Derivation of a reduced-order model for anaerobic digestion control

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Abstract

A simple model for anaerobic digestion (AD) is developed using data from the ADM1 model as our virtual plant. The reduction methodology consists in a systematic data driven-approach, which uses principal component analysis to deduce the dimension of the minimal reaction subspace explaining the data, followed by an identification of the kinetic parameters in the least-squares sense. The reduced-model includes variables widely available in waste treatment plants. Particularly, it contains hydrogen which has been found to be an important intermediate during AD and a key variable for process monitoring and control. The suitability of the model for control purposes is tested using two different hydrogen-based control strategies.

Keywords

Model reduction, parameter estimation, process control

INTRODUCTION

Anaerobic Digestion (AD) is an environmentally sustainable technology to treat waste (water) by biological means. Despite its numerous advantages, AD is still not used at its full potential, due to the high complexity of the process and its dependence on many operational variables. Moreover, under certain circumstances the stability of the AD process can be disturbed. Therefore, an important step towards an optimal operation and control is a better understanding of the interplay between the process dynamics and the operational conditions, which may be achieved by means of a reliable model. One of the most detailed and well-accepted description of the process is provided by ADM1 model (Batstone et al., 2002). However, from a control and optimization viewpoint, ADM1 is too complex. The present work presents a step-by-step methodology to derive a simplified dynamic model. The resulting mathematical model is envisioned as a good basis for an advanced (model-based) monitoring and control approach of the process. To date, most of the control strategies are based on COD, VFA and/or methane and only a few hydrogen-based control strategies have been proposed. In this study, two representative works, e.g., Rodriguez et al. (2006) and Dochain et al. (1991), are exploited to test our dynamic model and its consistency with respect to ADM1.

MODEL DERIVATION

ADM1 is used to generate synthetic data which are used to infer a low-dimensional dynamic model involving the main variables of interest. The model development method consists of 6 steps: (1) selection of the model variables and data collection, (2) determination of the minimum number of reactions and pseudo-stoichiometric matrix using principal component analysis, (3) model definition, (4) kinetic parameters identification and re-estimation of stoichiometric parameters, (5) sensitivity analyses for further model simplification and (6) model validation.

Model variable selection and data collection

ADM1 model is used as a plant emulator to generate virtual data. The advantage of using a simulator (over a real plant) is that informative data can be easily generated in various situations. This is a favorable situation to develop a reduced-order model that can capture the main process dynamics. Simulations are performed considering a 1 m³ reactor operating in continuous mode and treating mainly soluble waste matter with 50% biomass retention. Two data sets are built, one for parameter identification which runs over a period of 120 days, and another one for cross-validation over 170 days, both with a sampling time of 3.6 hours.

Six state variables of our reduced model, namely X₁, X₂, S₁, S₂, CH₄, H₂, are sampled from ADM1, and for the sake of realism are corrupted with independent, normally-distributed, additive white noises, with standard deviation of 1% of the error-free values for biogases and 5% for the rest of the variables.

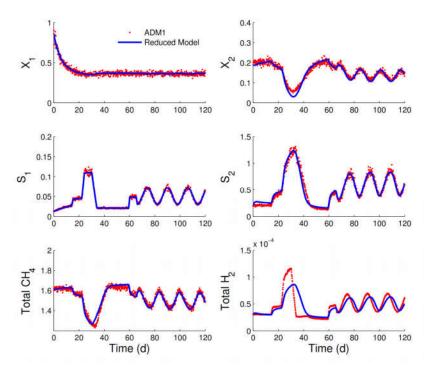


Figure 1: Model direct validation (red: ADM1 prediction; blue: reduced-order model prediction)

Reaction number, pseudo-stoichiometric matrix estimation and model definition

The minimum number of reactions and stoichiometric matrix are obtained using the Maximum Likelihood Principal Component Analysis (MLPCA) as described by Mailier et al. (2013). MLPCA is a systematic, optimization-based, model reduction procedure, which takes into account the noise corrupting the data. Test shows that a two-reaction scheme would be sufficient to represent the given data set. The following reaction scheme is obtained:

$$\begin{aligned} k_1 S_1 & \xrightarrow{r_1} X_1 + k_3 S_2 + k_7 H_2 + k_5 C H_4 \\ k_4 S_2 + k_8 H_2 & \xrightarrow{r_2} X_2 + k_6 C H_4 + k_2 S_1 \end{aligned}$$

Parameter identification and model validation

Identification of the kinetic parameters and re-identification of the stoichiometric parameters is performed using the maximum likelihood method, which consists in minimizing the prediction error between the experimental data and the model prediction (quadratic form in which the model deviation is weighted by the inverse of the covariance matrix of the measurement noise). Figure 1 shows direct

validation of the model, which is overall satisfactory, hydrogen being the component whose evolution is the most delicate to capture.

HYDROGEN-BASED CONTROLLERS

Two hydrogen-based controllers, which employ different principles are implemented and tested on the simplified model and ADM1, respectively. The first controller is developed based on experimental evidence; hence its development does not require the availability of the process model. The second controller is a linearizing feedback controller, which specifically employs the process model to develop the control law.

Heuristic-based controller

First, the control proposed by Rodriguez et al. (2006) is considered. One of the advantages of this control strategy is that it relies only on on-line sensors for the hydrogen concentration and methane flow rate, which are available on the market. The control described in Equation (1) is a proportional controller with variable gain, which uses the hydrogen concentration in the gas phase (ppmH₂) and the methane flow rate (Q_{CH4}) to determine the appropriate change in the inlet flow rate (D) to drive the process to the desired set-points.

$$\frac{dD}{dt} = DK f_{CH4} f_{H2} \tag{1}$$

In this expression, f_{CH4} and f_{H2} are described by Equations (2) and (3), respectively,

$$f_{CH_4} = \frac{\alpha Q_{CH4}^*}{Q_{CH4} + \alpha Q_{CH4}^*} \tag{2}$$

$$f_{H2} = \left(1 - \frac{ppmH_2}{ppmH_2^*}\right)^{1/m} \qquad \text{if } ppmH_2 \le ppmH_2^*$$
 (3)

$$f_{H2} = \left(\frac{ppmH_2^*}{ppmH_2}\right)^n - 1 \qquad \text{if } ppmH_2 > ppmH_2^*$$

 f_{CH4} is a decaying function of the methane flow rate Q_{CH4} . Hence, when a high methane productivity as defined by the parameter $Q_{CH_4}^*$, is achieved, this factor decreases to a low value, close to α (which is usually chosen around 0.1), dampening the control action. On the contrary, when this factor increases (when the production decreases), the controller becomes more agressive. On the other hand, the hydrogen factor f_{H2} is zero at the setpoint $ppmH_2^*$ and defines the direction of change in the dilution rate, correcting deviations from the hydrogen set-point with a reactivity depending on the shape parameters m and n.

Figure 2 shows a typical controller test. The hydrogen setpoint is well tracked but there are some discrepancies in the model prediction of the other variables, which highlight the limits of validity of the reduced-order model.

Model-based controller

The model-based controller belongs to the class of adaptive linearizing controllers introduced by (Bastin and Dochain, 1991). In this study, the algorithm proposed by (Dochain et al., 1991) is adapted to the structure of the developed model. More details on this implementation can be found in (Sbarciog et al., 2017).

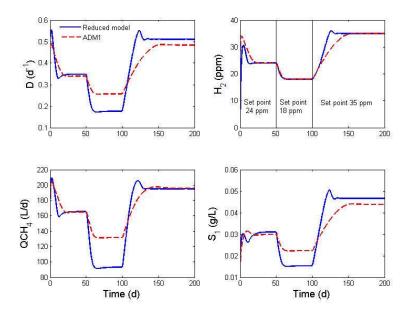


Figure 2. Heuristic controller and system responses with ADM1 (red dashed line) and reduced-order model (blue continuous line).

CONCLUSIONS

The reduced-order model derived from ADM1 predicts satisfactorily the dynamics of the state variables of interest, and can be exploited for model-based control.

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