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► **To cite this version:**

Younoussa Moussa Balde, Sihem Tebbani, Sette Diop, Cellou Kante. Modeling of a Continuous Anaerobic Digestion of Wastes. 24th International Conference on System Theory, Control and Computing (ICSTCC 2020), Oct 2020, Sinaia (virtual), Romania. pp.596-601, 10.1109/ICSTCC50638.2020.9259735 . hal-03034724

HAL Id: hal-03034724

<https://hal.science/hal-03034724>

Submitted on 1 Dec 2020

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Modelling of a Continuous Anaerobic Digestion of Wastes

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Abstract—Anaerobic digestion is widely used for waste treatment and the production of biogas. The automatization and optimization of the operation of the digester is still a challenging task. This study considers the first step in the design of the optimal continuous operation of an experimental anaerobic digester, namely its modeling. The well-known Anaerobic Digestion Model No.1 (ADM1) model is used, and its parameters identified from experimental data. Sensitivity analysis allows determining the more influential kinetic parameters of the model to be identified. The modeling procedure is assessed and its performance highlighted through the comparison between measured and predicted outputs.

Index Terms—Anaerobic digestion, biogas, modelling, identification, sensitivity analysis.

I. INTRODUCTION

Anaerobic digestion (AD) is a natural process of transforming organic matter into energy by bacteria in the absence of oxygen [1]. The digestion is conducted in confined chambers (called digesters) inside which the fermentation reactions are optimized and controlled. Biogas, mainly composed of methane, is produced while reducing by half the organic matter content of many biodegradable wastes or by-products. The residue from digestion (or digestate) is stable, deodorized, mostly free of pathogenic germs [1]. This kind of energy production, widely used and known for ages, presents a very promising solution for renewable energy production. It, however, raises some challenges linked to the operation of this kind of complex, uncertain systems [2], [3].

Indeed, anaerobic digestion is a multistage process in which a consortium of microorganisms acts upon composite organic matter to produce biogas (CH_4 , CO_2 , H_2 , and H_2S) [4]. The monitoring and control of an AD process, in order to maintain stable and optimal system operation, is a difficult task because of the complexity of the system and of the lack of online sensors for biological and biochemical variables. Mathematical modeling of the AD process is the first step in its automatization. The model will be used in a second step to develop

simulation models to test and assess estimation and control strategies [5], [6]. In this context, benchmark simulation models (BSMs) have been designed to develop, test, and evaluate local and/or plant wide wastewater treatment plant control and monitoring strategies, using dynamic models to realize good effluent quality at low operational cost [7]. Several models were proposed in the literature to model the AD process [8]–[10]. Among the models presented in the literature, the Anaerobic Digestion Model No.1 (ADM1), proposed in [9] is probably the most used one. ADM1 model has been tested in several applications such as municipal sewage sludge and solid waste, agricultural waste, livestock waste, and crop residues. ADM1 is a structured model, where physical, chemical, and biological processes are embedded in a kinetic biochemical matrix. A total of 19 biochemical processes are included such as disintegration, hydrolysis, acidogenesis, acetogenesis, and methanogenesis [9].

In this study, the ADM1 model is used to model an experimental AD system for cow dung. More specifically, the paper presents the ADM1 calibration and parameter identification for the studied experimental biodigester. The proposed procedure was developed as an analogy to aerobic respirometry used for the determination of influent COD fractions for activated sludge system models [11]. This procedure enables the simultaneous determination of some ADM1 input state variables and related hydrolysis kinetics [11].

In this paper, the kinetic parameters of the reactions of the decay, acetogenesis, and methanogenesis processes during anaerobic digestion are verified. Simulation results are then compared with some experimentally obtained data, namely biogas/methane production, chemical oxygen demand (COD) concentration, volatile fatty acid (acetate, propionate and valerate) concentration [12].

This paper represents the first step for the modeling, estimation and control of the studied experimental biodigester.

The paper is structured as follows. First, the process and

its modeling are presented in Section 1. Secondly, the identification procedure is detailed in Section 2. Experimental results are presented and discussed in Section 3. Finally, the conclusion and perspectives conclude the paper.

II. SYSTEM MODELING

A. Experimental setup

The simulation was carried out on the basis of data collected from an experimental biodigester built at the Superior Institute of Technology of Mamou (Guinea) (see Fig. 1).

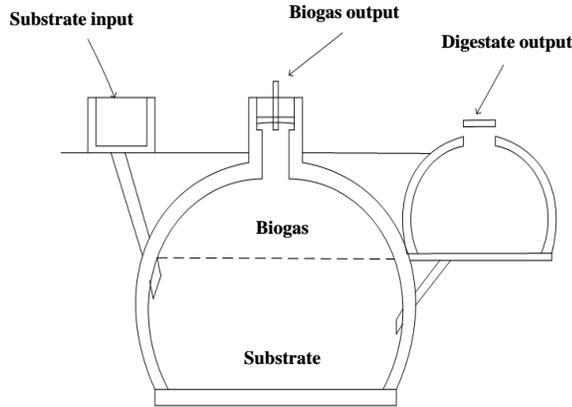


Fig. 1. Schematic representation of the studied anaerobic digester.

The bioreactor has a volume of 3 m^3 , operating under mesophilic conditions at 35°C . The liquid volume varies between 1.5 m^3 and 2 m^3 and the hydraulic retention time (HRT, or residence time) is about 45 days. It represents the duration that a soluble compound remains in bioreactor.

The digester is fed with 35 kg of raw material, cow dung in our study. The average inflow load is $0.34 \text{ kg}\cdot\text{m}^{-3}$. The average biogas production is about $2.1 \text{ N}\cdot\text{m}^3\cdot\text{d}^{-1}$ (d : day), and varies from a minimum of $0.73 \text{ N}\cdot\text{m}^3\cdot\text{d}^{-1}$ to a maximum of $2.49 \text{ N}\cdot\text{m}^3\cdot\text{d}^{-1}$.

The bioreactor is agitated everyday and the culture medium will be assumed to be homogeneous hereafter.

The characterization of the physical and biomechemical variables, namely dry matter (DM), organic matter (OM) and chemical oxygen demand (COD) are based on standard methods. Volatile fatty acids (VFA) were measured using a gas chromatograph.

Determination methods according to [13], [14], were used to characterize the substrate in terms of carbohydrates, proteins and fats [14].

The total biogas production was measured by the Itron/G4 GALLUS gas meter. The values of the biogas production were normalized. Biogas production, the distribution of the main biogas components (CH_4 and CO_2), temperature and pH were measured continuously throughout the experiment period.

The measurements of COD, VFA and biogas flow rate will be used hereafter for the model identification.

B. Mathematical modeling

The ADM1 model is a high-order nonlinear model widely used to model the anaerobic digestion.

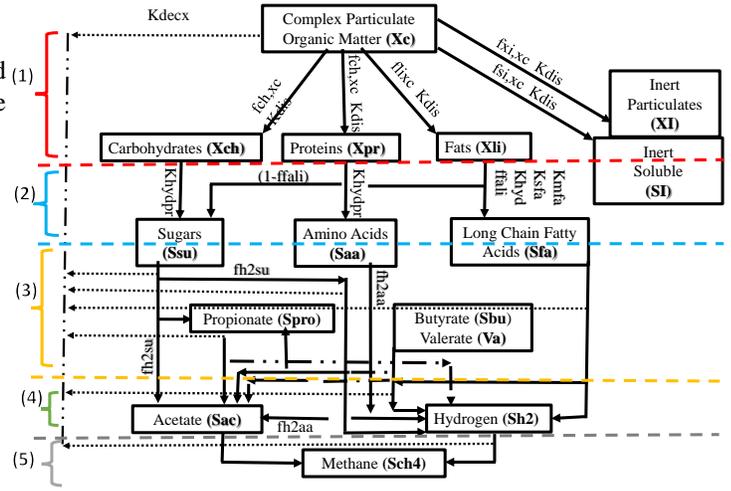


Fig. 2. Schematic representation of anaerobic digestion. (1) Desintegration, (2) Hydrolysis, (3) Acidogenesis, (4) Acetogenesis, (5) Methanogenesis.

In the ADM1 model, anaerobic digestion is divided into five basic processes, namely the desintegration, hydrolysis, acidogenesis, acetogenesis and methanogenesis (see Fig. 2).

All extracellular biochemical processes are assumed to be first-order type, while all intracellular reactions are Monod-type kinetics.

The influent chemical oxygen demand (COD) is split into 13 input state variables including 11 biodegradable COD fractions such as composite substrate, carbohydrates, proteins, lipids, sugars, amino acids, long chain fatty acids, butyrate, valerate, propionate and acetate. Inert COD of the influent is split into a soluble fraction and a particulate fraction [15]. Every substrate was considered as composed of fractions which degrade at different rates. Particulate fractions have by definition hydrolysis as limiting rate and therefore their rate of degradation was described by a first order hydrolysis kinetics [16].

In this study, a modified version of the ADM1 model as in [17] is considered. This modified version incorporates the concentration of particulate products arising from biomass decay in the state vector.

The ADM1 model is then described via a set of ordinary differential equations (ODE) and of algebraic differential equations (DAE). The ODE equations, about 35 equations, are derived from dynamics of state variable corresponding to a component in the liquid phase. It is determined from a mass balance consideration assuming a continuous well stirred-tank reactor. In [18], some ODE equation can be replaced by algebraic differential equations (DAE). The DAE equations concern 33 steady-state variables (substrates, reaction intermediates and gaseous products, i.e. methane, hydrogen, carbon

dioxide in the liquid and gaseous phase). The model includes 105 stoichiometric and kinetic parameters.

The MATLAB/SIMULINK software proposed by [9] and [18] was used as the simulation tool in this study.

III. MODEL CALIBRATION

A. Input flow-rate

First of all, the input flow rate of the waste, here cow dung, must be determined. The digester is operated in continuous mode (outlet flow-rate equals its inlet, leading to a constant cultivation volume). This flow rate must be sufficient to allow the growth of bacterial populations, but not too high to avoid growth inhibition by the substrate or a culture washout.

In this study, the inlet flow rate was determined experimentally, via the determination of the dilution rate (denoted D). The latter is defined as the inverse of the HRT. It can be also defined as:

$$D = \frac{Q_{in}}{V_{liq}} \quad (1)$$

Where Q_{in} is the feed-rate (in $\text{m}^3 \cdot \text{d}^{-1}$), V_{liq} is the volume of liquid (in m^3) and D is the dilution ratio (in d^{-1}).

For the determination of the appropriate value of the dilution rate for the identification procedure, several experiments were carried out (see Section IV). Anaerobic digestion experiments were performed for several values of dilution rate, over periods of 45 days.

B. Model parameters determination

From available experimental measurements of gas flow rate, VFA and DCO concentrations, model parameters are adjusted so that the experimental data are as close as possible to the predicted values with the ADM1 model. However, ADM1 model is a high-order nonlinear model, making the model calibration a difficult task. In this study, the model parameters were divided into two groups. The first group contains less influential parameters. Their value will be fixed from the literature. The second group of parameters represents the most influential model parameters on the system output. They will then be identified from the measured data. The model parameters to be identified are then determined by solving an optimization problem. The optimal value of parameters' values, Θ^* , minimizes the following cost function:

$$J = \|y - y_p\|_Q^2 \quad (2)$$

where y and y_p are measured and predicted data of gas flow rate, VFA, and DCO concentrations, respectively, the matrix Q is a normalization matrix. Bound constraints could be added to this optimization problem, e.g. to constrain each Θ component to be positive.

The determination of the influence of the parameters on the outputs were determined thanks to a sensitivity analysis.

In order to define which parameter can influence the most a defined variable, a sensitivity analysis of the outputs with respect to the parameters must be performed. Relative Sensitive Function (RSF) proposed in [19] is used. It is defined as:

$$\delta_{i,j} = \frac{P_i}{y_j(P_i)} \frac{y_i(P_i + \Delta P_i) - y_j(P_i)}{\Delta P_i} \quad (3)$$

where $\delta_{i,j}$ is the RSF between P_i and y_j , P_i the i^{th} parameter, $y_j(P_i)$ the j^{th} output, ΔP_i the variation on the parameter. A value up to 20% for ΔP_i is commonly used. In this study, the parameter variation, ΔP_i , is determined from the range of order of the parameter from the literature for similar application.

The value of RSF will help to determine the influence of parameter i^{th} on the j^{th} output [19]:

- RSF < 0.25: No influence, denoted "0"
- $0.2 \leq \text{RSF} < 1$: Sensitive, denoted "+"
- $1 \leq \text{RSF} < 2$: Very sensitive, denoted "++"
- RSF ≥ 2 : Extremely sensitive, denoted "+++"

For each parameter of the ADM1 model, the RSF value for all the outputs is calculated to determine the most influential parameters for each output.

It should be mentioned that one parameter can influence several state variables, just as it can be found that several parameters can influence the same state variable. Some adjustable parameters are shown in Fig. (2).

The influence of the parameters on the outputs also highly depends on the operating conditions. For example, in the case of inhibition conditions, parameters linked to the kinetics of inhibition are the most influential ones. On the contrary, if the system is operated far from inhibition conditions, these inhibition parameters have less influence on the outputs. It is then important to perform sensitivity analysis for operating conditions close to the optimal ones (since in our case the process will be operated later in the optimal conditions), or for several inputs to characterize the influence of parameters for several case studies.

However, the parameter identification of a biological model can be a difficult task, especially since there are few measured data. In this study, we choose to limit the identification to biochemical parameters only. The stoichiometric parameters will be either fixed to a value from the literature for similar AD processes, or to the default value of ADM1 model if their influence, for the considered inlet flow rate, is very small. In addition, the decay rates for all acetogens were increased to 0.04 d^{-1} in agreement with other research indicating decay rates higher than 0.02 d^{-1} [20]. In the next section, the results obtained by applying the proposed procedure are detailed and analyzed.

IV. EXPERIMENTAL RESULTS

A. Input flow-rate

The input flow rate was chosen with a piecewise constant evolution as illustrated by Fig. 3. The dilution rate of the substrate varies from a minimum of 0.2 d^{-1} to a maximum of 0.25 d^{-1} , with a progressive change in average of 0.02 d^{-1} .

TABLE I
DILUTION RATE VALUES.

Time	$D(d^{-1})$	Time	$D(d^{-1})$
0	0.252	22	0.216
2	0.252	23	0.253
3	0.186	34	0.253
8	0.186	35	0.223
9	0.238	39	0.223
15	0.238	40	0.200
16	0.216	45	0.200

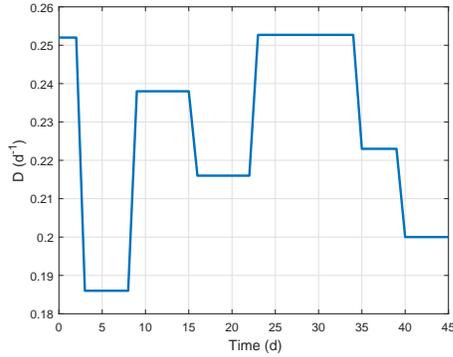


Fig. 3. Dilution rate evolution versus time.

V. EXPERIMENTAL BIOGAS PRODUCTION RESULTS

Figure (4) illustrates the measured gaz flow rate. It can be noticed that the transformation into gaseous compounds CO_2 and CH_4 of a defined quantity of the organic substrate occurs as follows: (i) over a period of 45 days, 50% of the total volume of the gas is produced in 10 days with a maximum between the 10th and 20th day, (ii) the process of anaerobic digestion continues from the 10th to the 45th day. This result is in agreement with the literature, which reports that the average time of anaerobic digestion varies between 10 and 15 days [21]. After 45 days of methanation in a temperature range of 27 to 35°C (mesophilic), in this experiment, a minimum biogas flow rate of 0.73 $Nm^3 \cdot d^{-1}$, a maximum flow rate of 2.49 $Nm^3 \cdot d^{-1}$, i.e. an average daily production of 2.05 $Nm^3 \cdot d^{-1}$. Future work will consider the optimization of this production by controlling the dilution rate profile.

Table (II) provides the results of the characterization of the physico-chemical parameters. The carbon-nitrogen ratio is about 21.4.

From these data, the initial values of the states is calculated from [20], [22], and [23]. The values of the states at initial time are given in Table III and Table IV. From all these data, the model simulation can be performed and its parameters are then identified.

A. Adjustment of model parameters

First, the classification of the model parameters according to their influence on the outputs is carried out as described in Section III-B.

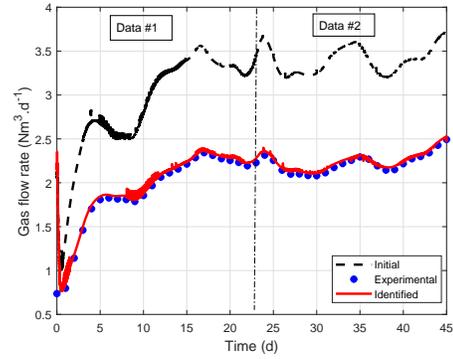


Fig. 4. Gas flow rate evolution versus time.

TABLE II
BIOGAS PRODUCTIVITY OF COW DUNG

Description	Unit	Cow dung
MS	(%)	57
MO	(%)	54
C	(%MS)	31
N	(%MS)	1.46
COD	($kgCOD \cdot m^{-3}$)	57.37
VFA	($kgCOD \cdot m^{-3}$)	2.035
pH	-	7.4
Ratio (C/N)	-	21.40

TABLE III
SOLUBLE COMPONENTS VALUES (^aESTIMATED FROM [23], ^bESTIMATED FROM [22]).

Description	Value	Unit
Monosacharides	5.00 ^a	$kgCOD \cdot m^{-3}$
Total valerate	0.125	$kgCOD \cdot m^{-3}$
Total butyrate	0.065	$kgCOD \cdot m^{-3}$
Total propionate	0.132	$kgCOD \cdot m^{-3}$
Total acetate	0.215	$kgCOD \cdot m^{-3}$
Carbohydrates	18 ^b	$kgCOD \cdot m^{-3}$
Proteins	31 ^b	$kgCOD \cdot m^{-3}$
Lipids	1.7 ^b	$kgCOD \cdot m^{-3}$
Particulate inerts	35.3 ^b	$kgCOD \cdot m^{-3}$

TABLE IV
DEGRADERS INITIAL VALUES (^aESTIMATED FROM [22]).

Description	Value	Unit
Acetate degraders	1.2 ^a	$kgCOD \cdot m^{-3}$
Hydrogen degraders	0.5 ^a	$kgCOD \cdot m^{-3}$
Sugar degraders	0.27 ^a	$kgCOD \cdot m^{-3}$
Amino acid degaders	0.78 ^a	$kgCOD \cdot m^{-3}$
LCFA degraders	0.15 ^a	$kgCOD \cdot m^{-3}$
Valerate and butyrate degaders	0.28 ^a	$kgCOD \cdot m^{-3}$
Propionate degraders	0.09 ^a	$kgCOD \cdot m^{-3}$

The sensitivity analysis is performed for the dilution profile described on Section V. The model parameters are in this case fixed either to values from literature or for values given by default in the ADM1 model. Some results of the sensitivity analysis are given in Table V. For example, it can be noticed that the composite substrate concentration, denoted X_c , is extremely sensitive to the change of the decay constant k_{dis} , whereas outputs COD concentration, VFA concentration, and gas flow rate are less sensitive to the change of this parameter (but are still sensitive). X_c , COD and VFA concentrations are not sensitive to the variation of the stoichiometric parameter $f_{xi,xc}$, on the contrary to gas flow rate which is very sensitive to this parameter. Parameter $f_{xi,xc}$ is the yield of desintegration of X_c into inerte soluble S_I (see Fig. 2). In general, X_c is obviously very sensitive to variation of $f_{xi,xc}$. However, for the range of the considered dilution rate, and in the operation conditions for which the sensitivity analysis was performed, it becomes less important than the other parameters. It is thus important to emphasize that the result of the sensitivity analysis depends on the considered operation conditions.

TABLE V
SENSITIVITY OF ADM1 MODEL PARAMETERS ON STATE VARIABLES

Parameters	X_c	COD	VFA	Gas flow
k_{dis}	+++	+	+	+
$f_{xi,xc}$	0	0	0	++
$f_{xi,xc}$	0	0	0	++
$k_{m,pr}$	0	0	+++	0
$k_{m,ac}$	0	+++	+++	+++

From the sensitivity analysis, 7 parameters among the 105 model parameters are found as the most influential parameters on the outputs. As mentioned previously, only the kinetic parameters are selected to be identified.

The parameters to be identified are: the decay constant (denoted k_{dis}), and the parameters describing the kinetics related to the absorption of butyrate, propionate and acetate. The three latter kinetics include limitation and inhibitory effects. Consequently, the parameters involved in these kinetics are the maximum absorption rate for butyrate (denoted $k_{m,c4}$), propionate (denoted $k_{m,pro}$), and acetate (denoted $k_{m,ac}$); the associated half-saturation coefficients (denoted $K_{S,c4}$, $K_{S,pro}$ and $K_{S,ac}$ respectively). The coefficients describing the inhibitory effects are not identified since the considered dilution profile does not lead the system to be operated in the inhibition conditions.

All the other parameters of the ADM1 model (excluding the 7 above mentioned ones) will be fixed to their values from literature and more specifically according to [9].

The 7 parameters k_{dis} , $k_{m,c4}$, $k_{m,pro}$, $k_{m,ac}$, $K_{S,c4}$, $K_{S,pro}$ and $K_{S,ac}$ are identified to obtain the best fit to the experimental data. The *fminsearch* function of the Optimization toolbox of Matlab is used. Other optimization algorithms were tested with similar results. The optimization algorithm was initialized with initial values from the default values of the parameters of the ADM1 model.

The measured data is split into two sets. First set, denoted Data #1, corresponding to the measured data from time=0 to time = 22 days, is used for the identification. Second set, denoted Data #2, from time=22 days to time = 45 days, is used for the model validation.

The adjusted parameters are shown in Table (VI). It can be noticed that for some parameters, the identified values are very close to their initial value (e.g. $K_{S,ac}$), whereas they can be very different (e.g. $K_{m,c4}$). However, all the obtained values are in accordance with the range of variation of these parameters reported in the literature.

TABLE VI
ADJUSTMENT OF THE MODEL PARAMETERS.

Parameter	Initial Value	Identified value
k_{dis}	0.5	0.21
$K_{m,c4}$	20	7.0
$K_{m,ac}$	8	6.289
$K_{m,pro}$	12	5.5
$K_{S,ac}$	0.15	0.137
$K_{S,c4}$	0.2	0.35
$K_{S,pro}$	0.1	0.392

B. Model validation

The predicted outputs with the identified parameters are illustrated by Fig. 4 to Fig. 6. These figures provide also the outputs with initial guess of the parameters values and the measured data. It is recalled that only data from the set Data #1 are used for identification, whereas data from the set Data #2 are used for validation. It can be noticed an agreement between predicted and measured data. Consequently, the obtained model seems to provide a good prediction of the system behavior.

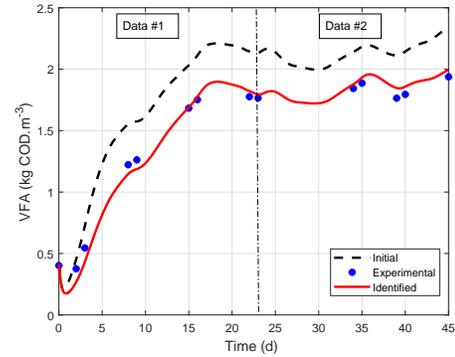


Fig. 5. VFA concentration evolution versus time.

CONCLUSION

In the present study, the ADM1 modeling of an experimental continuous bioreactor was considered. An identification procedure was proposed based on a sensitivity analysis of the outputs with respect to the parameter variations. Only 7 parameters among the 105 ADM1 model parameters were identified, whereas the other parameters were fixed to their

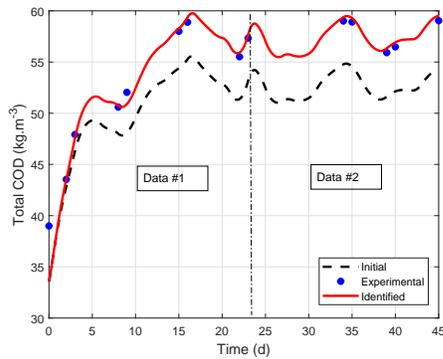


Fig. 6. COD concentration evolution versus time.

value from literature. Measured data of biogas production, VFA and COD concentrations were compared to the ones predicted by the obtained model, highlighting the performance of the obtained model. The ADM1 model is still a high-order complex model. Ongoing research concerns the development of a reduced model for the system as reported in the literature [10], [24]. The ADM1 model will be used as a reference model since real-life experiments are time demanding. Based on the reduced model, estimation and control strategies will be investigated, based on the gas flow rate, to monitor and control the biogas production so that the process operation is optimized.

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