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A generic and systematic procedure to derive a simplified model from the Anaerobic Digestion Model No. 1 (*ADM1*)

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Highlights

► We introduce the hydrolysis stage and the ammonium dynamics into the AM2 model. ► A generic and systematic state-association approach is proposed. ► The new proposed model AM2HN is calibrated. ► The AM2HN model gives an accurate description of the dynamics of the ADM1 model. ► The AM2HN is robust with regard to moderate variations in the influent composition.

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Abstract

The Anaerobic Digestion Model No.1 (*ADM1*) developed by the *IWA* Task Group for mathematical modelling of anaerobic digestion processes (Batstone et al. (2001) [1]) is a structural model which describes the main biochemical and physicochemical processes. For such purposes, other models have been proposed to describe anaerobic processes with a reduced set of parameters, state variables and processes. Among them, the Anaerobic Model No. 2 (*AM2*) proposed by Bernard et al. (2001) [2] which describes the degradation of soluble organic compounds appears as a model well-suited for control and optimization applications. In this work, we aimed at obtaining a model of reduced dimensions on the basis of which to synthesize regulators or observers with guarantees of performance, stability and robustness. Specifically, our contribution is twofold. First, a modified version of the *AM2* is proposed while preserving the simplicity of the new model "*AM2HN*". Second, we propose a systematic and generic state association procedure in order to obtain such a simplified model from any validated *ADM1*.

Simulations and comparisons with the predictions of the *ADM1* for a case study involving the anaerobic digestion of waste sludge are presented along with satisfactory results.

Keywords: Anaerobic Processes; Dynamic Modelling; Optimisation; Control; *AM2*; *AM2HN*.

Nomenclature

AD: Anaerobic Digestion

B: Bicarbonate concentration (mM)

C: total inorganic carbon concentration (mM)

COD: Chemical Oxygen Demand

CSTR: Continuous-Stirred Tank Reactor

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D: dilution rate coefficient (day^{-1})

S_i*: dynamic state variable of the component S_i

HCO_3: Bicarbonate concentration (mM)

HRT: Hydraulic Retention Time (day)

I_C: inorganic carbon concentration (mM)

I_N: inorganic nitrogen concentration (mM)

k_1: yield for substrate concentration

k_2: yield for VFA production (mmol g^{-1})

k_3: yield for VFA consumption (mmol g^{-1})

k_4: yield for CO_2 production by X_1 (mmol g^{-1})

k_5: yield for CO_2 production by X_2 (mmol g^{-1})

k_6: yield for CH_4 production (mmol g^{-1})

K_b: equilibrium constant (mol L^{-1})

K_H: Henry's constant (mmol L^{-1} atm^{-1})

k_{La}: gas-liquid transfer coefficient (day^{-1})

K_I: inhibition constant (mM)

K_{S1}: half-saturation constant (g L^{-1})

K_{S2}: half-saturation constant (mM)

N_{bac}: Nitrogen content of bacteria (kmole N (kg COD)$^{-1}$)

N_{S1}: Nitrogen content of substrate S_1 (kmole N (kg COD)$^{-1}$)

NH_3: free ammonia concentration (mM)

NH_4^+: ammonium concentration (mM)

P_C: CO_2 partial pressure (atm)

q_in: influent and effluent flow rate (m^3 day^{-1})

q_C: carbon dioxide flow rate (mmol L^{-1} d^{-1})

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q_M: methane flow rate (mmol L^{-1} d^{-1})

$\overline{S_i}$: steady-state value of the concentration of component S_i

S_1: organic substrate concentration (g L^{-1})

S_2: volatile fatty acids concentration (mmol L^{-1})

VFAs: Volatile Fatty Acids

V_{liq}: liquid reactor volume (m^3)

VS: volatile solids

X_1: concentration of acidogenic bacteria (gVS L^{-1})

X_2: concentration of methanogenic bacteria (gVS L^{-1})

Z: total alkalinity (mmol L^{-1})

μ_1: specific growth rate of acidogenic bacteria (d^{-1})

$\mu_{1,max}$: maximum acidogenic bacteria growth rate (d^{-1})

μ_2: specific growth rate of methanogenic bacteria (d^{-1})

$\mu_{2,max}$: maximum methanogenic bacteria growth rate (d^{-1})

ρ_j: rate for process j (kgCOD m^{-3} d^{-1} or kmol $m^{-3}d^{-1}$)

1. Introduction

Anaerobic digestion *(AD)* is a delicate and complex process involving several bacterial groups each of them having its own ideal working conditions. Both the optimization of the *AD* and the assessment of its operation as a function of varying feed or operating conditions are important objectives and can be best attained using suitable digestion models. In fact, modelling is the best way for developing, applying and validating on-line monitoring of digestion (Appels et al. (2008) [3]). Models can be in a steady-state mode but can also be more complex in order to describe process dynamics. However, those models which describe

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in detail all the processes involved in *AD* are generally difficult to use for control purposes (Bastin and Dochain (1990) [4]). Control theory aims at synthesizing control laws in predefining performance and robustness margins with respect to a model capturing the main dynamical characteristics of a process. For that purpose, it is irrelevant to have a very detailed model of the process as it is the case for a model "for thinking". It is rather the opposite: without being able to characterize the qualitative behaviour of a complex model (that can only be investigated numerically), we are not able to fix appropriate robustness and performance characteristics for its outputs. Rather, a model including only the main dynamical characteristics must be used.

Reduced models are available in the literature that can be used for control; they include the *AM2* that is a good compromise between the complexity of a model and its correspondence with the available experimental information.

This model involves two processes and two bacterial populations. In the first stage of acidogenesis, the acidogenic bacteria X_1 consume the organic substrate S_1 and produce volatile fatty acids *VFA* (S_2) and CO_2. In the second stage of methanization, the methanogenic population X_2 consumes *VFA* and produces methane and carbon dioxide. The biological reactions are as follow:

Acidogenesis (with reaction rate μ_1):

$$k_1 S_1 \xrightarrow{\mu 1} X_1 + k_2 S_2 + k_4 CO_2$$

Methanogenesis (with reaction rate μ_2):

$$k_3 S_2 \xrightarrow{\mu_2} X_2 + k_5 CO_2 + k_6 CH_4$$

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where k_i are stoichiometric coefficients, also referred to as yield coefficients.

The bacterial growth rate μ_1 (d^{-1}) of the acidogenic bacteria is of the Monod type whereas Haldane's kinetics describe the methanogenic bacterial growth rate μ_2 (d^{-1}), taking into account the inhibitory effects of *VFA* accumulation.

An additional state variable is the inorganic carbon concentration *C*, made up of CO_2 and bicarbonate, *B*. Total alkalinity (*Z*) is defined as the sum of dissociated acids in the liquid phase, that is to say bicarbonate and *VFAs*; the latter are considered as completely dissociated in the *pH* range concerned.

Assuming that the processes described above take place in an ideal continuous-stirred tank reactor (*CSTR*) with a dilution rate *D* (d^{-1}), the following differential equations describe the mass-balance for the six state variables:

$$\frac{dX_1}{dt} = (\mu_1(S_1) - aD)X_1 \tag{1.1}$$

$$\frac{dX_2}{dt} = (\mu_2(S_2) - aD)X_2 S \tag{1.2}$$

$$\frac{dS_1}{dt} = D(S_{1,in} - S_1) - k_1\mu_1(S_1)X_1 \tag{1.3}$$

$$\frac{dS_2}{dt} = D(S_{2,in} - S_2) + k_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)X_2 \tag{1.4}$$

$$\frac{dZ}{dt} = D(Z_{in} - Z) \tag{1.5}$$

$$\frac{dC}{dt} = D(C_{in} - C) - q_C + k_4\mu_1(S_1)X_1 + k_5\mu_2(S_2)X_2 \tag{1.6}$$

where: subscript 'in' refers to influent concentrations and q_C in Equation (1.6) is the CO_2 flow rate. A parameter α was introduced by the authors in order to model biomass retention: α

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$= 0$ corresponds to an ideal fixed-bed reactor while $\alpha = 1$ corresponds to an ideal reactor with no biomass retention system.

This system has been extensively studied in the literature. In particular, its qualitative behaviour (finding equilibrium points and their stability) was studied by Sbarciog et al. (2010) [5] for $\alpha = 1$ and was extended to the case $\alpha \approx 1$ by Benyahia et al. (2012) [6].

As for the inorganic equilibria and the *pH* calculations, Bernard et al. (2001) [2] assumed that inorganic carbon is composed mainly of dissolved carbon dioxide CO_2 and bicarbonate *B*, ignoring the amount of carbonate in normal operating conditions (*pH* range between 6 and 8, temperature between 35 and 38°C). The presence of the two species is regulated by the chemical equilibrium of the CO_2 in its aqueous form.

Nonetheless, the original *AM2* model was developed to describe the anaerobic degradation process applied to such industrial wastewater as winery effluent which contains mainly soluble, carbohydrates-based organic matter for which disintegration/hydrolysis is irrelevant (Bernard et al.(2001) [2]). Therefore, the *AM2* may need to be modified when describing the degradation of complex and proteinaceous substrates such as waste-activated sludge.

To this extent, our first contribution can be stated as follows:

- A modification of the *AM2* in order to take into account relevant processes including hydrolysis and the concomitant release of ammoniacal nitrogen. This has led to a new model which we propose to name "*AM2HN*" since it is based on the existing *AM2* model.

Today, the *ADM1* is recognized as a reference model by most people involved with liquid and solid wastes and an effective *ADM1* has been proposed and validated for a wide range of case studies ([7], [8]). Thus, proposing a new model has no real sense if its links with the *ADM1* have not been clearly established. A second contribution of this work is thus:

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- An association procedure that has been developed to facilitate a simple and systematic interfacing between the *AMD1* state variables and those of the simplified model so that the latter can be easily calibrated from simulated values generated from the available/validated *ADM1*.

Since the *ADM1* is a non-linear, physically-based model, our aim was to obtain a non-linear reduced model retaining a physical meaning. Indeed, the originality of the proposed approach is to keep both the nonlinear characteristics and the balance-type equations that are well known in biotechnology. In doing so, we can use specific robust control techniques proposed in the field of control theory for biochemical engineering.

This paper is organized as follows: first, we introduce the hydrolysis stage and the ammonium dynamics into the *AM2* to derive the *AM2HN* (section 2). Then we propose a generic and systematic state-association approach to find correspondences between the variables of the *ADM1* and those of the *AM2HN* (section 3). In Section 4, the proposed *AM2HN* is calibrated with data generated by the *ADM1*. The dynamic responses of the model are then compared in Section 5. Section 6 deals with a sensitivity analysis. Finally, in Section 7 conclusions and perspectives are drawn.

2. Introduction of the hydrolysis stage and the ammoniacal nitrogen release into the *AM2*

To broaden the field of applicability of the *AM2*, the first modification was to include the disintegration/hydrolysis step that describes the degradation into soluble organic substances (e.g. amino acids and fatty acids) of both the composite organic material and the high-molecular-weight compounds such as lipids, polysaccharides, and proteins. When the organic matter to be converted into methane is particulate, hydrolysis is often recognized as the rate-

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limiting step in the overall digestion process (Vavilin et al. (2001) [9]). This is typically the case for the anaerobic digestion of waste-activated sludge (*WAS*). In the *ADM1*, disintegration and hydrolysis are described as a whole process that converts particulate organics into soluble forms, and whose rate is described by first-order kinetics:

$$\rho_H = k_{hyd}.X \tag{2}$$

where k_{hyd} is the hydrolysis constant (d^{-1}), X is the particulate substrate concentration ($kg\ m^{-3}$) and ρ_H is the rate of hydrolysis of the particulate substrate ($kg\ m^{-3}\ d^{-1}$).

In the proposed modification of *AM2*, the substrate mixture that will undergo hydrolysis is represented by the total particulate substrate X_T including particulate substrates related to composite material (X_c), carbohydrates (X_{ch}), proteins (X_{pr}) and lipids (X_{li}). To preserve the simplicity of the model, we have made the choice not to consider the hydrolysis of each of these components separately but to consider them as a single particulate substrate.

The hydrolysis of X_T in the *AM2* can be represented by the following reaction scheme:

$$X_T \xrightarrow{\rho_H} S_1$$

Thus, there will be one additional state variable (X_T), i.e. one additional differential equation, and the differential system previously described (eqs. 1.1-1.6) needs to be modified by adding one more differential equation describing the X_T mass balance:

$$\frac{dX_T}{dt} = D(X_{T,in} - X_T) - k_{hyd}.X_T \tag{3}$$

and by modifying eq. 1.3 into the following:

$$\frac{dS_1}{dt} = D(S_{1,in} - S_1) - k_1\mu_1(S_1)X_1 + k_{hyd}.X_T \tag{4}$$

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Then, we introduced in the *AM2* the ammonium (NH_4^*)released from protein hydrolysis in order to consider its contribution to the alkalinity of the solution. In the *AM2*, three components contain nitrogen: the degradable substrate S_1 ,whose nitrogen content is N_{S1}, the acidogenic biomass (X_1) and the methanogenic biomass (X_2) whose nitrogen content is N_{bac}.

For the sake of simplicity, ammoniacal nitrogen was not included as an additional state variable, but the *N* release dynamics was included into the mass-balance differential equation of alkalinity Z :

$$\frac{dZ}{dt} = D(Z_{in} - Z) + [(k]_1.N_{S1} - N_{bac}).\mu_1(S_1)X_1 - N_{bac}.\mu_2(S_2)X_2 + k_{d,1}.N_{bac}.X_1 + k_{d,2}.N_{bac}.X_2$$

(5)

This modification makes alkalinity a reactive species whereas it was not so in the original *AM2*.

As a matter of fact, alkalinity is the sum of the concentrations of all bases in solution, i.e. all chemical species that can accept H^+.

In anaerobic digesters, the following chemical species and corresponding equilibria contribute to the total alkalinity:

Bicarbonate: $HCO_3^- + H^+ \leftrightarrow H_2CO_3$

$VFA: Ac^- + H^+ \leftrightarrow HAc$

Hydroxide ions: $OH^- + H^+ \leftrightarrow H_2O$

Free ammonia: $NH_3 + H^+ \leftrightarrow NH_4^+$

Ignoring any ammonium contribution to alkalinity, then bicarbonate and *VFA* are the main species that contribute to Z, i.e. the alkalinity considered in the AM2, so that the following applies:

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$$Z \approx [Cat] - [An]$$

Where [Cat] and [An] are the concentrations of those ions (cations and anions) that are unaffected by the anaerobic digestion process and is therefore a non-reactive specie, i. e. the so-called 'charge imbalance' (Mairet et al., 2012) [14]. However, this charge imbalance does not strictly coincide with alkalinity and it is a good approximation of alkalinity in those cases in which protein hydrolysis is irrelevant (e.g. when treating waste containing mainly sugars). On the contrary, when proteins are digested, ammonium is released with a consequent increase in the alkalinity concentration. This concept is generally accepted (Sialve et al., (2009) [15]). Indeed, the Eqs. 8 and 25 of Mairet's work refer to a quantity that corresponds to alkalinity only if the ammonia contribution to alkalinity is ignored. In this case, there is a difference between the 'charge imbalance' and the *Z* that we have used to describe 'alkalinity' in the *AM2HN*. Here the charge imbalance no longer coincides with alkalinity.

3. Associating the *ADM1* – *AM2HN* variables

In order to use the data simulated by *ADM1* to calibrate the original *AM2* or the modified *AM2HN* models, an interfacing procedure is here presented that establishes a correspondence between the large number of variables that are modelled by the *ADM1* and the fewer and aggregated *AM2* or *AM2HN* variables.

Similar aggregation procedures have been proposed in the literature in order to link and interface existing models that were originally developed separately and that use different sets of state variables. For example, Vanrolleghem et al. (2005) [10] presented a general framework for making this association possible. Their idea is based on algebraic equations that constitute interfaces between models. Here, a similar interface procedure is presented, aimed at interfacing the *ADM1* and the *AM2* and *AM2HN* models. The explanation of this

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association procedure and the line of reasoning leading to the aggregation are presented below.

The concentration of the organic substrate S_1 in the *AM2* corresponded to the soluble substrates in the *ADM1* i.e. sugars, amino and fatty acids and the particulate *COD* (composite, proteins, lipids and carbohydrates) since they often represent a significant percentage of the total *COD* and cannot be ignored.

On the other hand, the concentration of the organic substrate S_1 in the *AM2HN* corresponded to the *ADM1*'s soluble substrates only; the particulate components of the influent substrate are taken into account in the aggregated *AM2HN* variable X_T.

In the following, the variable association is the same for both the *AM2* and *AM2HN* models.

The total concentration of *VFA*s, comprising the soluble compounds valeric, butyric, propionic and acetic acids, is represented by S_2.

In the *AM2* and the *AM2HN*, the seven different *ADM1* bacterial populations belonged to just two families: one X_1, responsible for acidogenesis, while X_2 was responsible for acetogenesis and methanization. Micro-organisms responsible for the degradation of sugars, amino and fatty acids were grouped in the first family while those converting hydrogen and volatile acids into methane made up the second.

As for the inorganic carbon species, lumping was not necessary because the correspondence between the *ADM1* variables and the aggregated variables of the *AM2* and the *AM2HN* was straightforward. Total inorganic carbon C, bicarbonates B and dissolved carbon dioxide CO_2 corresponded to S_{ic}, S_{co_3} and S_{co_2} respectively (the same with regard to the pH).

Alkalinity Z, on the other hand, had to be calculated from the species that contributed to it: *VFA*s, bicarbonates and ammoniacal nitrogen.

The gas flows, expressed in the *AM2HN* as molar production rates (*mmol* L^{-1} d^{-1}), are expressed as a mass flow in the *ADM1*. Therefore, they correctly correspond to the *ADM1* gas

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transfer rates of methane and carbon dioxide. Hydrogen gas is not taken into account by the *AM2HN* so the partial pressure of CO_2 (P_C) must be computed as a ratio of the CO_2 partial pressure in the *ADM1* (p_{gas,CO_2}) and the sum of the partial pressures due to methane and CO_2, the sole biogas constituents in the *AM2HN*.

A comprehensive description of the above-described correspondences between the two groups of variables is summarised in Table 1. Since the respective units of measurement did not always correspond, a conversion factor was sometimes necessary.

4. Identification of *AM2* and *AM2HN* parameters

4.1 Data set

In order to compare the dynamic predictions of the different models, we had to calibrate both the *AM2* and the *AM2HN* parameters.

The modified *AM2* parameters were identified from a set of steady-state data obtained after running the *ADM1* simulations of the mesophilic single-stage anaerobic digestion of *WAS* in a *CSTR* without biomass retention ($\alpha = 1$).

Characterisation of the *WAS* in terms of *ADM1* state variables and *ADM1* parameters were assumed as suggested by Rosen and Jeppsson (2006) [11]; input characteristics are given in Appendix A.

Steady-state data sets were obtained by varying the hydraulic retention time ($HRT = 1/D$) between 5 and up to 90 days.

Simulations were obtained using *DYMOLA* (Dynamic MOdeling LAboratory), a simulation platform based on the Modelica language. The synthetic data set obtained for the calibration is reported in Table 2.

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4.2 Identification procedure

Model calibration is an awkward task when dealing with biotechnological processes. As for the *ADM1*, calibration is typically based on practitioners' knowledge who select the set of parameters to be calibrated according to their experience, without any guarantee that another set of parameters would ultimately predict the same dynamical behavior. On the contrary, a systematic identification procedure had been proposed by Bernard and co-workers and applied to the *AM2* (Bastin and Bernard, 2005). This procedure is based on the decoupling of yield and kinetic parameters and their separate identification. Specifically, the model was rewritten by using a number of basic transformations so that the resulting model form allows certain parameters to be identified using linear regression. To guarantee parameters identifiability, this same approach was applied in this work for the *AM2HN*.

First, the *AM2* model was calibrated and, to this purpose, the same procedure proposed by Bernard et al. (2001) [2] was applied. However, by considering simulation data obtained at high *HRT*s (more than 12 days) several parameter values gave negative results or had no physical meaning. This can be explained by the absence of a decay term in the biomass growth rate which becomes increasingly important at high *HRT* because the residence time of the biomass is enough to make the decay process relevant.

Thus, a decay rate, k_d, was introduced for both kinds of biomass and was estimated to be 10% of the maximum bacterial growth rates, respectively $\mu_{1,max}$ and $\mu_{2,max}$ as in Eqs. (6) and (7):

$$\mu_1(S_1) = \mu_{1,max} \cdot \frac{S_1}{S_1 + K_{s1}} - k_{d,1} = \mu_{1,max} \cdot \frac{S_1}{S_1 + K_{s1}} - 0.1.\mu_{1,max} \quad (6)$$

$$\mu_2(S_2) = \mu_{2,\max} \cdot \frac{S_2}{S_2 + K_{S2} + \frac{S_2^2}{K_I}} - k_{d,2} = \mu_{2,\max} \cdot \frac{S_2}{S_2 + K_{S2} + \frac{S_2^2}{K_I}} - 0.1.\mu_{2,\max} \quad (7)$$

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4.3 Modified estimation procedure

By introducing the decay process, the linearization procedure previously applied was no longer applicable. Therefore, a modified procedure was developed as described below.

Kinetic parameters

At steady state, we have from Eqs. (1.1) and (1.2):

$$\mu_1(S_1) = aD \tag{8}$$

$$\mu_2(S_2) = aD \tag{9}$$

and from Equation (6) the following expression:

$$\overline{S_1} = \frac{a}{0.9\mu_{1,max}}.D.\overline{S_1} + \frac{aK_{S1}}{0.9\mu_{1,max}}.D + 0.1\mathbf{1}K_{S1} \tag{10}$$

Expression (10) contains two operational parameters, α and D, that are known. Regression on this relationship gives the values of $\mu_{1,max}$ and K_{S1}.

Eqs. (7) and (9) provide the following relationship:

$$\overline{S_2} = \frac{a}{0.\mathbf{9}\mu_{2.max}}.D.\overline{S_2} + \frac{aK_{S2}}{0.\mathbf{9}\mu_{2.max}}.D + 0.1\mathbf{1}K_{S2} + \frac{a}{0.\mathbf{9}\mu_{2.max}K_I}D.\overline{S_2}^2 + \frac{0.1\mathbf{1}}{K_I}\overline{S_2}^2 \tag{11}$$

Regression on this relationship gives the values of $\mu_{2,max}$, K_{S2} and K_I.

The steady-state equilibrium of X_T leads to the following equivalent equation:

$$D(X_{T,in} - \overline{X}_T) = k_{hyd}.\overline{X}_T \tag{12}$$

Regression on this relationship gives the values of k_{hyd}.

Liquid-gas transfer coefficient

To estimate the value of the liquid-gas transfer coefficient k_{La}, we used the same equation as used by Bernard et al. (2001) [2] since the introduction of the decay term did not affect the physico-chemical equilibrium.

From Bernard et al. (2001) [2], the CO_2 flow rate q_C is given by the following equation:

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$$q_C = k_{La}(CO_2 - K_H P_C) \quad (13)$$

And the total inorganic carbon in the *pH* range considered is equal to:

$$C = CO_2 + B \quad (14)$$

From the measurements of pH, C and the partial pressure of carbon dioxide (P_C) at steady-state, the regression can be performed as follows:

$$\overline{q_C} = k_{La}\left[\frac{\overline{C}\mathbf{1}}{1+1\mathbf{0}^{pH-pK_b}} - K_H.\overline{P_C}\right] \quad (15)$$

where

$$pK_b = -\log(K_b) \quad (16)$$

$$\overline{CO_2} = \frac{\overline{C}}{1+1\mathbf{0}^{pH-pK_b}} \quad (17)$$

where K_b denotes the equilibrium constant for bicarbonate dissociation, i.e. $K_b = \frac{[H^+]B}{CO_2}$

Stoichiometric coefficients

From Eq. (8) and by rewriting the steady-state expression of S_1, Equation (18) was deduced, leading to the estimation of k_1:

$$D(S_{1,in} - \overline{S_1}) + k_{hyd}.\overline{X_T} = k_1.a.D.X_1 \quad (18)$$

Considering the expression of the outflow of methane, the following was obtained:

$$\frac{\overline{q_{Ch4}}}{\overline{X_2}} = a.k_6.D \quad (19)$$

The regression of the above relationship gives the estimation of k_6.

The parameters k_2 and k_3 were identified by starting from the steady-state expression of S_2 and obtaining the estimation shown in Eq. (20):

$$D(S_{2,in} - \overline{S_2}) = k_3.a.D\overline{X_2} - k_2.a.D.\overline{X_1} \quad (20)$$

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The last two yield coefficients k_4 and k_5 were identified from the regression of the following relationship obtained from the steady-state expression of the total inorganic carbon C:

$$q_C - D(C_{in} - \overline{C}) = k_4.a.D.\overline{X_1} + k_5.a.D.\overline{X_2} \quad (21)$$

The *AM2* and the *AM2HN* maximum growth rates ($\mu_{1,max}$ and $\mu_{2,max}$) correspond to the *ADM1* specific growth rates (i.e. $k_{m,i}$) multiplied by the respective yield coefficients (i.e. Y_i). Since several trophic groups are considered in the *ADM1*, the *AM2* and the *AM2HN* parameters were compared to the *ADM1* mean values for the maximum growth rate and the half-saturation constants.

The stoichiometric coefficients in the *AM2* and the *AM2HN* (i.e. k_i) correspond to the reverse of the *ADM1* yield coefficients (i.e. Y_i). Again, average yield values assumed in the *ADM1* model were used for comparison with the *AM2* and *AM2HN* calibrated parameters as shown in Tables 3 and 4. It should be stressed here that a conversion factor was used to take into account the change in the measuring unit.

The *AM2HN* yield coefficients were quite similar to those of the *ADM1* compared with those of the *AM2*. The *AM2* and *AM2HN* maximum growth rates were lower than that of the *ADM1* but the *AM2* and the *AM2HN* parameters only refer to two families of bacteria in which heterogeneous bacterial strains are grouped. The liquid-gas transfer coefficient (k_{La}) in *ADM1* was much higher than that in either the *AM2* or the *AM2HN*, a consequence of the model structure due to the simplifications applied in the *AM2* and the *AM2HN*.

5. Dynamic responses

The ability of the *AM2* and the proposed *AM2HN* model to predict the dynamic behaviour of an anaerobic digester fed on waste-activated sludge was studied by simulating the dynamic

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responses to step-type disturbances in the influent composition and by comparing such responses to those expected from using the *ADM1* model as a reference.

We chose to apply disturbances to the anaerobic digester by increasing and decreasing the influent *COD* concentration, mainly via the particulate components X_c, X_{ch}, X_{pr}, X_{li} whose concentrations were all increased by 20%. The disturbance was a square wave consisting in a step increase of +20%, followed by a step decrease to the initial input value. This disturbance started at day 20 and ended at day 100. The hydraulic retention time (*HRT*) was set at 20 days as proposed by Rosen and Jeppsson (2006) [11].

Dynamic simulations were again performed by using *DYMOLA* (Dynamic MOdeling LAboratory) [12].

The comparison of the outputs of the *ADM1*, the *AM2* and the *AM2HN* models was done by using dimensionless variables (X_i*) obtained by normalizing the dynamic values ($X_i(t)$) according to their steady-state value prior to the step variation ($\overline{X_i}$), as follows:

$$X_i^* = \frac{X_i(t)}{\overline{X_i}} \tag{24}$$

The comparison of the output of the models was done using dimensionless variables because, in terms of control, we are mainly interested in the dynamics of the variables. Indeed, we consider that the off-set among steady state values of AM2-like and ADM variable is not relevant when monitoring and control are the objectives.

If we compare the outputs without such dimensionless variables, we obtain results that are similar in absolute value, as shown in Figure 1 which describes the dynamic of the gas outflow of methane.

Simulations started at the equilibrium which meant that the initial values were set equal to those at steady state such that the value of dimensionless variables was equal to 1. After the disturbance, each variable reacted according to its own dynamics and the dimensionless

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variable reported the entity of the dynamic variation relative to the initial steady-state condition.

Particular attention must be paid to the dynamic response of S_1 (Fig. 2). It must be noted that WAS (Rosen and Jeppsson (2006) [11]) is composed mainly of particulate *COD* that, according to the *ADM1* model, undergoes the hydrolytic steps; therefore its dynamics followed the typical response to a step-like input of first-order systems. On the other hand, in the *AM2* model, S_1 is degraded according to the enzymatic Michaelis-Menten kinetics, therefore its dynamic response to a step-like input showed a very different behaviour. Concerning the responses of the *VFA*s (Fig. 3 (a)), the *ADM1* dynamics of S_2 were completely different from those simulated by the *AM2*. The *ADM1* dynamics showed a huge increase of the dimensionless variable, with a profile revealing a non-linear response; additionally, such an increase appeared despite the fact that *VFA* concentrations in the influent were not disturbed. By analyzing the *VFA* components in the *ADM1*, which were lumped together in S_2, it was found that the dominant dynamics was that of the acetate (i.e. S_{ac} in *ADM1*) and that the reason for such a massive increase lays in the inhibiting effect of free ammonia (NH_3) on the methanogens generated within the reactor. This inhibitory effect was not taken into account by the *AM2* because the ammonium equilibrium was not included. Another significant comment concerning S_1 and S_2 (Figs. 2 and 3 (a)) is that at day 100 the influent concentration changed which entailed a change in S_1 and S_2, though with different behaviour for the *ADM1* and the *AM2*. For the *AM2*, the concentrations became lower because during the first step increase the biomass concentration has increased and therefore the steady state at day 100 was different from the initial one; therefore, after the step decrease at day 100, S_1 and S_2 moved back to the previous steady state value which was reached at the end of the transient response.

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The biomass concentration of the two trophic groups were well simulated (Fig.3 (b), (c)) in the case of the *AM2* while alkalinity *Z* (Fig. 3 (e)) seemed to remain unaffected by the influent variation, revealing its non-reactivity. This is due to the fact that the *AM2* considered alkalinity *Z* as related to a non-reactive species. Consequently, the responses of B, C, pH and CO_2 (Fig. 3 (g), (d), (h), (f)) were far from reproducing the *ADM1*'s original dynamics. The results showed a very good prediction for the dynamics for gas outflow for carbon dioxide and methane (Fig. 3 (i), (j)).

It should be noted that all these simulations were repeated with a 20% decrease in the influent *COD* and the results obtained were symmetrical with the initial results.

Using the *AM2HN*, the comparison of the outputs by means of normalized dimensionless variables showed a large improvement in the modelling of inorganic species. With the introduction of the hydrolysis step (Fig. 4 (a)), the S_1 included only soluble components while the particulate components involved were expressed in the aggregated variable X_T (see Table 1). Thus, the S_1 dynamics from the *ADM1* in this case were no longer a first-order type. Thus, the introduction of X_T allowed for a much better description of the anaerobic digestion process of particulate organic matter as simulated by the *ADM1*. In fact, the *AM2HN* correctly described the first-order dynamics of the hydrolytic step (Fig. 4 (j)) and the enzymatic degradation of the soluble components included in S_1 (Fig. 4 (a)).

The dynamics of the alkalinity Z were modelled perfectly (Fig. 4 (b)) which was not the case in the *AM2*. There was a substantial improvement in the prediction of pH (Fig. 4 (i)) as well as in the prediction of C and B (Fig. 4 (e and h)) which displayed good correlation with the simulations. As for the gas producing gaseous species, the simulation results showed a good prediction of the dynamic gas outflow of carbon dioxide and methane (Figs. 4 (k) and (l)).

Furthermore, we checked the robustness of the *AM2HN* with regard to the input variability. We should stress here that the *ADM1* that we used as a case-study was calibrated on WAS as

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the typical feed. So, we made limited changes in the feed composition (percentage of proteins, sugars, and fats) to avoid:

- moving to conditions for which the *ADM1* itself may not larger be applicable;
- simulating conditions that are no longer realistic (if waste sludge is the typical feed, it is not realistic to expect great variations in the influent's chemical composition).

For these reasons we limited the percentage of variations of the individual components X_{ch}, X_{pr} and X_{li} of $X_{T,in}$ to 10% in addition to the 20% of variation in the total influent *COD*. This led to the following three cases:

- Case 1: $X_{T,in} = 1.2(X_{c,in} + 1.1X_{ch,in} + X_{pr,in} + X_{li,in})$ leading to a total change of 21,88% of the total influent COD
- Case 2: $X_{T,in} = 1.2(X_{c,in} + X_{ch,in} + 1.1X_{pr,in} + X_{li,in})$ leading to a total change of 27,5% of the total influent COD
- Case 3: $X_{T,in} = 1.2(X_{c,in} + X_{ch,in} + X_{pr,in} + 1.1X_{li,in})$ leading to a total change of 21,88% of the total influent COD

which means that we were exploring the case of an increase in the total load plus a "reasonable" modification in the quality of the feed. [1]

The results of these new simulations are reported in Figures 5, 6 and 7, where it can be seen that the results were very similar to those previously obtained (Fig. 4) which showed the same dynamics.

It is clear that by introducing variations in the influent load and composition did not significantly change predictions about the dynamics of the *AM2HN*, suggesting a definite robustness of this model for a limited variability in the quality of the input, i.e. in the chemical composition of the organic matter fed to the digester.

[1]We obtained similar values for the percentage of change in cases 1 and 3 because the input values $X_{pr,in}$ and $X_{li,\ in}$ were equal (see Appendix A).

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6. Assessment of sensitivity

It was important to evaluate the sensitivity of the *AM2HN* with respect to the hydrolysis parameter k_{hyd}, that was not formerly included in the AM2, and then compare it with that of the *ADM1* with respect to the same parameter. If we take a deviation Δp_i for the parameter p_i, we can estimate the sensitivity of a state with respect to the parameter involved using the index of sensitivity proposed by Dochain and Vanrolleghem (2001) [13], as follows:

$$\delta_{ij} = \frac{p_i}{y_i(p_i)} . \frac{y_j(p_i + \Delta p_i) - y_j(p_i)}{\Delta p_i} .100 \quad (25)$$

For each parameter p_i, an absolute variation Δp_i of 20% of the default value was applied. The index of sensitivity was then classified in the following way:

$1 = \delta_{ij} < 30\%$;

$2 = 30\% \leq \delta_{ij} \leq 60\%$;

$3 = \delta_{ij} > 60\%$.

The results of the study of the *ADM1*'s and *AM2HN*'s sensitivity to the hydrolysis parameter showed that the sensitivity of the states involving the hydrolysis parameter, i.e. S_1 and X_T, were the same: in the range of 3 in both models.

7. Conclusions and perspectives

The original *AM2* version proposed in Bernard et al. (2001) [2] reproduces quite faithfully the biological anaerobic digestion process, as simulated by the *ADM1*, assuming that the largest part of the organic matter was soluble.

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By modifying the original *AM2* and by using an association procedure, we obtained a reduced model that closely reproduced *ADM1* behaviour with far fewer variables, processes and parameters. Indeed, the *AM2HN* gave an accurate description of the dynamics of the *ADM1*, especially for the inorganic species. Moreover, gas outflows were perfectly reproduced, establishing the consistency of the *AM2HN* in its prediction of the dynamic response of the biogas and its components.

Furthermore, the sensitivity study showed that the state variables considered for the *ADM1* and the *AM2HN* have the same sensitivity with regard to the hydrolysis parameter, indicating that the introduction of new processes in the *AM2* preserved the sensitivity of the states in this respect. The *AM2HN* also revealed its robustness with regard to moderate variations in the chemical composition of the influent.

This study was successful for waste-activated sludge as the AD feed but a similar procedure can be applied in other case studies once a calibrated *ADM1* becomes available.

Perspectives for this work include the effective use of the *AM2HN* for control design purposes and the study of this model from a mathematical viewpoint, notably to progress in the study of the qualitative properties of the *ADM1* which are still not clearly understood.

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Figures And Tables:

Figure 1. Response of q_{ch_4} to 20% disturbance in the influent *COD* concentration. *ADM1*: solid line, *AM2*: dashed line.

Figure 2. Response of S_1^* to +20% disturbances in the influent *COD* concentration. ADM1: solid line, *AM2*: dashed line

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Figure 3. Response of (a) S_2^* (b) X_1^* (c) X_2^* (d) C^* (e) Z^* (f) CO_2^* (g) B^* (h) pH^* (i) q_{CH4}^* (j) q_C^* to +20% disturbance in the influent *COD* concentration. *ADM1*: solid line, *AM2*: dashed line.

Figure 4. Response of (a) S_1^* (b) S_2^* (c) X_1^* (d) X_2^* (e) C^* (f) Z^* (g) CO_2^* (h) B^* (i) pH^* (j) X_T^* (k) q_C^* (l) q_{CH4}^* to +20% disturbance in the influent *COD* concentration. *ADM1*: solid line, *AM2HN*: dashed line.

Figure 5. Response of (a) C^* (b) Z^* (c) CO_2^* (d) B^* (e) pH^* (f) X_T^* (g) q_C^* (h) q_{CH4}^* to case 1 (+21.88% disturbance in the influent COD concentration). *ADM1*: solid line, AM2HN: dashed line.

Figure 6. Response of (a) C^* (b) Z^* (c) CO_2^* (d) B^* (e) pH^* (f) X_T^* (g) q_C^* (h) q_{CH4}^* to case 2 (+27.5% disturbance in the influent COD concentration). *ADM1*: solid line, *AM2HN*: dashed line.

Figure 7. Response of (a) C^* (b) Z^* (c) CO_2^* (d) B^* (e) pH^* (f) X_T^* (g) q_C^* (h) q_{CH4}^* to case 3 (+21.88% disturbance in the influent COD concentration). *ADM1*: solid line, *AM2HN*: dashed line.

Table 1. *AM2* and*AM2HN* variables and their proposed correspondence with *ADM1* variables.

	Variable	Model	ADM1	Conversion
a r	X_T [kgCOD m^{-3}]	*AM2*	-	-

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		AM2HN	X_c, X_{ch}, X_{pr}, X_{li} [kgCOD m^{-3}]	$X_c + X_{ch} + X_{pr} + X_{li}$
	S_1[kgCOD m^{-3}]	AM2	S_{su}, S_{aa}, S_{fa}, X_c, X_{ch}, X_{pr}, X_{li}[kgCOD m^{-3}]	$S_{su} + S_{aa} + S_{fa} + X_c + X_{ch} + X_{pr} + X_{li}$
		AM2HN	S_{su}, S_{aa}, S_{fa}[kgCOD m^{-3}]	$S_{su} + S_{aa} + S_{fa}$
	S_2 [mM]	AM2, AM2HN	S_{va}, S_{bu}, S_{pro}, S_{ac}[kgCOD m^{-3}]	$\frac{Sva}{(208} + \frac{Sbu}{160} + \frac{Spro}{112} + \frac{Sac}{64)}.1000$
	X_1 [kgVS m^{-3}]	AM2, AM2HN	X_{su}, X_{aa}, X_{fa}[kgCOD m^{-3}]	$(X_{su} + X_{aa} + X_{fa}) / 1.55$
	X_2 [kgVS m^{-3}]	AM2, AM2HN	X_{ac}, X_{h_2}, X_{c_4}, X_{pro} [kgCOD m^{-3}]	$(X_{ac} + X_{h_2} + X_{c_4} + X_{pro}) / 1.55$
	C [mM]	AM2, AM2HN	S_{ic} [M]	$S_{ic} * 1000$
	Z [mM]	AM2, AM2HN	S_{va}, S_{bu}, S_{pro}, S_{ac} [kgCOD m^{-3}], S_{hco3} [M]	$\frac{Sva}{(208} + \frac{Sbu}{160} + \frac{Spro}{112} + \frac{Sac}{64)} + S_{hco_3}).1000$
Calculation variables	CO_2 [mM]	AM2, AM2HN	S_{co_2} [M]	$S_{co_2}.1000$
	B [mM]	AM2, AM2HN	S_{hco_3} [M]	S_{hco_3} 1000
	pH [-]	AM2, AM2HN	pH [-]	-
	Z_0 [mM]	AM2, AM2HN	S_{an} [M]	$S_{an} * 1000$
	q_C [mM d^{-1}]	AM2, AM2HN	$\rho_{T,10}$ [M d^{-1}]	$\rho_{T,10} * 1000$

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q_{ch4} [mM d^{-1}]	AM2, AM2HN	$\rho_{T,9}$ [M d^{-1}]	$\rho_{T,9}$ * 1000
P_C [atm]	AM2, AM2HN	P_{gas,co_2} [bar]	$\frac{P_{gas,co_2}}{P_{gas,co_2}+P_{gas,ch_4}}$

Table 2. Steady-state data set generated by the *ADM1* simulations (digestion of waste-activated sludge) and used to calibrate both the original *AM2* model and the proposed improved version *AM2HN*.

COD /m^3	S_2 mM	X_1 kgVS m^{-3}	X_2 kgVS m^{-3}	X_T kgVS m^{-3}	Z mM	C mM	CO_2 mM	B mM	pH -	q_C kmol m^{-3} d^{-1}	P_C atm
0.92	82.6	1.42	1.12	1.30	145	75	12.4	63	7.01	42.8	0.4
0.34	31.9	1.39	1.19	0.92	144	123	10.9	112	7.32	27.9	0.3
0.25	15.3	1.35	1.19	0.78	144	139	10.5	129	7.40	22.6	0.3
0.20	8.9	1.32	1.17	0.68	144	146	10.3	136	7.43	19.0	0.3
0.15	5.4	1.27	1.13	0.58	145	150	10.1	140	7.45	15.3	0.3
0.13	4.3	1.24	1.10	0.53	146	151	10.0	141	7.46	13.6	0.3
0.12	3.4	1.19	1.06	0.47	146	153	9.9	143	7.47	11.7	0.3
0.11	3.0	1.16	1.04	0.44	147	153	9.8	144	7.47	10.6	0.3
0.10	2.6	1.12	1.00	0.40	147	154	9.8	145	7.48	9.4	0.3
0.08	2.1	1.05	0.94	0.35	148	155	9.7	146	7.48	7.9	0.3
0.06	1.4	0.86	0.77	0.24	150	159	9.6	149	7.50	4.8	0.3
0.05	1.2	0.72	0.65	0.19	152	160	9.5	151	7.51	3.5	0.3
0.05	1.0	0.62	0.56	0.15	153	162	9.5	152	7.51	2.8	0.3

Table 3. Comparison between the yield coefficients of *AM2*, *AM2HN* and the *ADM1* mean values.

Yield coefficient	Unit	*ADM1*	*AM2*	*AM2HN*

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			Mean	St.dev.	Mean	St.dev.
Y_1	$kgCOD_X(kgCOD_S)^{-1}$	0.08				
$1/k_1$	$kgVS_X(kgCOD_S)^{-1}$		0.07	0.00	0.08	0.00
Y_2	$kgCOD_X(kgCOD_S)^{-1}$	0.052				
$1/k_3$	$kgVS_X(molCOD_S)^{-1}$		0.003	0.00	0.003	0.00

Table 4. Comparison between the kinetic parameters of *AM2*, *AM2HN* and the *ADM1* mean values.

Parameters	Unit	*ADM1*	*AM2*		*AM2HN*	
			Mean	St.dev.	Mean	St.dev.
$\mu_{1,max}$	$[d^{-1}]$	2.45	0.25	0.10	0.33	0.07
K_{S2}	$[gCOD\ L^{-1}]$	0.40	0.22	0.08	0.40	0.09
$\mu_{2,max}$	$[d^{-1}]$	1.06	0.13	0.16	0.13	0.16
K_{S2}	$[mmol\ L^{-1}]$	1.76	2.93	3.62	2.93	3.62
k_{hyd}	$[d^{-1}]$	10	-	-	5	0
k_{La}	$[d^{-1}]$	200	24	0	24	0

APPENDIX A

ADM1 constituents	Influent concentrations (input values)

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$S_{su,in}$	0.01kgCOD m^{-3}
$S_{aa,in}$	0.001kgCOD m^{-3}
$S_{fa,in}$	0.001kgCOD m^{-3}
$S_{va,in}$	0.001kgCOD m^{-3}
$S_{bu,in}$	0.001kgCOD m^{-3}
$S_{pro,in}$	0.001kgCOD m^{-3}
$S_{ac,in}$	0.001kgCOD m^{-3}
$S_{h2,in}$	1.0E-08kgCOD m^{-3}
$S_{ch4,in}$	1.0E-05kgCOD m^{-3}
$S_{ic,in}$	0.04kmol m^{-3}
$S_{in,in}$	0.01kmol m^{-3}
$S_{i,in}$	0.02kgCOD m^{-3}
$S_{cat,in}$	0.04kmol m^{-3}
$S_{an,in}$	0.02kmol m^{-3}
$X_{su,in}$	0kgCOD m^{-3}
$X_{aa,in}$	0.01kgCOD m^{-3}
$X_{fa,in}$	0.01kgCOD m^{-3}
$X_{c4,in}$	0.01kgCOD m^{-3}
$X_{pro,in}$	0.01kgCOD m^{-3}
$X_{ac,in}$	0.01kgCOD m^{-3}
$X_{h2,in}$	0.01kgCOD m^{-3}
$X_{i,in}$	25kgCOD m^{-3}
$X_{c,in}$	2kgCOD m^{-3}
$X_{ch,in}$	5kgCOD m^{-3}
$X_{pr,in}$	20kgCOD m^{-3}
$X_{li,in}$	5kgCOD m^{-3}

Table A.1 - Steady-state input values of the waste-activated sludge (Rosen and Jeppsson, 2006)

APPENDIX B

Parameter	Meaning	Units	*AM2* value	S.D	*AM2HN* value	*S.D*

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$\mu_{1,\max}$	Maximum acidogenic biomass growth rate	$[d^{-1}]$	0.25	0.10	0.33	0.07
K_{S1}	Half-saturation constant associated with S_1	$[gCOD\ l^{-1}]$	0.22	0.08	0.40	0.09
$\mu_{2,\max}$	Methanogenic biomass growth rate	$[d^{-1}]$	0.13	0.16	0.13	0.16
K_{S2}	Half-saturation constant associated with S_2	$[mmol\ L^{-1}]$	2.93	3.62	2.93	3.62
K_{I2}	Inhibition constant associated with S_2	$[mmol\ L^{-1}]$	207	76.14	207	76.14
k_{hyd}	Maximum specific hydrolysis rate	$[d^{-1}]$	n.a.	-	5.02	0
k_{La}	Liquid/gas transfer rate	$[d^{-1}]$	24	0	24	0
k_1	Yield for substrate COD degradation (acidogenesis)	$[gCOD\ gVS^{-1}]$	23	0	20	0
k_2	Yield for VFA production (acidogenesis)	$[mmol\ gVS^{-1}]$	464	0	464	0
k_3	Yield for VFA consumption (methanogenesis)	$[mmol\ gVS^{-1}]$	514	0	514	0
k_4	Yield for CO_2 production (acidogenesis)	$[mmol\ gVS^{-1}]$	310	0	310	0
k_5	Yield for CO_2 production (methanogenesis)	$[mmol\ gVS^{-1}]$	600	0	600	0
k_6	Yield for CH_4 production (methanogenesis)	$[mmol\ gVS^{-1}]$	253	0	253	0

Table B.1 - Estimated values for the *AM2* and the *AM2HN* parameters

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