) + b_2(t) \end{aligned} \quad (2)$$

where the m measured states have been included in $x_2(t) \in \mathfrak{R}_+^m$ and the variables to be estimated are represented by $x_1(t) \in \mathfrak{R}^s$ ($s = n - m$). Matrices $A_{11}(t) \in \mathfrak{R}^{s \times s}$, $A_{12}(t) \in \mathfrak{R}^{s \times m}$, $A_{21}(t) \in \mathfrak{R}^{m \times s}$, $A_{22}(t) \in \mathfrak{R}^{m \times m}$, $C_1(t) \in \mathfrak{R}^{s \times r}$, $C_2(t) \in \mathfrak{R}^{m \times r}$, $b_1(t) \in \mathfrak{R}^s$ and $b_2(t) \in \mathfrak{R}^m$ are the corresponding partitions of $A(t)$, C and $b(t)$, respectively.

The following hypotheses are introduced:

Hypotheses 1 (H1):

H1.1: $A(t)$ is known $\forall t \geq 0$ and it is bounded between two constant matrices A^- and A^+ such that $A^- \leq A(t) \leq A^+$. This hypothesis implies that guaranteed bounds on the dilution rates are given as: $D_i^-(t) \leq D_i(t) \leq D_i^+(t)$, $\forall i, i = 1, 2, \dots, l$.

H1.2: $f(x(t), t)$ is fully unknown, however, guaranteed bounds on the reaction rate vector $f(x(t), t)$ are known, i.e.:

$$\bar{f} \leq f^-(x(t), t) \leq f(x(t), t) \leq f^+(x(t), t) \leq \underline{f} \quad (3)$$

Remark 1 (R1): The operator “ \leq ” applied between vectors and between matrices should be understood as a collection of inequalities between elements.

2.1.1 Anaerobic Digestion Model AM2a

Anaerobic digestion (AD) processes involve several multi-substrate multi-organism reactions that are performed both in series and in parallel [10], [11]. Here, we consider a model of an anaerobic digestion process carried out in a continuous fixed bed bioreactor for the treatment of red wine vinasses, which has been proposed and successfully validated by [12]. This model, called AM2 model, has been used in the design of several control approaches that have been successfully tested in actual AD processes [13]; [14]; [15]; [16], [17], [18]). On the other hand, it is well known that operational stability of AD prevails when the physical-chemical equilibrium between the VFA and the alkalinity exists while the acidogenic and methanogenic bacteria are in a productive stage [17]. A procedure to preserve the physical-chemical equilibrium between the VFA and the alkalinity recommends addition of alkali (*i.e.* NaOH, KOH, etc.) [19]. Thus, the model AM2 can be modified if a second input flow that allows regularize the strong ion concentration (alkalinity) is considered. In [4] a second tank containing NaOH is considered as an extra dilution stage in the model. This addition to the process only modify the strong ion concentration within the digester. The mathematical model is similar to AM2 except that one input more is considered:

$$\begin{aligned}\dot{X}_1 &= (\mu_1 - \alpha D(t))X_1 \\ \dot{X}_2 &= (\mu_2 - \alpha D(t))X_2 \\ \dot{C}_{TI} &= (C_{TI}^{in} - C_{TI})D(t) + k_4\mu_1 X_1 + k_5\mu_2 X_2 \\ &\quad + k_{La}(K_H P_{CO_2} + Z - C_{TI} - S_2) \\ \dot{S}_1 &= (S_1^{in} - S_1)D(t) - k_1\mu_1 X_2 \\ \dot{S}_2 &= (S_2^{in} - S_2)D(t) + k_2\mu_1 X_1 - k_3\mu_2 X_2 \\ \dot{Z} &= (Z_1^{in} - Z)D_1(t) + (Z_2^{in} - Z)D_2(t)\end{aligned}\quad (4)$$

with

$$\mu_1 = \frac{\mu_{\max,1} S_1}{k_{s,1} + S_1}, \quad \mu_2 = \frac{\mu_{\max,2} S_2}{k_{s,2} + S_2 + (S_2 / k_{I,2})^2} \quad (5)$$

$$P_{CO_2} = \frac{\phi - \sqrt{\phi^2 - 4K_H P[CO_2]}}{2K_H}$$

$$\phi = [CO_2] + K_H P + \frac{k_6\mu_2 X_2}{k_{La}}$$

$$[CO_2] = C_{TI} + S_2 - Z$$

where X_1 , X_2 , S_1 , S_2 y C_{TI} are the concentrations of acidogenic and methanogenic biomass, COD, VFA

and the total inorganic carbon respectively. Z_1^{in} and Z_2^{in} are the respective strong ion concentrations in both tanks. P_{CO_2} is the CO_2 partial pressure. $\mu_{\max,1}$ and $\mu_{\max,2}$ (d^{-1}) are the maximum growth rates. The parameter α is related with the biomass fraction that is retained for the reactor bed, *i.e.*, $\alpha=0$ for an ideal fixed-bed reactor and $\alpha=1$ for an ideal continuous stirred reactor tank. This parameter is calculated experimentally. The specific growth rates (Monod type and Haldane type, respectively) are the main responsible for the highly nonlinear kinetic behavior of the system. Values of the model parameters can be found in [12].

The following assumption is introduced:

Assumptions 1 (A1):

The dilution rate $D_2(t) \lll D_1(t)$, where $D_1(t)$ represents the original dilution rate and $D_2(t)$ is the alkali dilution rate. Therefore $D(t) = D_1(t) + D_2(t) \approx D_1(t)$.

As it can be observed, the AM2a model provides a MIMO structure that will be of great importance for the design of the control laws proposed here.

2.2 Control Objectives

The first control objective in any WWT system is the regulation of COD. However, as it has been mentioned previously, AD is susceptible of substrate inhibition, and then, a second objective, not less important, is to guarantee the operational stability of the bioreactor. In this paper we propose to achieve this second objective by regulating both, Total Alkalinity (TA) and the Intermediate Alkalinity (IA). Nevertheless, strictly speaking, neither TA nor IA appears as state variables in the AM2 model but they may be related to the true state variables S_2 and Z in the following form [6]:

$$TA \equiv f_{Tc} Z(t) + (f_{Ta} - f_{Tc}) F_a S_2(t) \quad (6)$$

$$\frac{IA}{TA} \equiv \frac{f_{Ic} Z(t) + (f_{Ia} - f_{Ic}) F_a S_2(t)}{f_{Tc} Z(t) + (f_{Ta} - f_{Tc}) F_a S_2(t)} \quad (7)$$

with

$$f_{Tc} = \left(1 - \frac{10^{-pH(t)} + K_c}{10^{-4.3} + K_c}\right), \dots, F_a = \left(\frac{K_a}{10^{-pH(t)} + K_a}\right)$$

$$f_{Ta} = \left(1 - \frac{10^{-pH(t)} + K_a}{10^{-4.3} + K_a}\right) \quad f_{Ic} = f_{Tc} - f_{Pc}$$

$$f_{Ia} = f_{Ta} - f_{Pa}$$

$$f_{Pc} = \left(1 - \frac{10^{-pH(t)} + K_c}{10^{-5.75} + K_c}\right), f_{Pa} = \left(1 - \frac{10^{-pH(t)} + K_a}{10^{-5.75} + K_a}\right)$$

where K_a and K_c are the equilibrium constants for VFAs and carbonates (first dissociation), respectively. On the other hand, a number of practical operational criteria have been established for TA and IA/TA in order to guarantee the operational stability of AD processes. For instance, [20] and [21] have suggested that VFAs and TA should be kept in 25 mmol/L and 60 mEq/L respectively. Others studies have been based on Total Alkalinity (TA) and the relationship between Intermediate Alkalinity (IA, due to VFA concentration) and Total Alkalinity (IA/TA). For instance, [5], have established these criteria as

$$TA \geq TA_{\min} \equiv 60mEq/l \quad (8)$$

$$IA/TA \leq (IA/TA)_{\max} \equiv 0.3,$$

while [22] suggested a similar criteria based on the partial alkalinity (PA) instead of TA as

$$IA/PA \leq (IA/PA)_{\max} \equiv 0.3 \quad (9)$$

Thus, taken into account any of these criteria, the control objectives in terms of state variables can be stated as follows:

$$S_2^r(t) \leq \frac{TA_{\min} (f_{Ic} - (IA/TA)_{\max} f_{Tc})}{F_a (F_1 + F_2)} \quad (10)$$

with

$$F_1 = f_{Tc} ((IA/TA)_{\max} (f_{Ta} - f_{Tc}) - (f_{Ia} - f_{Ic}))$$

$$F_2 = (f_{Ta} - f_{Tc})(f_{Tc} - (IA/TA)_{\max} f_{Tc})$$

$$Z^r(t) \geq \frac{TA_{\min} - F_a (f_{Ta} - f_{Tc}) S_2^r(t)}{f_{Tc}} \quad (11)$$

Expressions (10-11) mean that the set-point values for the VFA and strong ions concentrations S_2^r and Z^r respectively, must fulfil these inequalities in order to guarantee the operational stability criteria denoted by equations (8-9).

3 Problem Solution

3.1 Control law

This section is devoted to develop the main idea in this contribution. The goal is design a MIMO system able to regulate variables $S_2(t)$ and $Z(t)$ towards chosen operating points $S_2^r(t)$ and $Z^r(t)$, respectively by using dilution rates $D_1(t)$ and $D_2(t)$ as control inputs.

Let $x_2(t) = [S_1 \ S_2 \ Z]^T$ be the measurable state vector and S_2 and Z (*i.e.*, $l = 2$) the variables which it is desired to regulate. Let $y_1 = S_2$, $y_2 = Z$ with $y_{21}^{in} = Z_1^{in}$ and $y_{22}^{in} = Z_2^{in}$. Thus, according to AM2a their dynamic are the following:

$$\dot{y}_1(t) = k_2 \mu_1 X_1 - k_3 \mu_2 X_2 + D_1(t)(y_1^{in} - y_1(t)) \quad (12)$$

$$\dot{y}_2(t) = D_1(t)(y_{22}^{in} - y_2(t)) + D_2(t)(y_{21}^{in} - y_2(t)) \quad (13)$$

In order to guarantee the feedback regulation the following hypotheses are introduced:

Hypotheses 2 (H2):

H2.1: The manipulated variables $D_i(t) \in [\underline{D}_i, \overline{D}_i] \subset \mathfrak{R}_+$ for $i=1,2$, are limited by the following saturation law:

$$sat(D_i(t)) = \begin{cases} \overline{D}_i, & D_i(t) \geq \overline{D}_i \\ \tilde{D}_i(t), & \overline{D}_i < \tilde{D}_i(t) < \underline{D}_i \\ \underline{D}_i, & D_i(t) \leq \underline{D}_i \end{cases} \quad (14)$$

where \underline{D}_i is the lower permissible value for the dilution rate and \overline{D}_i the upper permissible value.

H2.2: Consumption mode for $S_2(t)$ and $Z(t)$ variables, *i.e.*:

For $S_2(t)$: $k_2 \mu_1 X_1 - k_3 \mu_2 X_2 \leq 0$; $S_2^{in} > S_2(t)$.

For $Z(t)$: $Z_1^{in} < Z(t)$; $Z_2^{in} > Z(t)$.

Notice that Hypothesis *H2.2* is met in most industrial effluents. Furthermore, a rigorous analysis on the stability of the steady state of model AM2 [17] reveals that normal operational conditions of this systems are only possible when this hypothesis holds

Proposition 1 (PI): Under hypotheses H1-H2, the following output control laws exponentially stabilizes the variables $S_2(t)$ and $Z(t)$ about $S_2^r(t)$ and $Z^r(t)$ references values:

$$D_1 = \frac{-\eta - \lambda_1^* \frac{1 - e^{-\frac{1}{2}(S_2(t) - S_2^r)^2}}{(S_2(t) - S_2^r)}}{(S_2^{in} - S_2(t))} \quad (15)$$

$$D_2 = \frac{-D_1(Z_1^{in} - Z(t)) - \lambda_2^* \frac{1 - e^{-\frac{1}{2}(Z(t) - Z^r)^2}}{(Z(t) - Z^r)}}{(Z_2^{in} - Z(t))} \quad (16)$$

where $\lambda_i^* \in \mathfrak{R}_+$ for $i=1,2$, are suitably chosen constant values. Moreover, η represents the uncertain kinetics $(k_2\mu_1 X_1 - k_3\mu_2 X_2)$. Then, in order to ensure robustness to control laws presented here, the following Luenberger observer has been used in this paper to reconstruction of these uncertainties:

$$\begin{aligned} \dot{\hat{S}}_2 &= \hat{\eta} + D_1(S_2^{in} - \hat{S}_2) + \Gamma g_1(S_2 - \hat{S}_2) \\ \dot{\hat{\eta}} &= \Gamma^2 g_2(S_2 - \hat{S}_2) \end{aligned} \quad (17)$$

where Γ_1 is a tuning parameter to the observer and g_1, g_2 are chosen properly to fulfill the Hurwitz polynomial $s^2 + g_2s + g_1 = 0$. Thus the observer (17) guarantee that state vector $[S_2 - \hat{S}_2, \eta - \hat{\eta}]^T \rightarrow \varepsilon$ as $t \rightarrow \infty$, where ε is arbitrarily small around of the origin [4], [17]. Other observers are possible. For example, in Alcaraz et al., 2012, a rigorous analysis was made by using interval observers. Thus, once the problem of the uncertainties is solved, the following control laws are proposed.

$$D_1 = \frac{-\hat{\eta} - \lambda_1^* \nu_1}{(S_2^{in} - S_2(t))} \quad (18)$$

$$D_2 = \frac{-D_1(Z_1^{in} - Z(t)) - \lambda_2^* \nu_2}{(Z_2^{in} - Z(t))} \quad (19)$$

$$\nu_1 = \frac{1 - e^{-\frac{1}{2}(S_2(t) - S_2^r)^2}}{(S_2(t) - S_2^r)}; \quad (20)$$

$$\nu_2 = \frac{1 - e^{-\frac{1}{2}(Z(t) - Z^r)^2}}{(Z(t) - Z^r)} \quad (21)$$

with the following adaptive parameters:

$$\left\{ \begin{aligned} \lambda_1^- &= \frac{-\hat{\eta} - \bar{D}_1(S_2^{in} - S_2(t))}{\nu_1}; \\ \lambda_1^* S_2 - S_2^r &< 0 \\ \lambda_1^+ &= \frac{-\hat{\eta}}{\nu_1}; \\ S_2 - S_2^r &\geq 0 \end{aligned} \right. \quad (22)$$

$$\left\{ \begin{aligned} \lambda_2^- &= \frac{-D_1(Z_1^{in} - Z(t)) - \bar{D}_2(Z_2^{in} - Z(t))}{\nu_2}; \\ \lambda_2^* Z - Z^r &< 0 \\ \lambda_2^+ &= \frac{-\bar{D}_1(Z_1^{in} - Z(t))}{\nu_2}; \\ Z - Z^r &\geq 0 \end{aligned} \right. \quad (23)$$

$$\underline{D}_1 \geq 0; \quad \underline{D}_2 \geq 0;$$

$$\bar{D}_1 \geq \frac{-\hat{\eta}}{(S_2^{in} - S_2(t))}; \quad (24)$$

$$\bar{D}_2 \geq \frac{(Z_2^{in} - Z(t))}{(Z_1^{in} - Z(t))}$$

The proof on the stability of this control in a general case is depicted in [23].

3.2 Experimental Implementation

Experimental runs were carried out on a pilot plant located at the Laboratoire de Biotechnologie de l'Environnement de l'Institut National de la Recherche Agronomique (INRA-LBE) in Narbonne, France. The anaerobic reactor used is an up-flow fixed bed type, with a useful volume of 0.528 m³ and is highly instrumented on-line to

soluble chemical oxygen demand (COD) every half hour using mid an infra-red [24], total volatile fatty acids (VFA) bicarbonate concentrations and total and partial alkalinity in the liquid phase with a titrimetric sensor [25]. Measurements of input and recirculation liquid flow rates, pH of the reactor, heater and reactor temperatures, biogas output flow rate, CO₂, CH₄ and H₂ composition in the gas phase and total organic carbon (TOC) in the reactor are available every 2 minutes. More details about the process and evaluation of its on-line instrumentation are available in [26].

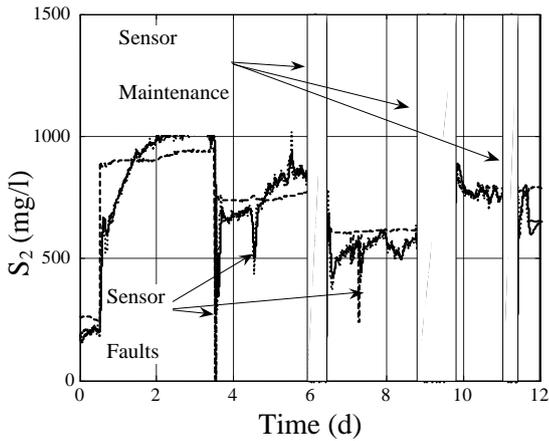


Fig. 1. VFA Concentration. (--) S_2^r , (—) S_2 .

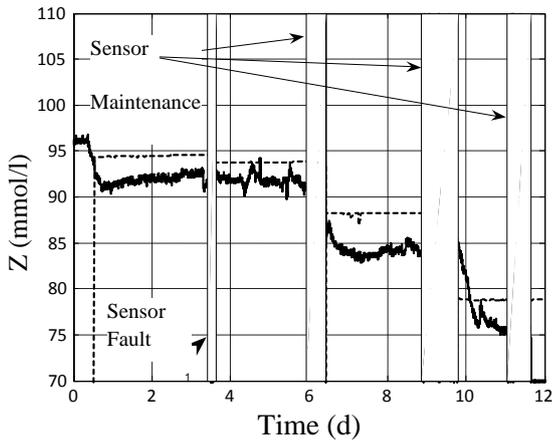


Fig. 2. Strong ions cocentration. (--) Z^r , (—) Z .

The following values on process inputs and saturation parameters for the dilution rate were considered: $S_2^{in} = 5050 \text{ mg/l}$, $Z_1^{in} = 90, 80$ and 75 mmol/l , $Z_2^{in} = 18.870 \text{ mol/l}$, $\underline{D}_1 = 0$, $\underline{D}_1 = 0$ (d^{-1}); $\underline{D}_2 = 0$ (d^{-1}); $\overline{D}_1 \geq 1$ (d^{-1}); $\overline{D}_2 \geq 0.022$ (d^{-1}).

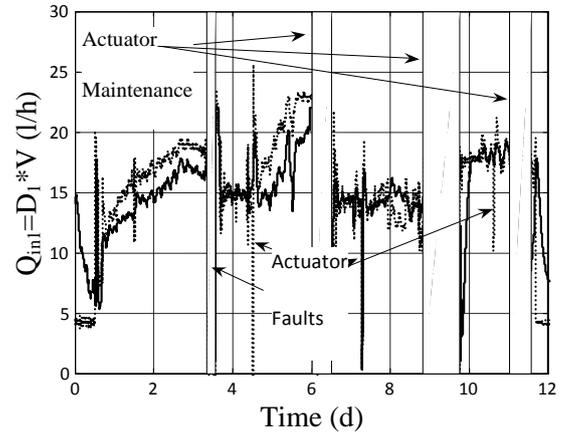


Fig 3. Input flow rate. (··) \hat{D}_1 (calculated), (—) D_1 (real).

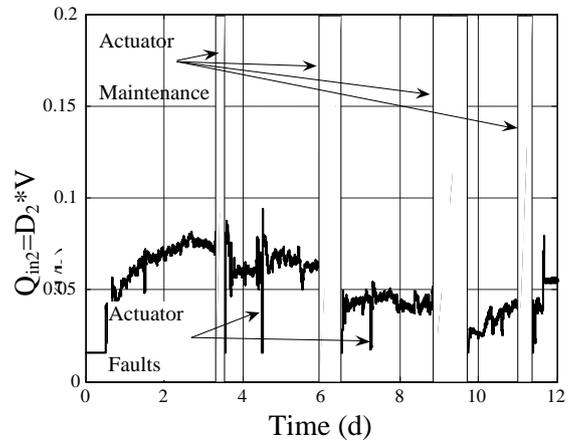


Fig. 4. Alkali input Flow rate. (—) \hat{D}_2 (real).

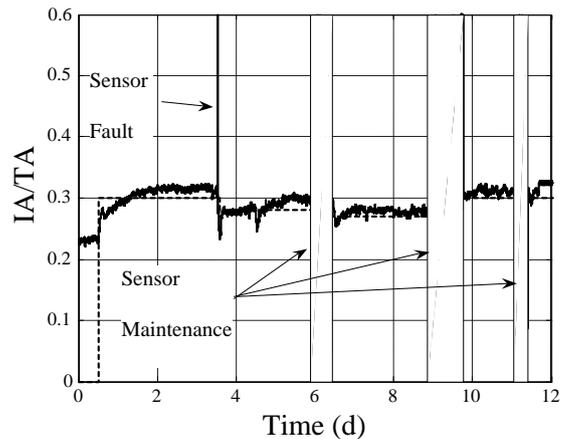


Fig. 5. (--) $(AI/AT)^r$, (—) AI/AT .

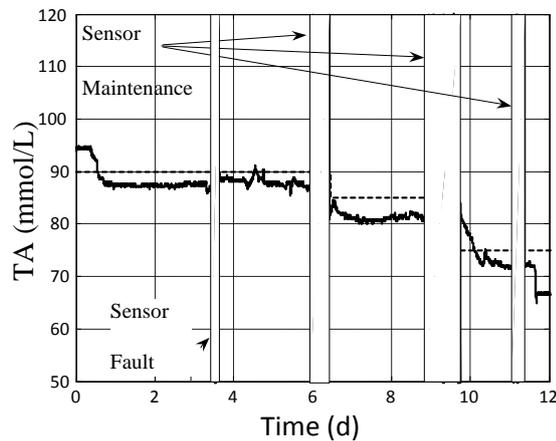


Fig. 6. (--) $(AT)^r$, (—) AT .

In order to show the versatility of this approach and how the operational stability can be easily manipulated by the user, a flexible operation was allowed by fixing the control objectives (8)-(9) as inequalities in the whole sense (i.e., greater/smaller or equal than) and this was applied also for the regulation of Z (i.e., $Z \geq Z^r$). Notice that only S_2 was regulated strictly around its set-point S_2^r . Figures 1 and 2 show the constant references (dashed line) (that actually area function of pH) as well as the measured variables S_2 and Z (continuous line). The time evolution of the dilution rates D_i (the regulation laws), expressed as input flow rates, can be seen in Figures 3 and 4. Experimental runs show how the control laws (18) and (19) are able to regulate the effluent concentrations S_2 and Z around the desired set-points S_2^r , Z^r fulfilling in this form the operational stability criteria (8)-(9). Experimental runs were performed over a 12 days period, using only operational stability criteria (8) (Bernard et al 2000). Different set-points were used as shown in table 1. The objective was to regulate the ratio IA/TA and TA as $(IA/TA)^r \leq 0.3$ (see Fig. 5) and $TA^r \approx 90 \text{ mmol/l}$ (see Fig. 6) respectively. Notice that these control objectives were obtained in an indirect way by regulating the true states variables S_2 and Z .

Table 1. Set points used I the experimental phase

Period	1	2	3	4
AT (mmol/l)	90	90	85	75
AI/AT	0.30	0.28	0.27	0.30

4 Conclusion

A multivariable robust control law for regulating TA and the relationship IA/TA in an anaerobic digestion process was proposed and validated experimentally. Even though not TA nor IA/TA state variables, the correspondence with actual state variables like VFA and Strong Ions Concentration was established in terms of the chemical equilibrium. Thus the control problem was stated indirectly for operational criteria upon alkalinities and then adapted for the actual state variables. Despite a large variation in the process inputs as well as a high uncertainty in the process inputs and kinetic parameters, the control law was able to maintain the regulated variables around the set-points pre-specified for operational stability. The well control law performance held even though it used as inputs the estimates of the unmeasured variables given by a Luemberger which operated under a high uncertainty on the process kinetics.

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