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Experimental estimation of unmeasured inputs in anaerobic wastewater treatment processes

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Abstract This paper presents a virtually controlled observer (VCO) used to estimate both, unmeasured states and unknown influent substrate concentrations in an anaerobic digestion process. This VCO is experimentally implemented in a pilot-scale AD process used for the treatment of wine distillery vinasses. This implementation was carried out under the complete ignorance of the process kinetics. Results indicate that the VCO is able to reconstruct the influent substrate concentration under moderate changes on the operating conditions, while showing also robustness and accuracy against model uncertainties and even sensor faults.

Keywords Anaerobic wastewater treatment; experimental implementation; state and inputs estimation; unknown input observers

1. Introduction – In recent years, Control and Automation (CA) of Wastewater Treatment Process (WWTP), has been revealed as a need for guaranteeing stability, safe operation, and maintaining of a good performance in WWTP [1]. Nevertheless, CA of WWTP requires also of Instrumentation that is not always easy to implement. This is true particularly in Anaerobic Digestion (AD) processes, that are complex WWTP in which organic matter determined as Chemical Oxygen Demand (COD) is first degraded into Volatile Fatty Acids (VFA) and then, from those, into CO₂ and CH₄. Despite AD is nowadays widely used in the agro-industrial field, it is well known that this kind of processes may become unstable under some operational conditions (e.g., high organic loads, low hydraulic retention times) [2] and then control process is necessary in order to guarantee stability efficiency and a good performance [3]. Furthermore, given the strong nonlinear behavior of this kind of processes, different estimation and control schemes have been proposed in the past [4], [5]. Nevertheless, most control laws are function of process inputs that usually are unknown, but actually, relatively few works has been paid attention regarding their estimation when is difficult to measure it [6]. Recently, [7] developed an observer-based estimator named Virtually Controlled Observer (VCO), to reconstruct simultaneously the influent COD and some unmeasured state variables in continuous anaerobic digestion processes. In the current paper, this approach is improved and extended to the estimation of influent VFA as well. In addition, this VCO is experimentally implemented in a 1 m³ fixed bed anaerobic digester used for the treatment of red wine vinasses from the Narbonne (France) area. This paper is organized as follows: First, some details about the data acquisition are provided and then, the AD model used in this work is briefly described. After, the VCO design is presented and the results on the experimental implementation are shown and discussed. Finally some conclusions are drawn.

2. Material and methods - The experimental runs were carried out in a 0.948.35 m³ up-flow fixed-bed pilot-scale anaerobic reactor [8]. The measurements of pH, inflow flow rate (l/h), total organic carbon concentration (mg/l), partial pressure (mbar), volatile fat acids concentration (mg/l) and bicarbonate concentration (mmol/l) were taken every two minutes. The VCO design requires a dynamical model of the process [9], and it consist of an observer and an output feedback controller, in which, one of the observer's inputs (the hypothetical -unmeasured- influent substrate concentration) is updated by a feedback control, which regulates the estimation error of a measured output [7]. In order to deal with the kinetic process uncertainties, a classical asymptotic observer (CAO) was used, because it does not require

the knowledge of the process kinetics and because of its excellent robustness and stability properties [10]. The control variable of the VCO is the error between the measured variables and the estimated ones. The manipulated variable is the input concentration used in the asymptotic observer. Once the error becomes less than an arbitrarily chosen value it is considered that the estimated influent concentration is approximately equal to the real. In the following, the model, the CAO and the VCO are briefly described.

2.1 The anaerobic digester model. In this paper we use the structure of the model AM2 [9] that was validated precisely in the same up-flow fixed-bed pilot-scale anaerobic reactor considered in this paper. However, most of parameters were later updated in [8] and they were used in this work.

$$\begin{aligned}
\dot{S}_1 &= (S_1^{in} - S_1)D - k_1\mu_1(S_1)X_1 & q_c &= k_L a [CO_2 - K_H P_c] \\
\dot{S}_2 &= (S_2^{in} - S_2)D + k_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)X_2 & P_c &= \frac{f - \sqrt{f^2 - 4K_H P_T CO_2}}{2K_H} \\
\dot{C} &= D(C^{in} - C) - q_c + k_4\mu_1(S_1)X_1 + k_5\mu_2(S_2)X_2 & f &= CO_2 + K_H P_T + \frac{k_6}{k_L a} m_2(S_2)X_2 \\
\dot{Z} &= (Z^{in} - Z)D_1
\end{aligned} \tag{1}$$

In this model, S_1 (g/l), S_2 , Z and C (mmol/l) represent the concentrations of organic material measured as COD (which does not include volatile fatty acids), VFA, strong ions and total inorganic carbon, respectively, while X_1 and X_2 (g/l) are the concentrations of acidogenic and methanogenic bacteria respectively. In this paper biomass concentrations may be considered reasonably constants [8]. The superscript "*in*" is used to identify the influent concentration of each component while the dilution rate, D (d⁻¹), is defined as the ratio between the volumetric inlet flow rate and the digester volume. Parameters k_1 , k_2 , k_3 , k_4 , k_5 and k_6 are the respective yield coefficients. q_c (mmol/l-d) represents the CO₂ gas flow rate, $k_L a$ (d⁻¹) is the liquid-gas transfer coefficient, $CO_2 = C + S_2 - Z$ is the dissolved CO₂ concentration, and K_H (mmol/l-atm) is the Henry's constant. P_c and P_T (atm) are the CO₂ partial pressure and total pressure, respectively. The specific growth rates, $m_1(S_1)$ and $m_2(S_2)$ (d⁻¹) are the unknown specific growth rates described by Monod and Haldane-type functions, respectively.

2.2 The Classical Asymptotic observer. In this paper, a CAO was designed to estimate \hat{Z} and \hat{S}_1 from the measurements of the state variables S_2 , and C . Other measurements like D , C^{in} and Z^{in} were considered available as well. Thus, using the model (1) and following the methodology described in [10], this CAO is depicted by the following equations:

$$\begin{aligned}
\begin{bmatrix} \dot{\hat{w}}_1 \\ \dot{\hat{w}}_2 \end{bmatrix} &= \begin{bmatrix} -D\hat{w}_1 + \frac{k_1 k_3 k_7 (\hat{w}_2 - S_2 - C)}{k_2 k_5 + k_3 k_4} + S_1^{in} D + \frac{k_1 k_5 S_2^{in} D}{k_2 k_5 + k_3 k_4} + \frac{k_1 k_3 (C^{in} D + k_L a k_H P_c)}{k_2 k_5 + k_3 k_4} \\ -D\hat{w}_2 + Z^{in} D \end{bmatrix} \\
\begin{bmatrix} \hat{S}_1 \\ \hat{Z} \end{bmatrix} &= \begin{bmatrix} \hat{w}_1 - \frac{k_1 k_5}{k_2 k_5 + k_3 k_4} S_2 - \frac{k_1 k_3}{k_2 k_5 + k_3 k_4} C \\ \hat{w}_2 \end{bmatrix}
\end{aligned} \tag{2}$$

Notice that the CAO is also function of S_1^{in} , and S_2^{in} which are unknown and that are just the variables that, besides \hat{Z} and \hat{S}_1 we want to estimate. These variables, S_1^{in} , and S_2^{in} are actually recursively modified and estimated by the VCO as is described in the next subsection.

2.3 Virtually Controlled Observer. In this subsection we present the main approach used in this paper. Besides of S_2 and C , it is considered that the measurement of S_1 is also available. It will serve to be compared with his estimation by the CAO. As it can be seen in Fig. 1, the VCO (dotted line) consists of an asymptotic observer and an output feedback controller. Measurements of S_2 , C and D are fed both,

to the asymptotic observer and to the controller. The observer output variables are \hat{Z} and \hat{S} . The control variable is \hat{S} , which is feedback to the controller via the observation error, $e_0 = \hat{S} - S$. The estimation of \hat{S}^n , and \hat{S}_2^n is made in two steps. In the first step, \hat{S}_2^n is estimated using the nominal value of S_2^n which was $S_2^n = 6$ gCOD/l at $0 < t < 7$ and $12 < t < 14$ d, and $S_2^n = 12$ gCOD/l at $8 < t < 12$ d. Since the observer performance depends on the right value of the hypothetical influent substrate concentration, \hat{S}_2^n , then the goal of the controller is to lead the observation error asymptotically to zero, by manipulating \hat{S}_2^n . Once the absolute value of the observation error becomes less than an arbitrarily chosen value, within a reasonable time, it is considered that the estimated influent VFA concentration is approximately equal to the real one. Then, in the second step, following a similar procedure [7], \hat{S}^n is estimated by using \hat{S}_2^n , which was estimated in the first step. Notice that the bioreactor is in open-loop while the controller operates only upon the observer. The control laws were obtained by using the Lyapunov function $V = e_0^2$ and by demanding the observation error to have the stable dynamics $\dot{e}_0 = -k_c e_0$ resulting in the following equations:

$$\hat{S}_1^m = \frac{1}{D} \left[D\hat{w}_1 - \frac{k_1 k_3 k_7 (\hat{w}_2 - S_2 - C)}{k_2 k_5 + k_3 k_4} - \frac{k_1 k_5 S_2^m D}{k_2 k_5 + k_3 k_4} - \frac{k_1 k_3 (C^m D + k_L a k_H P_C)}{k_2 k_5 + k_3 k_4} \right] + \hat{S}_1 + \frac{k_1 k_3 \dot{S}_2}{k_2 k_5 + k_3 k_4} + \frac{k_1 k_3 \dot{C}}{k_2 k_5 + k_3 k_4} - k_c (\hat{S}_1 - S_1) \quad (3)$$

$$\hat{S}_2^m = \frac{(k_2 k_5 + k_3 k_4)}{D k_1 k_5} \left[D\hat{w}_1 - \frac{k_1 k_3 k_7 (\hat{w}_2 - S_2 - C)}{k_2 k_5 + k_3 k_4} - S_1^m D - \frac{k_1 k_3 (C^m D + k_L a k_H P_C)}{k_2 k_5 + k_3 k_4} \right] + \hat{S}_1 + \frac{k_1 k_5 \dot{S}_2}{k_2 k_5 + k_3 k_4} + \frac{k_1 k_3 \dot{C}}{k_2 k_5 + k_3 k_4} - k_c (\hat{S}_1 - S_1)$$

In equation (3), $k_c = 10 \text{ d}^{-1}$ was used as controller gain. The derivatives \dot{S}_2 and \dot{C} were calculated numerically using the filtered data with a 50 min (25 data) floating window.

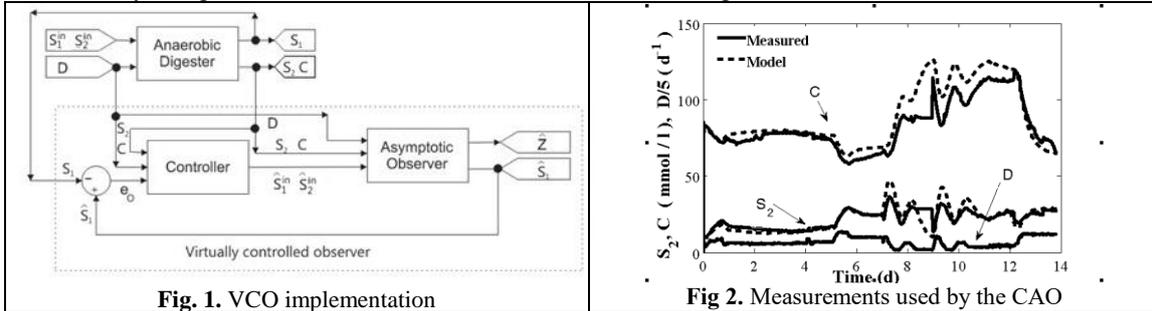


Fig. 1. VCO implementation

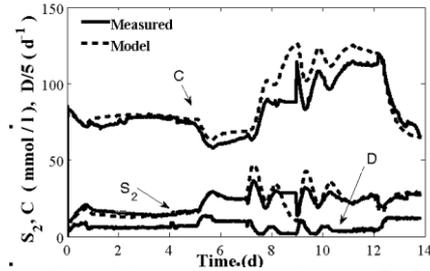
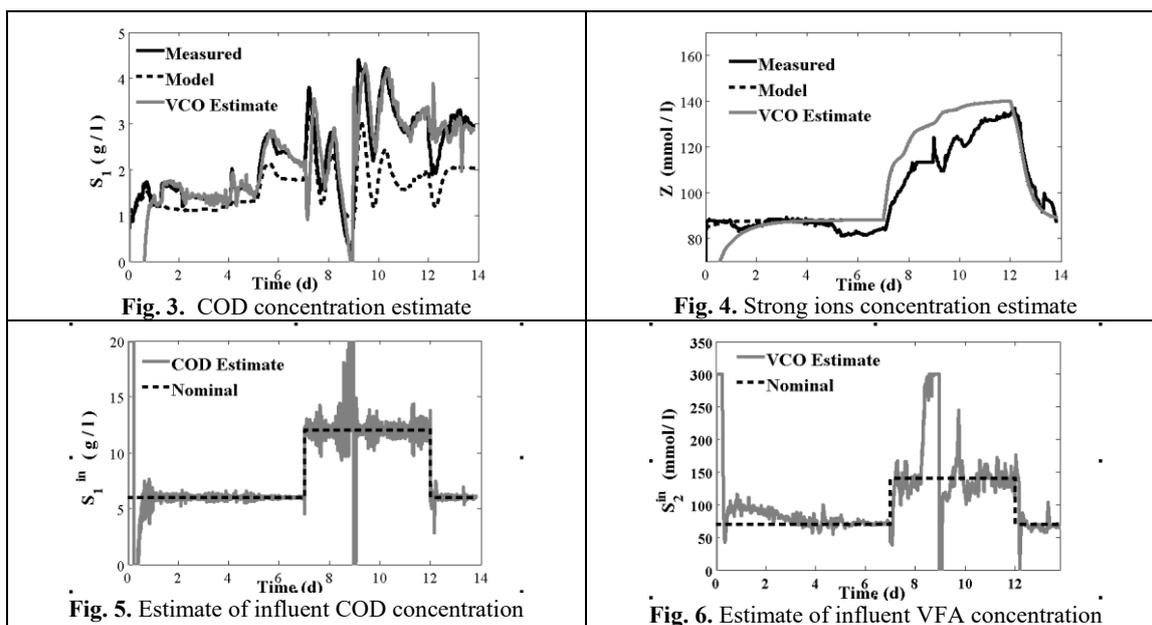


Fig 2. Measurements used by the CAO

3. Results and Discussion – Fig. 2 shows the measurements of D , S_2 and C . The predictions given by the model are shown also in this figure. Despite a small lack of accuracy at $8 < t < 12$ d, that was caused for a mismatch in sensors, we confirm that the model is reasonably acceptable. Once sensors were recalibrated, at time $t = 12$ d, the model recovered its good performance. Estimations of \hat{S} and \hat{Z} given by the CAO using these measurements are shown in Figures 3 and 4 respectively. As it is known this observer exhibits very good stability, convergence and performance properties, but it is not possible in general to tune its convergence time [10]. However, in our case, after a very short time (only 1 d), the CAO achieved a reasonable convergence and then their estimates could be used with certainty by the VCO. Only some small differences in the estimation of \hat{Z} at $8 < t < 12$ d, caused again for the small sensor faults in this time period, were observed. However, this does not affect significantly the performance of the VCO. Figures 5 and 6 show the estimation of \hat{S}^n and \hat{S}_2^n . From these figures it can be seen that the VCO showed a very good performance estimating influent concentrations with a reasonable accuracy, even in the presence of perturbations, noise, and a full lack of knowledge on process kinetics. The only mismatch was observed at $t = 8$ d, due to the fault sensor already mentioned, but even when this sensor mismatch lasted for 4 days, the VCO recovered its performance in only a half of this time period, showing its robustness against to a fully lack of kinetics knowledge, noise and sensor faults.



4. Conclusions - Results show that the VCO has an acceptable performance to reconstruct the influent substrate concentration under different operating conditions, in spite of the full ignorance of the process kinetics and sensor faults. Moreover, the use of the VCO induced an exponentially stable dynamic to the observer. Thus, the VCO is a viable and useful alternative to estimate the influent composition in AD processes.

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