

Control and estimation of anaerobic digestion processes using hydrogen and volatile fatty acids measurements

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Abstract: The anaerobic digestion technology is widely used in the treatment of waste and wastewater. To ensure the treatment efficiency and to increase the production of biogas, which can be reused as a renewable energy source, a good understanding of the process and tight control are needed. This paper presents an estimation and control scheme, which can be successfully used in the operation of the anaerobic digestion process. The process is simulated by ADM1 model, the most complex and detailed model developed so far to characterize anaerobic digestion. The controller and the observer, which provides estimates of the unmeasurable variables needed in the computation of the control law, are designed based on a simplified model developed in a previous work. Since it has been shown that hydrogen concentration is an accurate and fast indicator of process stability, it was chosen as controlled variable. Aside the hydrogen concentration, the only measurement employed by the proposed control structure is the volatile fatty acids concentration. Simulation results prove the effectiveness of the proposed control structure.

INTRODUCTION

Anaerobic digestion (AD) is an efficient technology to treat various types of waste and wastewater. Additionally, biogas is produced, which can be used as a renewable energy source. However, the process is very complex and needs expertise to be properly operated. Aside the numerous variables and the interaction between them, the difficulty in operating these systems is also caused by the lack of measurement of key variables. Among the measurements which can be taken from an AD process, the gaseous compounds are quite common. Experimental evidence and various studies reviewed by Giovannini et al. (2016) have shown that hydrogen is an accurate and fast indicator of process stability, particularly in the case of high strength influents characterized by well-defined sugars (Pauss & Guiot 1993). However, hydrogen concentration or outflow rate are less used in estimation and control schemes in comparison to volatile fatty acids concentration and methane outflow rate. Among the limited number of studies involving hydrogen, one may recall the results of Cord-Ruwisch et al. (1997) who observed that during normal operating conditions a linear relationship exists between the dissolved hydrogen partial pressure and the digester loading rate and that an increase in the hydrogen concentration above a certain threshold indicates the accumulation of volatile fatty acids. Based on these observations they implemented a control algorithm to keep the concentration of the dissolved hydrogen at the critical value, thus controlling the digester near its maximum sustainable loading capacity. Similarly, based on the relationship between

the steady state hydrogen concentration and the organic loading rate characterizing a pilot plant treating winery effluents, Rodriguez et al. (2006) propose a controller which computes the dilution rate driving the AD process to the desired set-point based on the hydrogen concentration and methane outflow rate. Dochain et al. (1991) develop a nonlinear adaptive controller for the hydrogen concentration regulation in an AD model without employing analytical expressions for the reaction kinetics, while Ryhiner et al. (1993) implement classical PI and PID controllers tuned in simulation to successfully control (experimentally and in simulation) pH, dissolved hydrogen and organic acids in an AD process treating whey wastewater.

A wealth of control and estimation techniques have been applied to AD processes, which generally employ organic substrate and/or volatile fatty acids and methane outflow rate as measurements. Some of these control structures are developed and validated on simplified models, others employ simplified models in the development phase but are validated on complex models such as ADM1 or on pilot plants. The soft sensors (observers) are developed either for monitoring or control purposes and the techniques employed range from the classical Kalman filters to the modern sliding mode observers. Kalchev et al. (2011) developed a Kalman filter for a second order AD model to estimate the system states from the outflow rate of methane, which could facilitate the implementation of already proposed control algorithms. Haugen et al. (2014) implemented an unscented Kalman filter that uses only the measurement of the methane outflow rate and evaluated in simulation various control strategies and control objectives. A successful application of predictive control on a pilot plant is also presented. Employing the same AD model and measurement, Rocha-Cózatl et al. (2015) implemented an extended Kalman filter, which in addition to the system states provides also estimates of the unknown inlet substrate concentration, and propose a continuous-discrete unknown input observer for improved accuracy. García-Diéguez et al. (2011) propose a multi-objective cascade control based on volatile fatty acids concentration and methane outflow rate, which is first validated on ADM1 and subsequently on an AD reactor treating wastewater containing ethanol. Petre et al. (2013) develop an asymptotic observer, an interval observer, parameter estimation schemes and linearizing control laws and combine these techniques into adaptive and robust-adaptive control strategies for an AD model. A robust control scheme is also proposed by Méndez-Acosta et al. (2010), who develop a multi-input multi-output feedback loop that includes an extended Luenberger observer to control the volatile fatty acids concentration and total alkalinity. Montiel-Escobar et al. (2012) introduce a robust interval observer which reconstructs, within guaranteed lower and upper bounds, the key variables of ADM1 from a minimum number of measurements, while Gaida et al. (2012) use pattern recognition methods to predict the state of ADM1 from online measurements such as biogas production, methane and carbon dioxide content in the biogas, pH value and substrate feed volume of known substrates. The maximization of methane production is achieved in Lara-Cisneros et al. (2015) by extremum-seeking based on sliding mode control in conjunction with an observer which estimates unknown terms related to the growth kinetics and the inlet composition, while Kil et al. (2017) propose a nonlinear predictive controller to control the methane production in an AD process simulated by ADM1, methodology based on a reduced process model whose parameters are estimated online.

This paper presents a control loop which controls the hydrogen produced by an AD process treating winery wastewater at imposed set-point values using the principles presented by Dochain et al. (1991). Low levels of hydrogen imply increased process

stability and high biogas production. Except of the hydrogen measurement, the proposed loop employs also the measurement of volatile fatty acids for estimating the unmeasurable variables needed by the controller. Measurements of volatile fatty acids can be obtained by titrimetry, Fourier Transformed Infra-Red spectroscopy (Steyer et al, 2002), headspace gas chromatography (Boe et al, 2007). The estimations are provided by a second-order sliding mode observer, characterized by finite time convergence and robustness. Simulation results are provided, which demonstrate the effectiveness of the control structure. Note that although the control and estimation algorithms are designed based on a simplified process model, the process is emulated here by the complex ADM1 (Batstone et al, 2002).

CONTROL STRUCTURE DESIGN

The proposed control structure is illustrated in Figure 1. The controlled variable is the hydrogen concentration, while the manipulated variable is the dilution rate. The control aim is to make the hydrogen concentration H_2 follow the reference value (set-point) H_2^* in spite of the disturbances acting on the system, which may arise from unmodelled dynamics, simplifying assumptions and measurement noise. The set-point values are imposed by the plant operator (the control design is independent of the precise value or the variations of the set-point). Since high values of the hydrogen concentration are associated to process destabilization and imply also a low methane production, the reference is usually set at reasonably low values. The only measurements required by the control loop are the hydrogen concentration in gas phase and the volatile fatty acids (VFA) concentration. The working principle is quite simple: the observer estimates a non-measurable variable ϕ , which is a scaled image of the methanisation rate, from the VFA concentration S_2 and the controller computes a new value for the dilution rate based on the control error and the estimated ϕ . Both observer and controller are designed based on a reduced order model of the full process (ADM1), which is further simplified.

Subsequently, each component of the control loop is briefly described.

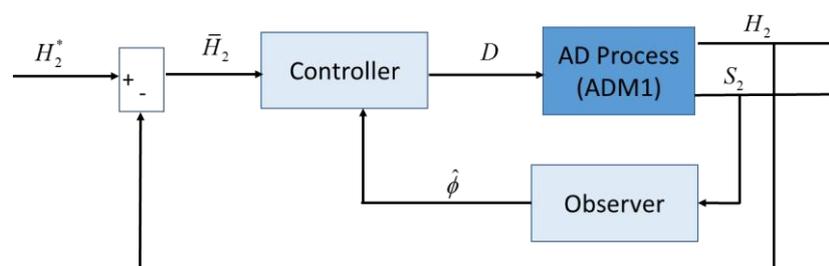
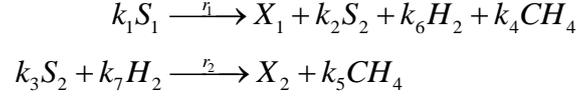


Figure 1. Layout of the control structure.

The simplified model

The model employed in the design of the control law has been developed by Giovannini et al. (2018), who built a simplified two step model of the complex ADM1 using model reduction techniques. The model structure has been also calibrated and validated with experimental data from an anaerobic digestion process treating winery wastewater.

The model implements the commonly used reaction scheme (acidogenesis and methanogenesis)



where the concentrations of acidogenic microorganisms X_1 , methanogenic microorganisms X_2 , organic substrate S_1 , volatile fatty acids S_2 , methane in the gas phase CH_4 and hydrogen in the gas phase H_2 are respectively given by

$$\frac{dX_1}{dt} = \mu_1 X_1 - \alpha D X_1 \quad (1) \quad \frac{dS_2}{dt} = D(S_{2in} - S_2) + k_2 \mu_1 X_1 - k_3 \mu_2 X_2 \quad (4)$$

$$\frac{dX_2}{dt} = \mu_2 X_2 - \alpha D X_2 \quad (2) \quad \frac{dCH_4}{dt} = -D \cdot CH_4 + k_4 \mu_1 X_1 + k_5 \mu_2 X_2 \quad (5)$$

$$\frac{dS_1}{dt} = D(S_{1in} - S_1) - k_1 \mu_1 X_1 \quad (3) \quad \frac{dH_2}{dt} = -D \cdot H_2 + k_6 \mu_1 X_1 - k_7 \mu_2 X_2 \quad (6)$$

The reaction rates are $r_1 = \mu_1 X_1$ and $r_2 = \mu_2 X_2$. The growth functions μ_1, μ_2 assume Monod kinetics $\left(\frac{\mu_{m1,2} S_{1,2}}{K_{S1,2} + S_{1,2}} \right)$. D is the dilution rate (the ratio between the inlet flow rate and the liquid volume) and represents the manipulated input used to control the process. α is the microorganisms retention factor and $k_i, i=1..7$ are the stoichiometric parameters. The numerical values of the model parameters are given in Table 1.

Table 1. Numerical values of model parameters.

Name	Value	Name	Value	Name	Value	Name	Value
α	0.5	K_{S1}	0.608 kg/m ³	k_2	7.526	k_5	3.308
μ_{m1}	3.585 d ⁻¹	K_{S2}	0.445 kg/m ³	k_3	11.167	k_6	5.14e-04
μ_{m2}	0.478 d ⁻¹	k_1	9.792	k_4	6.811	k_7	6.4e-04

The reduced model includes also expressions for the methane and hydrogen outflow rates, but they are not detailed in the sequel since they are not used in the control design or performance evaluation.

The matching between the states of the reduced order model and those of ADM1 (in the implementation and notations of Rosen & Jeppsson, 2006) is as follows:

$$X_1 = X_{su} + X_{aa} + X_{fa}, \quad X_2 = X_{ac} + X_{H_2} + X_{c4} + X_{pro}$$

$$S_1 = S_{su} + S_{aa} + S_{fa} + X_c + X_{ch} + X_{pr} + X_{li}, \quad S_2 = S_{va} + S_{ac} + S_{bu} + S_{pro}$$

$$CH_4 = S_{gasCH_4}, \quad H_2 = S_{gasH_2}$$

while the influent concentrations are the ones reported in (Giovannini et al., 2018).

Controller design

The model based controller presented here belongs to the class of adaptive linearizing controllers introduced in Bastin & Dochain (1990). More specifically, we adjust here the algorithm proposed by Dochain et al. (1991) for an anaerobic digestion model, which includes hydrogen dynamics, to fit the structure of the model (1)-(6). In the development of the control algorithm it is assumed that the first step in the bioconversion, the acidogenesis, is much faster than the subsequent steps, such that the system operates in a quasi-steady state, where the supply rate of substrate approximately equals the utilization rate of substrate. Mathematically this can be shown using the singular perturbation method (Dochain et al. 1991; Stamatelatos et al. 2009) but it will not be detailed here. The quasi-steady state approximation reads

$$DS_{in} = k_1 \mu_1 X_1 \quad (7)$$

and it is further used as a replacement of the differential equation (3) in the control law development.

Using (7) in the dynamics of the controlled variable (6), leads to

$$\frac{dH_2}{dt} = -D \cdot H_2 + KDS_{in} + \theta(t)\mu_2 X_2 \quad (8)$$

where $K = \frac{k_6}{k_1}$. Note that in order to cope with the various uncertainties affecting the

control loop, such as unmodelled dynamics, measurement noise, uncertainties of the kinetic and stoichiometric parameters, the measurement equation has been slightly modified. The time-varying parameter $\theta(t)$ replaces the stoichiometric coefficient $-k_7$ multiplying the reaction rate $\mu_2 X_2$ in (6). Hence, $\theta(t)$ describes the combined effect of all uncertainties occurring in the system and it is continuously adapted based on the control error variation.

Denoting by H_2^* the imposed reference for the hydrogen concentration and by $\bar{H}_2 = H_2^* - H_2$ the control error, a first-order linear closed loop dynamics is imposed

$$\frac{d\bar{H}_2}{dt} + C_1 \bar{H}_2 = 0 \quad (9)$$

where $C_1 > 0$ is a tuning parameter. Using (8) in (9) the control law is computed as

$$D = \frac{\frac{dH_2^*}{dt} - \theta(t)\mu_2 X_2 + C_1 (H_2^* - H_2)}{KS_{in} - H_2} \quad (10)$$

and the parameter $\theta(t)$ is adapted by

$$\frac{d\theta}{dt} = -C_2 \mu_2 X_2 (H_2^* - H_2) \quad (11)$$

where $C_2 > 0$ is a second tuning parameter.

Note that aside the measurement of the controlled variable H_2 the implementation of the control law (10) and of the adaptation rule (11) requires the knowledge of the

reaction rate $r_2 = \mu_2 X_2$, which cannot be measured in practice. Therefore an observer is designed for estimating this unmeasurable variable.

Observer design

The observer design relies on the principles introduced by De Batista et al. (2012) and uses the approach described by Sbarciog et al. (2014) to estimate the image ϕ of the reaction rate $r_2 = \mu_2 X_2$ from the measurement of the volatile fatty acids S_2 . The observer belongs to the class of second order sliding mode observers and ensures finite time convergence and robustness. In the observer development, the assumption of fast acidogenesis (7) is used to rewrite the dynamics of S_2 as

$$\frac{dS_2}{dt} = f(S_2, t) + \phi(t) \cdot S_2 \quad (12)$$

where $f(S_2, t) = D(S_{2in} + K_1 S_{1in} - S_2)$, $\phi(t) = -k_3 \frac{\mu_2 X_2}{S_2}$, $K_1 = \frac{k_2}{k_1}$. The proposed observer for (12) is

$$\dot{z}_1 = \left(\frac{f(S_2, t)}{S_2} + \rho z_2 + 2\rho b |\sigma|^{1/2} \text{sign}(\sigma) \right) z_1 \quad (13) \quad \sigma = \frac{1}{\rho} \ln \left(\frac{S_2}{z_1} \right) \quad (15)$$

$$\dot{z}_2 = a \cdot \text{sign}(\sigma) \quad (14) \quad \hat{\phi} = \rho \cdot z_2 \quad (16)$$

where z_1 is the estimate of the measurement S_2 and $\hat{\phi}(t)$ is the estimate of $\phi(t)$, σ is an image of the estimation error and ρ , a and b are the observer parameters. The control law and the adaptation rule become now

$$D = \frac{\frac{dH_2^*}{dt} - \theta \cdot \hat{\phi} \cdot S_2 / (-k_3) + C_1 (H_2^* - H_2)}{KS_{1in} - H_2} \quad (17),$$

$$\frac{d\theta}{dt} = -C_2 \cdot \hat{\phi} \cdot S_2 / (-k_3) (H_2^* - H_2) \quad (18)$$

SIMULATION RESULTS & DISCUSSION

The process (ADM1) and the estimation, control and adaptation algorithms are implemented in Matlab. Figure 2 presents the open loop response of the process and the reduced model for stepwise variations in the dilution rate. Some of the process states are better approximated by the reduced model than the others, but overall the model reproduces accurately the process dynamics and may be successfully used in the design of control policies. A visual inspection of the dynamics of VFA concentration S_2 and hydrogen concentration H_2 provides the confirmation for the

claim that hydrogen is a faster indicator of process destabilization: for changes in the dilution rate which lead to accumulation of VFA, the hydrogen concentration reaches the steady state at least few times faster than VFA concentration, which after 50d still increases slowly. The open loop response also shows that the assumption of fast acidogenesis and the quasi-steady state approximation employed in the observer and controller developments are fully entitled: the organic substrate concentration S_1 and the acidogenic microorganisms concentration X_1 exhibit faster dynamics, which seems instantaneous in comparison to the dynamics of the other states.

Figure 3 shows the observer validation with data generated by the model (1)-(6). Although these results may seem somehow artificial as the goal is to control the real AD process (simulated here by ADM1), this validation is useful for the observer tuning. A poorly tuned observer deteriorates (in the best case scenario) the performance of the control loop. Since the model predicts quite well the process dynamics, we may assume that the reaction rate is also well represented. The observer parameters are set to $\rho=1.2$, $a=1$, $b=1.5$ and measurements are collected with a sampling period $T_s=0.15$ d. The initial state of the observer is chosen as $[z_1(0) \ z_2(0)]'=[1.5S_2(0) \ 0]'$, the estimate of $S_2(0)$ is 50% higher, while for the estimate of ϕ it is assumed that no information is available. In spite of the uncertain initial condition, the observer converges very fast and tracks the changes in the volatile fatty acids concentration without errors. The non-measurable variable $\phi(t)$ is also fast and accurately estimated.

Figure 4 shows the control results for three imposed reference values. To reproduce the real—life situations, the measurements used in the control and estimation algorithms are corrupted by zero-mean white noise. For an easily readable scale, the controlled variable and the set-point are represented in ppm (parts per million). An effective control of hydrogen concentration is obtained, in spite of modelling errors, simplifying assumptions and measurement noise.

The controller can be easily implemented and tuned. The controller parameters (set here to $C_1=0.4$, $C_2=80$) are similar to the parameters of a standard PI-controller (see expressions (17) and (18)): increasing C_1 will decrease faster the control error, while increasing C_2 will make faster the control error equal to zero. Note that the implementation of the proposed control structure does not require any information on the reaction kinetics (which may be completely unknown) and some of the stoichiometric parameters. Only three parameters are needed: k_6/k_1 (the ratio between H_2 production yield and S_1 consumption yield), k_2/k_1 (the ratio between S_2 production yield and S_1 consumption yield) and k_3 (S_2 consumption yield).

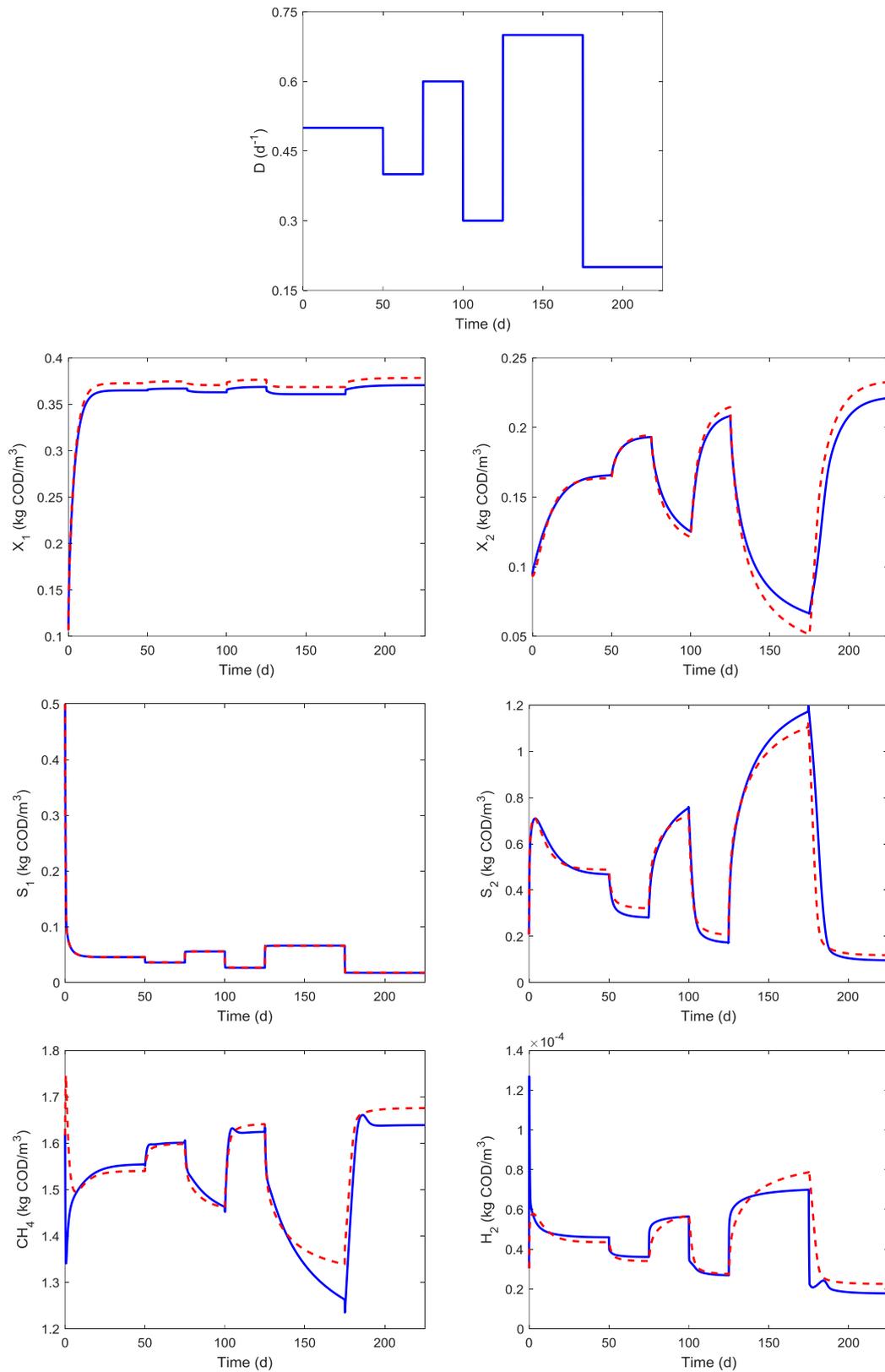


Figure 2. Open loop response of the process (ADM1) – continuous line and reduced model (1)-(6) – dashed line to variations in the dilution rate.

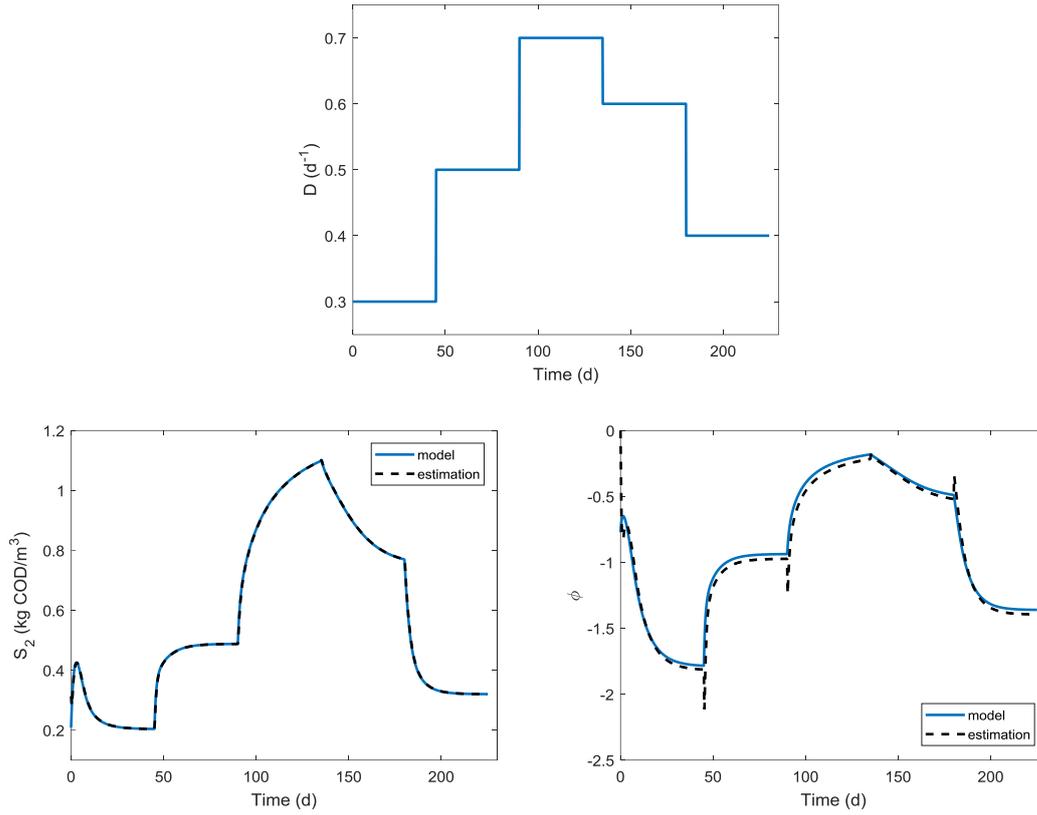
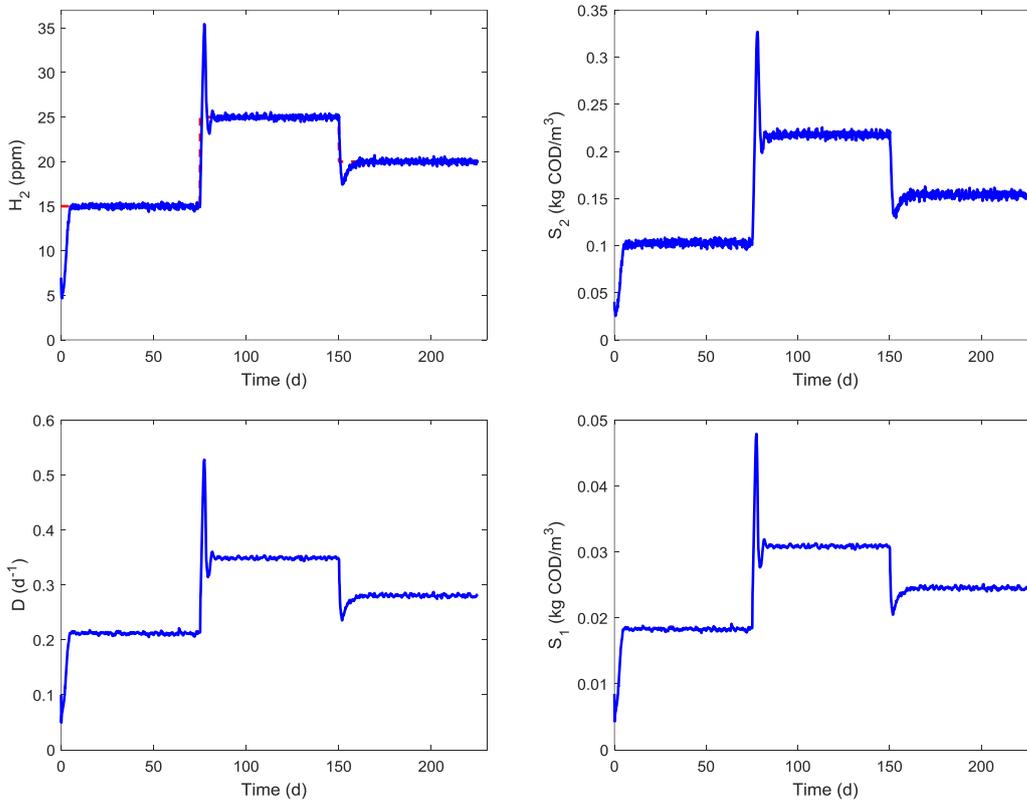


Figure 3. Open loop validation of the observer: model (1)-(6) response – continuous line, estimations provided by the observer – dashed line.



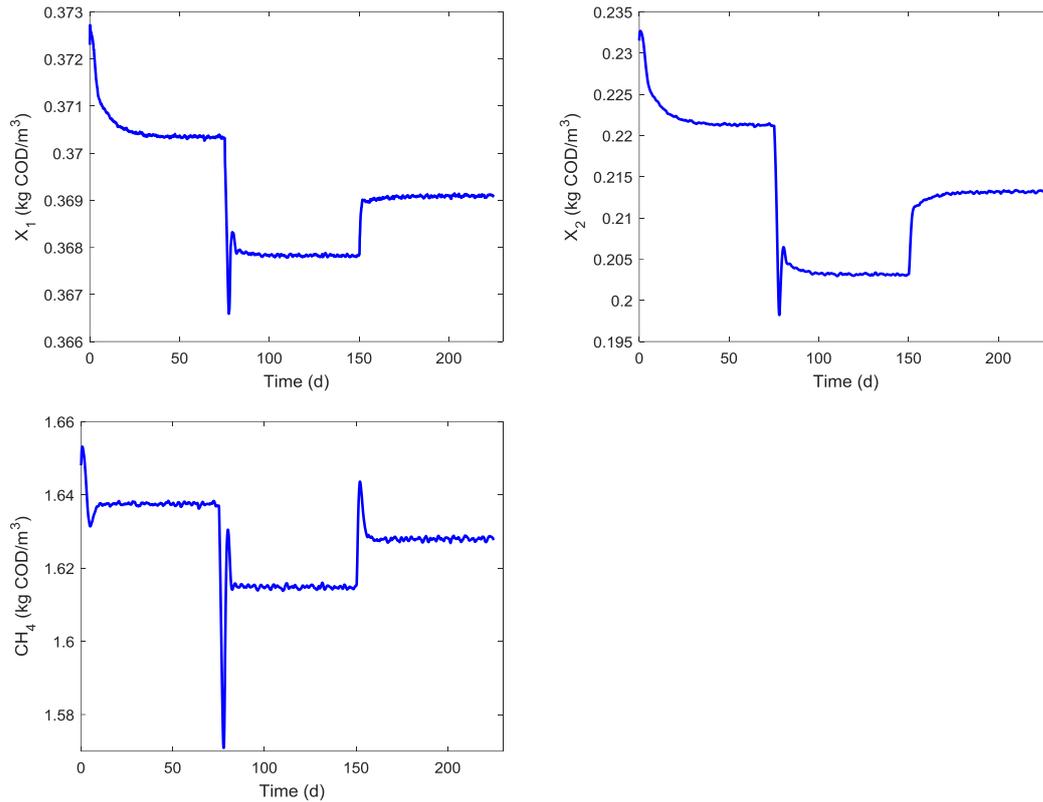


Figure 4. Closed loop process response: controlled variable H_2 - continuous line and imposed set-point – dashed line; S_2 measurement employed in the estimation algorithm; dilution rate computed by the controller; process states S_1 , X_1 , X_2 , CH_4 .

CONCLUSIONS

A control loop was presented in this paper to control the hydrogen concentration in an AD process, simulated here by ADM1. The hydrogen concentration was chosen as control variable based on the observation that for certain types of wastewater it is a faster indicator of process destabilization than the volatile fatty acids concentration. Additionally, hydrogen concentration measurements can be easily obtained in practice. The control loop consists of an adaptive control algorithm and a sliding mode observer, which are particularly suited for control and estimation of bioprocesses. Developed based on a reduced order model which was further simplified, the control loop is effective in achieving the control objective and robust with respect to modeling errors and measurement noise.

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