Dynamic model adaptation to an anaerobic digestion reactor of a water resource recovery facility

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Abstract

This study deals with model adaptation of the AM2 model to an anaerobic digestion reactor of a water resource recovery facility, namely a 6000 m^3 reactor at VEAS WWRF, the largest of Norway. The model is based on the mass balance with six states including acidogens, methanoges, alkalinity, organic substrate, volatile fatty acid and inorganic carbon. The model adaptation is applied firstly to simulated reactor data for testing the algorithms, and then to experimental data. The experimental data are collected from laboratory analysis and online measurements from January to October 2017. The data of the first 100 days are used for model identification, and the remaining data for model validation. Identification analysis is based on the Fisher Information Matrix and the Hessian matrix. Also, a sensitivity analysis of the parameter estimates is accomplished.

Keywords: Anaerobic digestion, Fisher Information Matrix, identifiability analysis, mathematical model adaptation, sensitivity analysis, sloppiness, water resource recovery facility.

1. Introduction

Anaerobic digestion (AD) of wastewater is a biological process to produce biogas consisting of methane and carbon dioxide in the absence of oxygen. Mathematical models of the AD process can be useful for control system design and testing, controller tuning, model-based control, state and parameter estimation, optimization of reactor design and operation, analysis, training, etc.

Several mathematical models of the AD process exist. The Anaerobic Digestion Model Number 1 (ADM1) is a well-known model with five stages including disintegration, hydrolysis, acidogenesis, acetogenesis and methanogenesis Batstone et al. (2000). The ADM1 model has 35 state variables with around 100 model parameters, and it represents the gases methane (CH$_4$), carbon dioxide (CO$_2$) and hydrogen (H$_2$). The Hill model is a relatively simple model for representing the behaviour of a biogas reactor with four state variables from which CH$_4$ gas is calculated Hill and Barth (1977). In the present study, the Anaerobic Digestion Model number 2 (AM2) with six states and 13 model parameters is applied Bernard et al. (2001). The model is implemented in MATLAB.

Before using a model effectively, the values of unknown model parameters have to be estimated from experimental data. The main goal of this study is dynamic model adaptation to a simulated biogas reactor and also to experimental data from the VEAS. The model adaptation comprises estimation of the model parameters and model validation. Root Mean Square Error (RMSE) is used to evaluate both the model identification and the model validation. Identifiability analysis and sensitivity analysis are investigated. The identifiability analysis is based on calculating and
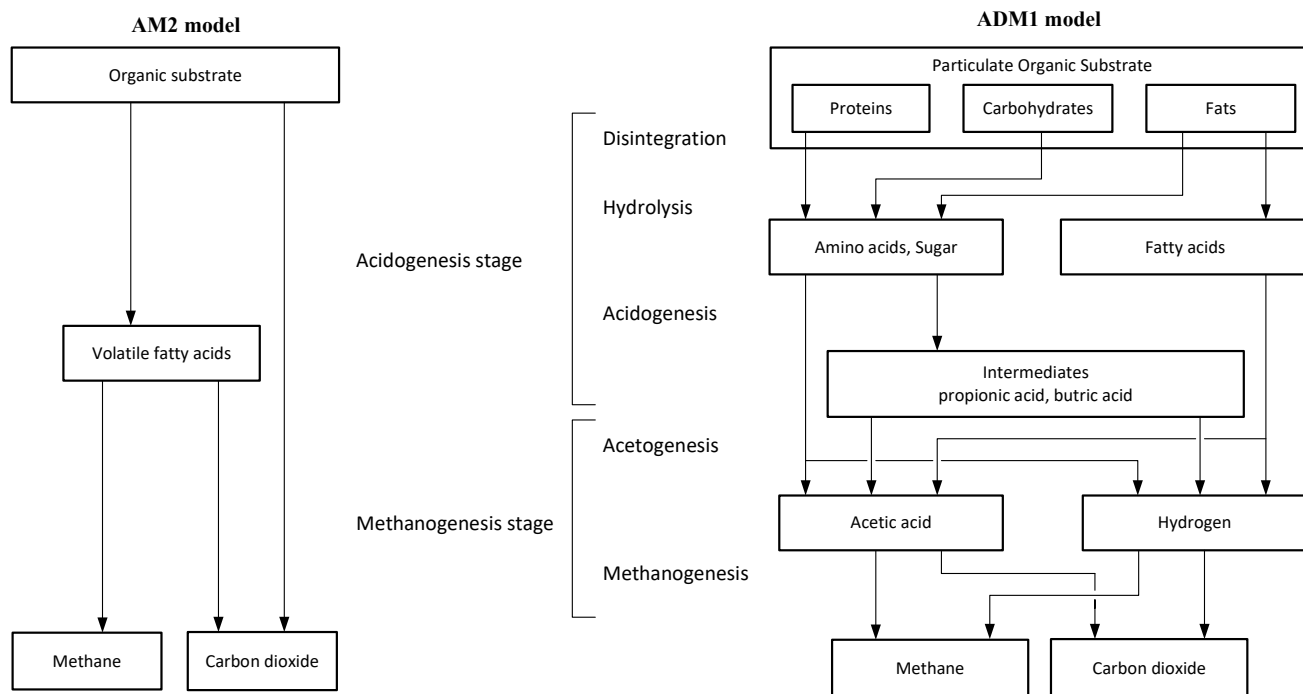
Figure 1: Comparison between ADM1 and AM2 models.

analyzing the Fisher Information Matrix (FIM). The convexity of the optimization problem of the model adaptation is analyzed with the Hessian matrix at the estimated model parameters Ljung and Chen (2013). The model identifiability is addressed also with a sensitivity analysis. The need for identifiability analysis can be stated as follows. When the measurement variables are not influenced by one or several model parameters, it is possible to have several different identified model parameter sets.

There exist several studies about the model adaptation to experimental data from different biogas reactors based on different models. A pilot anaerobic reactor fed with diary manure at Foss farm in Skien, Norway has been adapted to the Hill model Haugen et al. (2013). The AM2 model is used for production of biogas in the raw industrial wine distillery vinasses in a local winery at Narbonne, France Bernard et al. (2001). There are several studies using the ADM1 model for biogas reactors, such as olive mill solid waste Boubaker and Ridha (2008), lignocellulosic biomass Koch et al. (2010), and sewage sludge digestion for various water resource recovery facilities Shang et al. (2004, 2005).

The outline of the article is as follows. Section 2 in-

cludes a process description and the AM2 model equations. Section 3 explains about dynamic model adaptation of the AM2 model to a simulated biogas reactor. The parameters of the model are identified and the model will be evaluated based on the estimated model parameter. Also a practical identifiability analysis is described based on the Fisher Information Matrix (FIM) and the Hessian matrix. Then the model is validated on a wide range of the operating conditions covering 150 days. A sensitivity analysis for all model parameter estimation is presented. Dynamic model adaptation of the AM2 model to experimental data from the VEAS reactors will be discussed in Section 4. Discussion and Conclusions are given respectively in Section 5 and Section 6.

2. Process and model descriptions

2.1. Process description

The reactor at the VEAS plant has the form of a cylindrical tank. The diameter of the tank is 19 m, and the maximum volume of the tank is 6000 m^3. The reactor is equipped with a level sensor. The effective volume

can be calculated based on the height of the material inside the reactor which is measured by the level sensor. The reactor temperature is measured. The density of the sludge is assumed same as water density, 1000 kg/m^3.

The alkalinity ratio (AR), also denoted the FOS/TAC ratio[1], is the ratio between volatile fatty acid, VFA, and alkalinity, cf. (1).

$$AR = \frac{S_2}{Z} \qquad (1)$$

The AR expresses the reactor stability Lee et al. (2015). AR less than 0.3 indicates a stable AD process Drosg (2013).

An important parameter in AD processes is pH which is included in the AM2 model. The reactor temperature and pH have effects on the performance of AD processes Hajji et al. (2016)Jayaraj et al. (2014). Appropriate pH values for methane production in the mesophilic temperature range is investigated in Kheiredine et al. (2014).

2.2. Selection of a dynamical model

In this study, the AM2 model is selected because it is considerably simpler than the ADM1 model, while comprising the relevant parameters and variables. In Figure 1, the AM2 model is compared with the ADM1 model.

2.3. The original AM2 model

Figure 2 depicts an AD reactor with variables according to the AM2 model.

In the AM2 model, organic material is converted by microorganisms in two phases which are called acidogenesis and methanization. In the first phase, the acidogenic bacteria, X_1, consume the organic substrate, S_1, and produce CO_2 and volatile fatty acids, S_2. In the second phase, the population of methanogenic bacteria, X_2, uses the volatile fatty acids to produce CO_2 and methane. Z and C are the total alkalinity and total inorganic carbon, respectively. Mass balances give the following differential equations, which constitute a state space model of the AD reactor Bernard et al. (2001).

$$\frac{dX_1}{dt} = [\mu_1 - \alpha D] X_1 \qquad (2)$$

$$\frac{dX_2}{dt} = [\mu_2 - \alpha D] X_2 \qquad (3)$$

[1] Flchtige Organische Suren/Totales Anorganisches Carbonat (German)
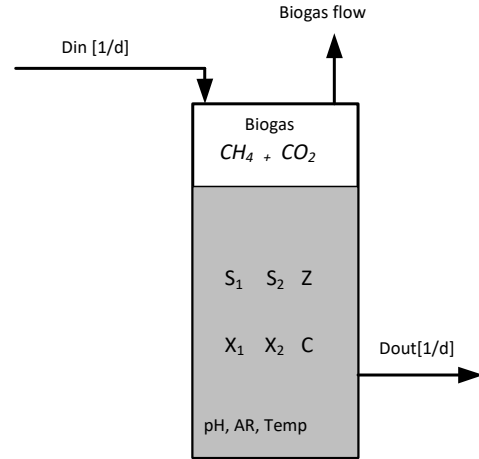

Figure 2: An anaerobic digestion reactor with variables according to the AM2 model.

$$\frac{dZ}{dt} = D(Z_{in} - Z) \qquad (4)$$

$$\frac{dS_1}{dt} = D(S_{1in} - S_1) - k_1 \mu_1 X_1 \qquad (5)$$

$$\frac{dS_2}{dt} = D(S_{2in} - S_2) + k_2 \mu_1 X_1 - k_3 \mu_2 X_2 \qquad (6)$$

$$\frac{dC}{dt} = D(C_{in} - C) - q_C + k_4 \mu_1 X_1 + k_5 \mu_2 X_2 \qquad (7)$$

where Z_{in}, S_{1in}, S_{2in}, C_{in} in (4)-(7) are, respectively, concentration of the inflow of alkalinity, substrate, VFA and dissolved inorganic carbon. D is the dilution rate, or normalized flow, defined in (8).

$$D = \frac{F}{V} \qquad (8)$$

F is flow rate and V is the effective volume of the reactor.

The flow of inorganic carbon from the liquid phase to the gas phase, q_C, is calculated accordance to Henry's law, cf. (9).

$$q_C = k_L a(C + S_2 - Z - K_H P_C) \qquad (9)$$

where $k_L a$ is liquid-gas transfer coefficient, K_H is Henry's constant, and P_C is CO_2 partial pressure. Methane flow is directly related to the methanogenic rate, μ_2, cf. (10).

$$q_M = k_6 \mu_2 X_2 \qquad (10)$$

The growth of acidogenic bacteria, μ_1, is based on Monod type kinetics and the growth of methanogenic

Table 1: Experimental data from VEAS

Data	Description	Lab. analysis	Measured	Unit
F	Inflow rate		$\checkmark$	L/s
TS_{in}	Inflow total solid	$\checkmark$		%
VS_{in}	Inflow volatile solid	$\checkmark$		%
T_{reac}	Reactor temperature		$\checkmark$	°C
q_m+q_c	Biogas production		$\checkmark$	m³/h
CH_4	Methane production		$\checkmark$	%
h	Height of the material inside the reactor		$\checkmark$	m
TS	Total solid	$\checkmark$		%
VS	Volatile solids	$\checkmark$		%
S_2	Volatile fatty acid	$\checkmark$		mmeq/L
Z	Alkalinity	$\checkmark$		mmeq/L
B	Bicarbonate	$\checkmark$		mmeq/L
pH	pH		$\checkmark$	-

bacteria, μ_2, is assumed based on Haldane type kinetics. The growth of bacteria depends on temperature and temperature change. Generally, an increase in temperature before reaching the optimum growth temperature will increase bacteria activity and the growth of bacteria. If temperatures get more than the optimum growth temperature, enzyme activity will decrease Eddy et al. (2003). The consensus is that temperature changes greater than 1°C/d affect process performance, thus temperature variations of less than 1°C/d are recommended. In general, the variables in the AM2 model are divided in three groups called state variables, environmental variables, and model parameters, respectively. The state variables and the environmental variables are shown in Figure 3. In this study, the model parameters are estimated based on observing input-output and some of state variables are measured.
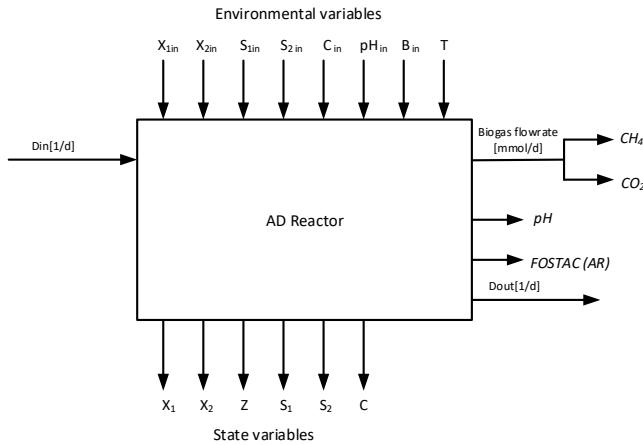

Figure 3: A block diagram of an AD reactor with the AM2 model requirements.

2.4. Modified AM2 model

It can be assumed that a part of the microorganisms continuously die during the process. In this study, we propose to enhance the AM2 model with death rates of acidoges and methanoges microbes, k_{d1}, k_{d2}, both with values of 0.2 d⁻¹, as in the AMD1 model Batstone et al. (2000). Thus, (2) and (3) are modified to become (4) and (5), respectively.

$$\frac{dX_1}{dt} = [\mu_1 - k_{d1} - \alpha D]X_1 \qquad (11)$$

$$\frac{dX_2}{dt} = [\mu_2 - k_{d2} - \alpha D]X_2 \qquad (12)$$

In the VEAS reactor, the inflow and outflow rates may be different, implying a variation of the level and hence the volume of the materials in the reactors varies. Consequently, (4)-(7) are modified to become (13)-(16).

$$\frac{dZ}{dt} = D_{in}Z_{in} - D_{out}Z \qquad (13)$$

$$\frac{dS_1}{dt} = D_{in}S_{1in} - D_{out}S_1 - k_1\mu_1 X_1 \qquad (14)$$

$$\frac{dS_2}{dt} = D_{in}S_{2in} - D_{out}S_2 + k_2\mu_1 X_1 - k_3\mu_2 X_2 \qquad (15)$$

$$\frac{dC}{dt} = D_{in}C_{in} - D_{out}C - q_C + k_4\mu_1 X_1 + k_5\mu_2 X_2 \qquad (16)$$

Temperature has effect on reaction rates but is not considered in the original AM2 model. The temperature dependency of the reaction rates may be based on the van't Hoff-Arrhenius model Eddy et al. (2003) or

on the Hashimoto model Hashimoto et al. (1995). We assume here the Hashimoto model, as it is based on a study of the behaviour of a large number of real reactors. The Hashimoto model was proven to represent very well the temperature-dependency of AD reactor dynamics in Haugen et al. (2013).

The Hashimoto model implies that the temperature dependency of the maximum reaction rates is modelled as in (17).

$$\mu_{\max}(T_{\mathrm{reac}}) = c_H\, T_{reac} - \mu_0 \qquad (17)$$

for temperatures between 20°C and 60°C. c_H is the Hashimoto's factor. μ_0 is a constant value. We assume that $\mu_{i_{\max}}$ in 35°C will be identified as a model parameter. Thus, the temperature dependency is applied based on (18) for enhancement of the original AM2 model.

$$\mu_{i_{\max}}(T_{\mathrm{reac}}) = c_H.(T_{\mathrm{reac}} - 35) + \mu_{i_{\max}}(35) \qquad (18)$$

The modified AM2 model is the original AM2 model with aforementioned modifications.

2.5. Experimental data

Experimental data are collected daily from laboratory analysis and from sensors installed on the pertinent VEAS reactor for the period of 1st of January to 10th of October 2017. The list of the collected data is mentioned in Table 1.

3. Model adaptation to a simulated biogas reactor

Model adaptation is applied to a simulated model, where of course the true parameter values are known, as a necessary check of the selected parameter estimation algorithm.

The model adaptation consists of two parts: (1) Parameter estimation, and (2) model validation where the reliability of the model is validated with data not used in the estimation Stare et al. (2006). Simulated data over the first 100 days are used for estimation, and data over 150 days for model validation.

15 model parameters are estimated, of which 13 model parameters are in the original AM2 model while the remaining two are one parameter of Hashimoto's formula, (18), and Z_{dis}, which is a parameter to represent uncertainty in the influent alkalinity, cf. (19).

$$\frac{\mathrm{d}Z}{\mathrm{dt}} = D_{\mathrm{in}}(Z_{\mathrm{in}} + Z_{\mathrm{dis}}) - D_{\mathrm{out}}Z \qquad (19)$$

3.1. Estimation method

3.1.1. Selection of a criterion

The parameter estimates are those minimizing the quadratic criterion in (20).

$$\mathrm{J}(\theta) = \sum_{i=1}^{N} [Y_{p,i}(\theta) - Y_{r,i}]^T Q[Y_{p,i}(\theta) - Y_{r,i}] \qquad (20)$$

where $Y_{r,i}$ is the simulated "real" data vector, and $Y_{p,i}(\theta)$ is the prediction vector with respect to the model parameters vector, θ, at the same instants t_i. In this study, Y is the so-called measurement vector defined by (21).

$$Y = [\ CH_4 \quad CO_2 \quad pH \quad S_2 \quad Z\ ]^T \qquad (21)$$

Q is a weight matrix defined by (22).

$$Q = W^{-1} \qquad (22)$$

where W is the inverse of the measurement error covariance matrix, (23).

$$\mathrm{W} = \begin{bmatrix} w_{CH_4} & 0 & 0 & 0 & 0 \\ 0 & w_{CO_2} & 0 & 0 & 0 \\ 0 & 0 & w_{pH} & 0 & 0 \\ 0 & 0 & 0 & w_z & 0 \\ 0 & 0 & 0 & 0 & w_{S_2} \end{bmatrix} \qquad (23)$$

where

$$w_{\mathrm{y}} = \frac{1}{n}\sum_{i=1}^{n}(y - \bar{y})^2 \qquad (24)$$

$\bar{y}$ is the mean of measurement values for n samples which is a proper subset of the original data.

3.1.2. Computational solution of the optimization problem

We use the *fmincon* NLP solver in MATLAB to minimize the criterion (20). In general, *fmincon* solves the optimization problem of (25).

$$\min_{\theta} J(\theta) \text{ subject to}: A\theta \leq B,\ A_{eq}\theta = B_{eq}$$
$$\mathrm{LB} \leq \theta \leq \mathrm{UB} \qquad (25)$$

In the present parameter estimation problem, neither the inequality constraints nor the equality constraints are included. Thus, A, B, A_{eq} and B_{eq} are empty matrices. LB and UB are chosen respectively 10 time smaller and larger than the model parameters in Bernard's work Bernard et al. (2001).

3.1.3. Assumptions

We do not have measurement data of the inflow inorganic carbon. However, it is assumed that C equals to 0.0058 mol/L in a reactor fed with waste waster Bergland and Bakke (2016). The initial relation between

Table 2: The initial state in the AM2 model

Parameter	Description	Unit	Value
$X_{1_{\text{init}}}$	Concentration of acidogenic bacteria	g/L	0.06
$X_{2_{\text{init}}}$	Concentration of methanogenic bacteria	g/L	0.22
Z_{init}	Total alkalinity	mmol/L	194
$S_{1_{\text{init}}}$	Organic substrate concentration	g/L	17.78
$S_{2_{\text{init}}}$	Volatile fatty acid concentration	mmol/L	16
C_{init}	Total inorganic carbon concentration	mmol/L	194.29

acidogens and methanoges bacteria is assumed as in Haugen et al. (2013):

$$X_1 = 3.4 X_2 \tag{26}$$

Note that during the simulation, X_1 and X_2 evolve individually and according to their material balances.

The assumed initial states are shown in Table 2.

Figure 4 shows the real inputs used as inputs to the simulation.

Analysis of the feed sludge taken at representative conditions shows $S_{2_{in}} = 82$ mmol/L, $Z_{in} = 72$ mmol/L, and $pH_{in} = 6.37$. It is supposed that concentrations of VFA and alkalinity and pH in the feed sludge are constant during the simulation.

One of the parameters to be estimated is the alkalinity offset, Z_{dis}, cf.19. Since Z_{in} is not measured during the preparing the data and also to satisfy the alkalinity ratio threshold, Z_{dis} must be estimated to have a reasonable and stable process.

We assume that the simulated AM2 model has model parameters as shown in Table 3. The initial model parameter values are according to Bernard et al. (2001).

3.2. Results of the parameter estimation

We decided to use simulated data over 100 days for the parameter estimation. The time-step of 0.1 d. The results of the parameter estimation are shown in Table 3. The table shows the results for noise-free measurements and for noisy measurements where a uniformly
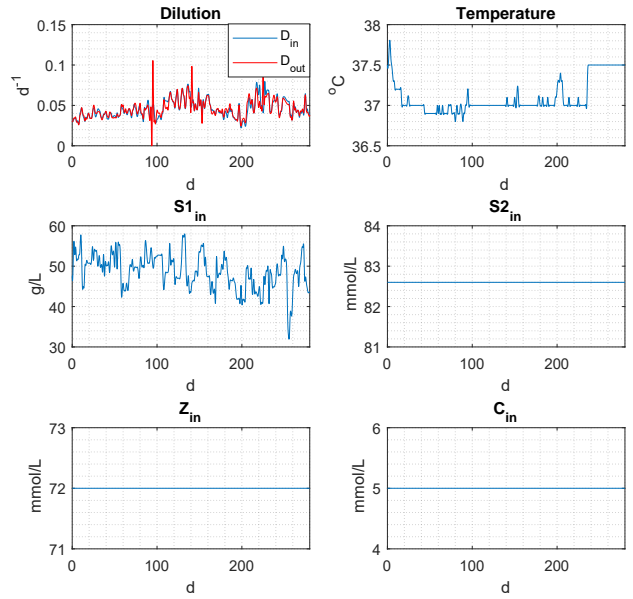

Figure 4: Real inputs used as inputs to the simulation

distributed random noise is added to the noise-free simulated measurement. The noise was set to have amplitude $\pm 0.5\%$ of the mean values of the parameter values. For the noise-free case, the parameter estimates are virtually equal to the parameter values used in the simulator, indicating that the parameter estimation procedure outlined in Section 3.1 works satisfactorily. There are however parameter offsets in the case of noisy simulated measurements, which is to be expected.

3.2.1. Evaluation of impact of measurement noise

Root-Mean-Square Error, RMSE, is a useful criterion to evaluate the relative quality of a parameter estimation procedure Muroi and Adachi (2015). RMSE is defined in (27).

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{N} \left[y_{p,i}\left(\hat{\theta}\right) - y_{r,i} \right]^2}{N}} \tag{27}$$

where $y_{p,i}\left(\hat{\theta}\right)$ is model-predicted measurement and $y_{r,i}$ is assumed real (but here: simulated) measurement sample number i. Here, we use RMSE to evaluate the impact of assumed measurement noise on the parameter estimation. Table 4 shows RMSE for five simulated measurements. It indicates small differences between the simulated methane and carbon dioxide gas flows. Therefore, both biogas productions resemble quite well with the measured methane and carbon dioxide gas flows. RMSE for pH, S_2 and Z are also small with acceptable differences.

Table 3: Model parameter values for simulation model, initial states and estimated values with and without added simulated measurement noise

Model Parameters	Initial values[*]	Simulated model	Estimated values noise-free	Estimated values 1% noise	Unit
k_1	42.14	100	100	102.06	-
k_2	116.5	280	280	287.68	mmol/g
k_3	268	300	300	316.62	mmol/g
k_4	50.6	415	415	424.17	mmol/g
k_5	343.6	385	385	404.34	mmol/g
k_6	453	500	500	525.67	mmol/g
α	0.5	0.8	0.8	0.73	-
$\mu_{1_{max}}$	1.2	1	1	0.89	d^{-1}
$\mu_{2_{max}}$	0.74	0.8	0.8	0.77	d^{-1}
K_{S_1}	7.1	5	5	5.09	g/L
K_{S_2}	9.28	60	59.99	68.37	mmol/L
K_{I_2}	256	350	350.27	92.68	mmol/L
$k_L a$	19.8	8.2	8.2	8.21	d^{-1}
c_H	0.013	0.013	0.013	0.053	-
Z_{dis}	100	100	100	100.16	mmol/L

[*]The initial values of the model parameters are based on Bernard et al. (2001).

Table 4: Evaluation of the parameter identification based on RMSE

Simulated meas.	RMSE noise-free	RMSE 1% noise	Unit
CH_4	1.59×10^{-5}	6.76×10^{-2}	mmol/L/d
CO_2	4.6×10^{-6}	3.34×10^{-2}	mmol/L/d
pH	6.9×10^{-8}	5.93×10^{-4}	-
Z	1.9×10^{-6}	1.26×10^{-1}	mmol/L
S_2	6.1×10^{-4}	3.05×10^{-2}	mmol/L

Table 5: The RMSE index for noise-free and noisy measurements

Simulated meas.	Mean value	Maximum value	Maximum difference	Unit
CH_4	15.384	20.34	0.489	mmol/L/d
CO_2	13.972	18.050	0.407	mmol/L/d
pH	7.463	7.552	0.003	-
Z	176.730	190.250	0.174	mmol/L
S_2	5.015	5.986	0.361	mmol/L

The mean and maximum of the measurement values are calculated based on the identification data set (150 days). The maximum difference between the estimated data and the simulated one in the identification period are mentioned in Table 5. Comparison between the maximum differences and the mean of the measurements indicates that the model error is acceptable.

3.2.2. Identifiability analysis

3.2.2.1. Structural and practical identifiability

Identifiability analysis is used to assess whether the selected parameter estimation method will work. Two methods of identifiability analysis are presented in the following.

Structural identifiability

Structural identifiability, so-called theoretical identifiability, depends on the model and it is a property of model structure Zhang et al. (2010). The structural identifiability is based on a mathematical approach to show the correlations among the parameters for noiseless data under ideal conditions. For correlated parameters, a change in one parameter can be compensated

by a change in another parameter, and the model fitness remain still satisfied. Therefore, structural identifiability is not sufficient to determine if the model parameters can be estimated uniquely for poor data Saccomani (2013).

Since there are 15 model parameters in the modified AM2 model to identify and 5 measurement values, algebraically evaluating the structural identifiability of the parameters is complicated. Also, since the goal of this study is model adaptation to practical data it is possible that parameters which are structurally identifiable are practically unidentifiable. Consequently, we do not focus on the structural identifiability in this study.

Practical identifiability

Practical identifiability depends on experimental condition and quality and the quantity of the measurement variables Petersen et al. (2001). The practical identifiability is a numerical method to determine whether it is possible to achieve a unique estimated parameter set from the available data Dochain (2013). The effect of a small deviation in each model parameter will be monitored to check the output sensitivity. In fact, the practical identifiability of model parameters is based on the output sensitivity function. The Fisher Information Matrix (FIM), and the Hessian matrix are used for this purpose. They are presented in the following subsections.

3.2.2.2. Identifiability analysis with Fisher Information Matrix

FIM is based on the sensitivity function, $\frac{\partial y}{\partial \theta}$, and the measurement accuracy, cf. (28).

$$\text{FIM} = \sum_{i=1}^{N} \left[\frac{\partial y_i}{\partial \theta}\right]^T Q \left[\frac{\partial y_i}{\partial \theta}\right] \qquad (28)$$

where Q is the weight matrix. The size of the FIM is $p \times p$, where p is the number of the estimated parameters. FIM provides information about estimation accuracy. Practical identifiability analysis is a numerical approach which is performed by calculating the FIM locally at the estimated parameters. If the determinant of the FIM becomes zero, some sensitivity functions are linear combination of each other. Thus, the unique parameter values cannot be obtained from the measurement data. The parameters are practically identifiable when the determinant of FIM becomes non-zero Li et al. (2018) or, in other terms, the FIM rank becomes full and equals the model parameter number Komorowski et al. (2011)Petersen et al. (2001).

Quality of identifiability analysis

It is necessary to check the quality of identifiability to be certain about reliability of the estimated parameters.

One way to examine the quality of identifiability is investigation on convexity of the model at the estimated parameters based on condition number of the FIM. The condition number of the FIM shows whether the parameter estimation is in well-condition or ill-condition.

Another way is investigation on sloppiness of model based on distribution of the eigenvalues of the FIM. Investigation on the eigenvalues of the FIM is useful to determine if the model is a so-called sloppy model. The concept of sloppiness was introduced in Brown and Sethna (2003) when the model output is not sensitive to changes in some of the model parameters which are called sloppy parameters. Meanwhile, stiff parameters are the model parameters that the model output is sensitive on their changes. If there is a clear gap between the eigenvalues of the FIM of model, it means there are some sloppy model parameters. The large eigenvalues are corresponding to stiff parameter and the small eigenvalues are corresponding to sloppy parameters. The existence of sloppy parameters causes the case that it is impossible to identify all model parameters uniquely Villaverde (2019). In fact, the small eigenvalues indicate that there are combinations among some model parameters.

Identifiability analysis for the case study

We compute numerically the FIM at the estimated model parameters with one percent changes. The determinant of the FIM becomes non-zero, so the FIM is full-rank matrix. The quality of identifiability analysis based in the convexity of the model at the estimated parameter set can be checked by computing the condition number of the FIM at this point. The identifiability of model parameters depends on the condition number of the FIM Cintrón-Arias et al. (2009).

$$\text{cond}(\text{FIM}) = \frac{\lambda_{\max}(\text{FIM})}{\lambda_{\min}(\text{FIM})} \qquad (29)$$

The amount of the condition number of the FIM becomes 2.75×10^{12} which presents an ill-condition.

The eigenvalues of the FIM are as follows:

$$\lambda(\text{FIM}) = \left[\begin{array}{cccc} 7.5 \times 10^8 & 2.45 \times 10^8 & 5.7 \times 10^7 & ... \end{array}\right.$$
$$\left. \begin{array}{ccc} 15.975 & 1.198 & 0.0003 \end{array}\right]$$

It shows there are sloppy parameters for AM2 model in respect of the collected measurements. Consequently, there are some unidentifiable model parameters.

The FIM has another outcome which is computing the standard deviation of the estimated parameters. The square root of the diagonal elements on the inverse matrix of the FIM is the standard deviation of the parameter estimation, SD in Table 6.

Table 6: The estimated model parameters with their standard deviations

parameter	Estimated value	SD*	Target value
k_1	102.06	0.22	100
k_2	287.68	0.003	280
k_3	316.62	1.131	300
k_4	424.17	0.005	415
k_5	404.34	0.001	385
k_6	525.67	0.001	500
α	0.73	0.002	0.8
$\mu_{1_{\max}}$	0.89	0.003	1
$\mu_{2_{\max}}$	0.77	0.011	0.8
K_{S_1}	5.09	0.018	5
K_{S_2}	68.37	0.84	60
K_{I_2}	92.68	52.14	350
$k_L a$	8.21	0.021	8.2
c_H	0.053	0.0007	0.013
Z_{dis}	100.16	0.02	100

* SD: Standard Deviation.

3.2.2.3. Identifiability analysis with Hessian matrix

The Hessian (matrix), H, of a function describes the local curvature or convexity or positive definiteness of a function. If all eigenvalues of the Hessian are positive, the function is convex. The larger eigenvalues of the Hessian, the stronger convexity. When the *fmincon* function is used for parameter estimation, the Hessian returned by the function expresses the identifiability of the parameters Rothenberg et al. (1971). A weak local identifiability occurs when eigenvalues of the Hessian matrix are positive but close to zero Little et al. (2010).

For our parameter estimation problem using simulated measurements, all of the eigenvalues of the Hessian are positive indicating identifiability of the parameters. However, the Hessian condition number, which is the ratio of the highest eigenvalue to the lowest eigenvalue Strang et al. (1993), indicates the degree of identifiability. The condition number is calculated. Its high value of 1.8425×10^{12} expresses that the parameter estimation problem is ill-conditioned, and hence, the degree of identifiability is low.

3.3. Model validation method

Since the quality of the parameter estimation depends on the amount and quality of the measurement data during the identification procedure, the performance of the model with the estimated model parameter should be evaluated in a wide range Dochain and Vanrolleghem (2001). The model validation is to determine if the model is good enough for the presenting the be-

Table 7: The evaluation on the validation based on RMSE for the simulated model

Simulated meas.	Mean value	Max. value	Max. diff.	RMSE 1% noise	Unit
CH_4	17.22	27.02	0.424	4.22×10^{-2}	mmol/L/d
CO_2	14.48	25.79	0.462	2.19×10^{-2}	mmol/L/d
pH	7.46	7.56	0.005	9.25×10^{-4}	–
Z	171.8	177.60	0.123	1.63×10^{-1}	mmol/L
S_2	4.66	7.88	0.448	9.56×10^{-2}	mmol/L

haviour of a biogas process Guidi (2008). Based on the estimated model parameters, we assess the behaviour of the process on the validation data set. The validation is based on data from 150 days from mid of April till October.

3.3.1. Evaluation of validation

RMSE is suggested for evaluation of both the parameter identification and the model validation. The mean values, maximum amounts and RMSE of the measurement variables are computed on the validation set, and are listed in Table 7. Based on the results, the model error is ignorable comparing the mean values of the measurement variables.

The results show that the model with estimated model parameter can track a simulated biogas reactor with 1% noise.

3.4. Sensitivity analysis

The sensitivity of the parameters expresses the reliability of model parameter estimation. We calculate the sensitivity of variable y to the parameters with (30) Bernard et al. (2001).

$$\sigma_y^{\Delta\theta} = \frac{1}{T} \sum_0^T \frac{y(\theta + \Delta\theta, u, x_0) - y(\theta, u, x_0)}{y(\theta, u, x_0)} \quad (30)$$

where $y(\theta, u, x_0)$ is the simulated measurement variable vector with the model parameter vector θ, the initial state values, x_0 and the input, u.

Figure 5 shows the sensitivity of the methane and carbon dioxide production and pH and also on the amount of VFA and alkalinity to the yield coefficients which are part of the estimated model parameters.

According to the result of sensitivity plots in Figure 5, we may conclude:

- S_2 is influenced by k_1, k_2 and k_3. The effect of k_1 is ignorable comparing to the effects of k_2 and k_3.

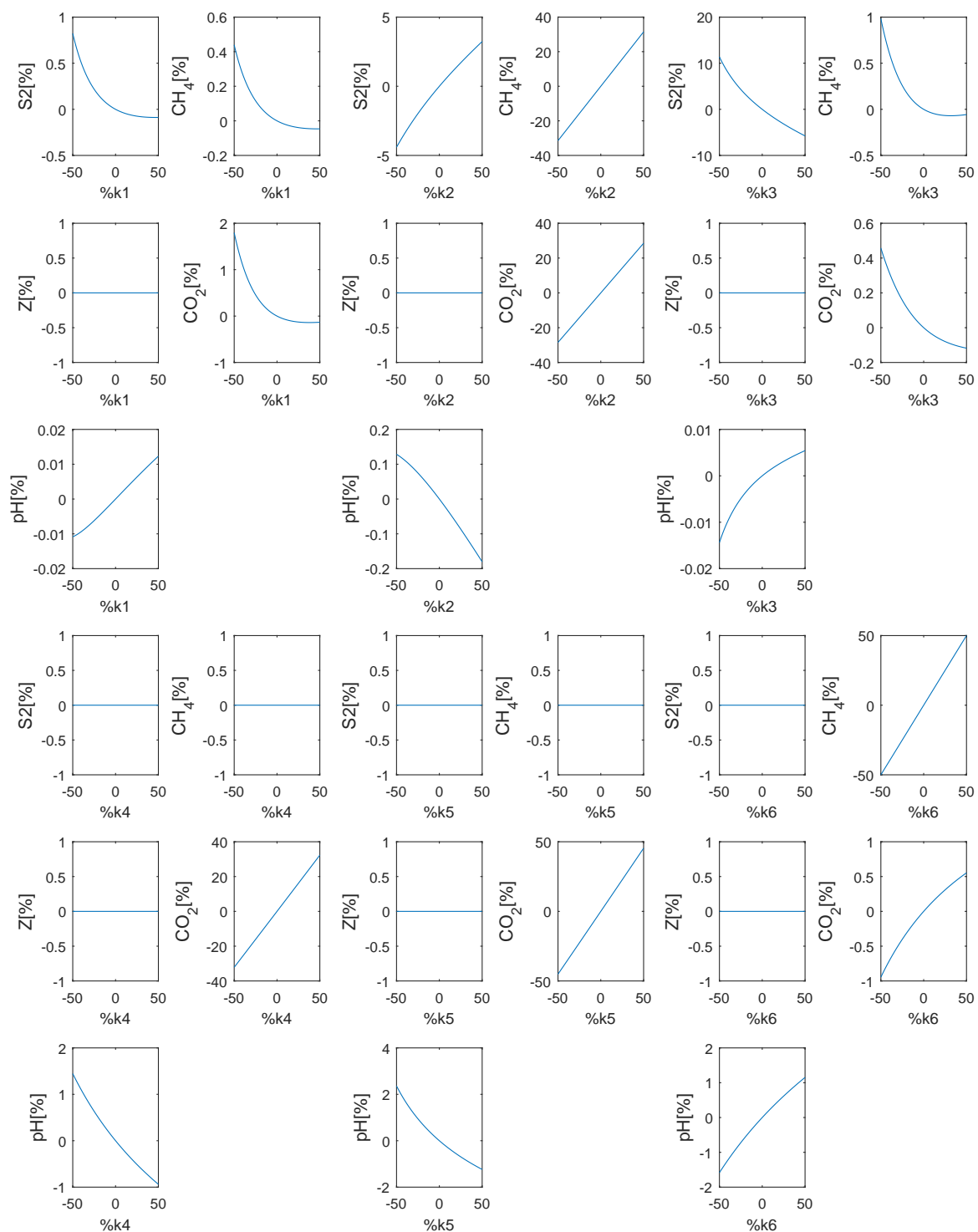- Z is not influenced by yield coefficients.

Figure 5: The sensitivity for the yield coefficient model parameters.

Table 8: The initial values and the estimated model parameter values regarding the experimental data from the VEAS reactor

Model Parameter	Initial values*	Estimated values	Unit
k_1	42.14	230.56	-
k_2	116.5	5315.20	mmol/g
k_3	268	1453.30	mmol/g
k_4	50.6	32.47	mmol/g
k_5	343.6	1886	mmol/g
k_6	453	2465.70	mmol/g
α	0.5	0.3	-
$\mu_{1_{max}}$	1.2	0.022	d^{-1}
$\mu_{2_{max}}$	0.74	0.23	d^{-1}
K_{S_1}	7.1	0.71	g/L
K_{S_2}	9.28	92.72	mmol/L
K_{I_2}	256	2396.2	mmol/L
$k_L a$	19.8	39.01	d^{-1}
c_H	0.013	0.006	-
Z_{dis}	100	115.48	mmol/L

*The initial values of the model parameters are based on Bernard et al. (2001).

- CH_4 is influenced by k_1, k_2, k_3, k_6. The effects of k_1 and k_3 are ignorable comparing to the effects of k_2 and k_6.

- CO_2 is influenced by all yield coefficients, but the most influences are regarding k_5, k_4 and k_2 respectively.

- pH is influenced by all yield coefficients. k_4, k_5 and k_6 have the most influences on pH. These effects are less than 2%.

Among the yield coefficients as model parameters, k_6 has a strong and direct effect on the methane production. pH and carbon dioxide production are influenced by k_6 changes but these influences are just around 1 % with regard to a 50% change in k_6.

Sensitivity analysis regarding the rest of the model parameters is discussed in Appendix A.

4. Model adaptation using experimental VEAS data

In this section, we estimate the AM2 model parameters using experimental data from the VEAS reactor. The parameter estimates minimize the optimization criterion (20).

Two methods are considered for minimization, the gridding method, also known as the brute force

method, implemented from scratch in MATLAB, and nonlinear programming (NLP) using the *fmincon* function in MATLAB. As the number of parameters to be estimated is 15, the gridding method is impractical because of an execution time of days based on an acceptable accuracy of the parameter estimation. Hence, *fmincon* function is chosen. Its execution time was a few minutes. The initial values of the model parameters are based on Bernard's work Bernard et al. (2001) and are shown in Table 8. The dilution rate, the reactor temperature and the feed sludge profile are depicted in Figure 4.

4.1. Parameter estimation and model validation

The parameter estimation is implemented on 1200 samples over 100 days. The estimated model parameters from the simulation are stated in Table 8. Both experimetal and simulated variables with the estimated parameter values are shown in Figure 6. Comparison between simulation results and measurements indicate that the AM2 model can reproduce the behaviour of the AD reactor in the VEAS for the pertinent period.

To evaluate the model adaptation, RMSE is calculated for both the model identification and validation, see Tables 9 and 10.

Table 9: RMSE of error (deviation) between experimental and simulated measurements with adapted model for estimation data set

Measurement	Mean	RMSE	Unit
CH_4	45.68	6.03	mmol/L/d
CO_2	31.57	5.65	mmol/L/d
pH	7.67	0.11	-
Z	187.12	5.42	mmol/L
S_2	15.45	0.81	mmol/L

Table 10: RMSE of error (deviation) between experimental and simulated measurements with adapted model for validation data set

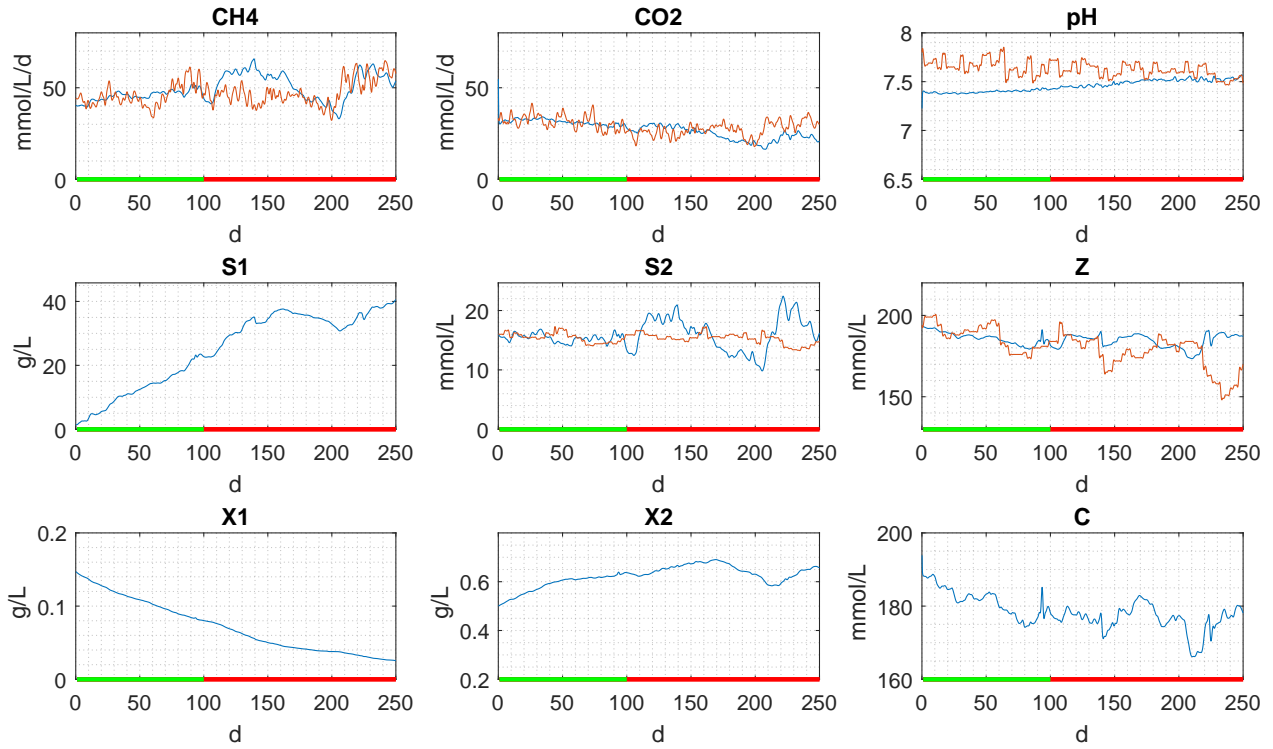| Measurement	Mean	RMSE	Unit
CH_4	47.84	7.83	mmol/L/d
CO_2	26.88	5.65	mmol/L/d
pH	7.70	0.63	-
Z	173.75	15.79	mmol/L
S_2	15.06	1.40	mmol/L

Figure 6: The results of the model adaptation based on the experimental data collected from the VEAS. The red curve is the experimental data and the blue curve is the AM2 model based on the estimated model parameters. In time axis, the green band shows the identification period and the red band shows the validation period.

4.2. Identifiability analysis

The RMSE values shown in Tables 9 and 10 indicate that the model adaptation is acceptable. As an alternative approach to identifiability analysis, Table 11 shows the FIM and the Hessian.

Table 11: The FIM and Hessian analysis for the identifiability analysis

	Rank	Condition number	Maximum eigenvalue	Minimum eigenvalue
FIM	12	1.09×10^{20}	3.5×10^{12}	3.2×10^{-8}
Hessian	13	1.23×10^{23}	9.7×10^{12}	5.7×10^{-8}

The condition numbers of both the FIM and the Hessian are very large, indicating that the model parameters are hardly identifiable using the given data set. Which of the parameters which are not identifiable, however, can not be identified.

5. Discussion

The modified AM2 model which has been adapted to the VEAS reactor is a relatively simple model compared with ADM1 model. Comparing with Hill's model, this model contains the pH, CO_2, alkalinity and inorganic carbon. Considering alkalinity is important to calculate alkalinity ratio and monitor impact on the stability and performance quality.

The modified AM2 model is assumed to be a sufficient accurate model to represent the behaviour of the biogas process.

In the original AM2 model, the impact of temperature is not considered. In addition, it was assumed that the effective reactor volume is constant. Temperature and volume variations are taken into account in the modified AM2 model.

In our study, the model adaptation is an optimization problem to minimize the prediction error. Estimation of model parameters is implemented for both a simulator, where of course the true parameter values are known, and for a real VEAS plant from which we have experimental data. In the simulation-based model adaptation, the effect on measurement noise and uncertainties are investigated. Regard to identifibility

analysis based on FIM and Hessian matrix, the model identification is in ill-condition and it shows the selective data are hardly sufficiently informative to estimate reliably the model parameters.

The sensitivity analysis states which model parameters have the most effect on measurements such as the biogas production.

In this study, collected data is not enough informative to estimate the model parameters and there has been lack of data in the inflow sludge. In the next project, first of all, the characteristics of the sludge in the VEAS including the concentration of the influent VFA, Alkalinity and inorganic carbon should be measured during preparing the data. Uncertain measurement of the influent alkalinity, Z_{in} implies that we had to add a new parameter, Z_{dis}, to compensate alkalinity disturbance and also to satisfy the AR condition to have a stable performance.

Each model parameter has specific physical concept. It is possible to measure and analyze some of them indirectly. For example, k_{La} as a model parameter, can be identified by measuring pH, C, flow rate and partial pressure of CO_2 at steady state Bernard et al. (2001). Specially, k_{La} is an unidentifiable parameter because of a low sensitivity on the measurement variable. In this study, we could not compute this parameter because of the lack of experimental measurements.

Volatile Suspended Solids, VSS is an informative parameter consisting of information about concentration of acidogenic and methanogenic bacteria. VSS helps us to be able to track the behaviour of X_1 and X_2 more accurately.

Study on temperature dependence based on the Hoff-Arrhenius model is suggested. It should be compared with the Hashimoto temperature model.

6. Conclusions

In this study, we have adapted on the AM2 model to both a simulated biogas reactor and to a real reactor at the VEAS plant. The biogas process has some experimental limitation such as alkalinity ratio. We state the model adaptation as an optimization problem. To have reliable identified model parameter set, we need to analyze the identifiability to be sure that there is just one unique set. We focused on the practical identifiability analysis. Investigation on convexity and sensitivity and sloppiness are carried out around the estimated points. The Hessian matrix and the Fisher Information Matrix provide a good information which is useful for a practical identifiability analysis. In spite of the acceptable model error in the considered period, the collected data is hardly not enough informative to obtain reliable model parameters for the modified AM2 model.

A. Sensitivity analysis

Here, there is a discussion about the sensitivity of the AM2 model based on the kinetics model parameters, α, Hashimoto's factor and Z_{dis}.

Figure 7 shows that the sensitivity of the methane and carbon dioxide production and pH and also on the amount of the VFA and alkalinity concentrations to the kinetic model parameters.

Based on Figure 7, we conclude:

- S_2 is influenced by $\mu_{1_{max}}$, $\mu_{2_{max}}$, K_{S_1}, K_{S_2} and K_{I_2}. The effects of $\mu_{2_{max}}$ and K_{S_2} are remarkable comparing of the effects of the rest of the kinetic parameters.

- Z is not influenced by the kinetic parameters.

- CH_4 is influenced by $\mu_{1_{max}}$, $\mu_{2_{max}}$, K_{S_1}, K_{S_2} and K_{I_2}. These influences are less than 2%.

- CO_2 is influenced by $\mu_{1_{max}}$, $\mu_{2_{max}}$, K_{S_1}, K_{S_2} and K_{I_2}.

- pH is influenced by $\mu_{1_{max}}$, $\mu_{2_{max}}$, K_{S_1}, K_{S_2} and K_{I_2}.

- k_{La}, K_{S_1} and K_{I_2} have a little influence on the simulated model measurement variables.

Table 12: The percent of the change on each measurement variable regarding 50% changes in each model parameter

%/50%	S_2	Z	CH_4	CO_2	pH
k_1	$< 1^{\downarrow *}$	0	$< 1^{\downarrow}$	$< 2^{\downarrow}$	$\ll 1^{**}$
k_2	< 5	0	35	35	$< 1^{\downarrow}$
k_3	$10^{\downarrow}$	0	$< 1^{\downarrow}$	$< 1^{\downarrow}$	$\ll 1$
k_4	0	0	0	35	$< 2^{\downarrow}$
k_5	0	0	0	50	$< 2^{\downarrow}$
k_6	0	0	50	< 1	< 1
α	20	0	$< 1^{\downarrow}$	$< 1^{\downarrow}$	$\ll 1$
$\mu_{1_{max}}$	$< 3^{\downarrow}$	0	$< 1^{\downarrow}$	$< 6^{\downarrow}$	$\ll 1$
$\mu_{2_{max}}$	$100^{\downarrow}$	0	< 1	$< 1^{\downarrow}$	< 1
K_{S_1}	< 1	0	$< 1^{\downarrow}$	< 1	$\ll 1$
K_{S_2}	40	0	$< 1^{\downarrow}$	$\ll 1$	$\ll 1^{\downarrow}$
K_{I_2}	$< 1^{\downarrow}$	0	$\ll 1^{\downarrow}$	$\ll 1$	0
k_{La}	0	0	0	< 1	< 1
c_H	$< 2^{\downarrow}$	0	$\ll 1$	$< -1^{\downarrow}$	0
Z_{dis}	0	20	0	$15^{\downarrow}$	< 2

$*^{\downarrow}$ means a reverse effect.
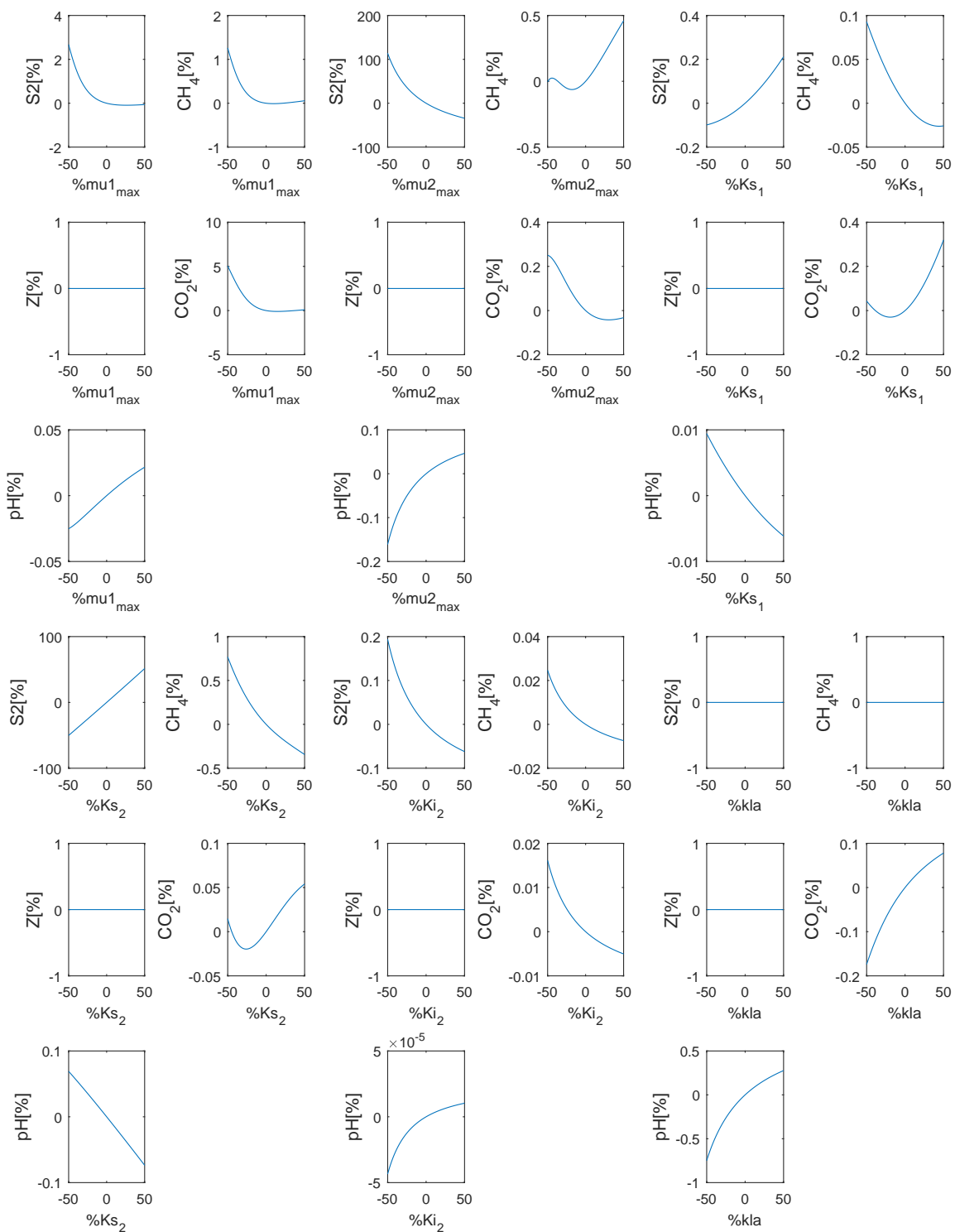
$**\ll 1$ means the effect is less than 0.1 %.

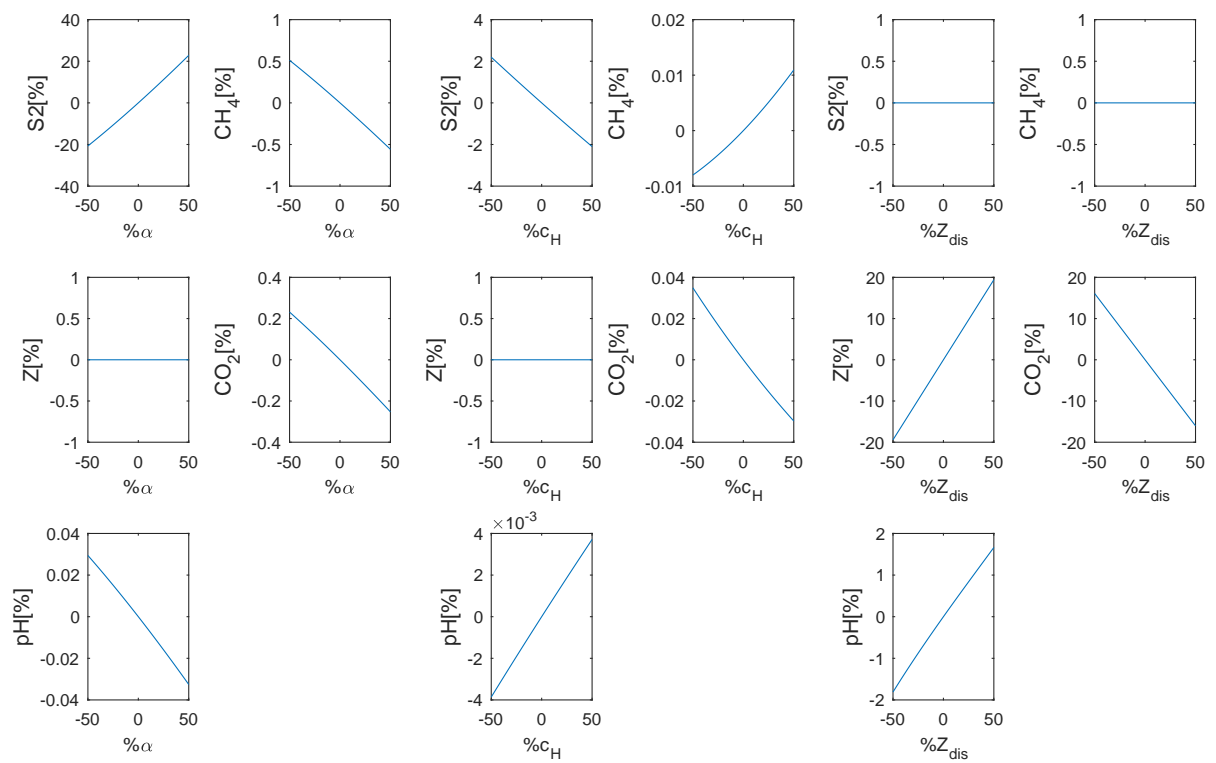Figure 7: The sensitivity for the kinetic and k_{La} model parameters.

Figure 8: The results of the sensitivity analysis for α, the Hashimoto factor and alkalinity disturbance.

Figure 8 shows that the sensitivity of the methane and carbon dioxide production and pH and also on the amount of VFA and alkalinity concentrations to α, c_H and Z_{dis}. The results of sensitivity analysis shows:

- S_2 is influenced by α, c_H. α has a direct effect on VFA while as c_H has reverse effect on VFA. Their effects are 20% and 2%, respectively.

- Z is influenced by Z_{dis}. There is no effect on alkalinity by changing in α or c_H.

- CH_4 is negligibly influenced by α, c_H.

- CO_2 is influenced by α, c_H and Z_{dis}.

- pH is influenced by α, c_H and Z_{dis}. The effects of α and c_H are ignorable comparing the effect of Z_{dis} on the pH.

Table 12 shows the percentage of the each individual model parameter effect on the each measurement variable with regard to 50% changes in each model parameter.

This table shows that K_{s_1}, K_{I_2}, k_{La} have ignorable effects on the all five measurements so we can assume these model parameters are unidentifiable based on the collected data.

Nomenclature

The nomenclature is in alphabetical order.

C	total inorganic carbon concentration (mmol/L)
c_H	Hashimoto's factor
D	dilution rate (d^{-1})
k_1	yield for substrate degradation
k_2	yield for VFA production (mmol/L)
k_3	yield for VFA consumption (mmol/L)
k_4	yield for CO2 production (mmol/L)
k_5	yield for CO2 production (mmol/L)
k_6	yield for CH4 production (mmol/L)
k_{d}	death rate (d^{-1})
K_{H}	Henry's constant (mmol/L per atm)
k_{La}	a liquid-gas transfer constant (d^{-1})
K_{I_2}	inhibition constant (mmol/L)
K_{S_1}	half-saturation constant (g/L)
K_{S_2}	half-saturation constant (mmol/L)
P_{T}	total pressure (atm)

q_C	carbon dioxide flow rate (mmol/L per d)
q_M	methane flow rate (mmol/L per d)
S_1	organic substrate concentration (g/L)
S_2	volatile fatty acids concentration (mmol/L)
T_{reac}	reactor temperature (°C)
X_1	concentration of acidogenic bacteria (g/L)
X_2	concentration of methanogenic bacteria (mmol/L)
V	effective volume of medium in the reactor (L)
Z	total alkalinity (mmol/L)
α	fraction of bacteria in the liquid phase
$\mu_{\max}$	maximum specific growth rate (d^{-1})

Abbreviations

The abbreviations are in alphabetical order.

AD	Anaerobic Digestion
ADM1	Anaerobic Digestion Model no.1
AM2	Anaerobic digestion Model no. 2
AR	Alkalinity Ratio
FIM	Fisher Information Matrix
RMSE	Root Mean Square Error
TS	Total Solid
VFA	Volatile Fatty Acid
VS	Volatile Solid
VSS	Volatile Suspended Solids
WRRF	Water Resource Recovery Facility

Acknowledgment

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