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Chemical Engineering Journal 141 (2008) 75–88

Chemical Engineering Journal

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# Implementation of IWA anaerobic digestion model No. 1 (ADM1) for simulating the thermophilic anaerobic co-digestion of olive mill wastewater with olive mill solid waste in a semi-continuous tubular digester

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Received 15 January 2007; received in revised form 26 July 2007; accepted 24 October 2007

**Abstract**

The anaerobic digestion model No. 1 (ADM1) developed by the international water association (IWA) task group for mathematical modelling of anaerobic digestion processes is the most sophisticated model established for full-scale industrial plants design, systems operational analysis and control, assisting technology transfer from research to industry and a common basis for further model development and validation studies. In this work the original ADM1, implemented in the simulation software package MATLAB/Simulink, was adapted and applied to replicate with reasonable degree of accuracy the thermophilic anaerobic co-digestion of olive mill wastewater (OMW) with olive mill solid waste (OMSW) in a semi-continuous tubular digester. The data set from lab-scale experiments described in our previous work was used to calibrate and validate the model. The simulations results indicated that the modified ADM1 was able to predict reasonably well the steady-state results of gas flows, methane and carbon dioxide contents, pH and total volatile fatty acids (TVFA) observed with all influents concentrations (43, 67 and 130 g COD/l) digested at the hydraulic retention times (HRTs) of 24 and 36 days. Also the reactor failure observed at a HRT of 12 days for an influent concentration of 67 g COD/l was predicted and well justified by the modified ADM1.


*Keywords:* Anaerobic co-digestion; Mathematical modelling; Simulation; ADM1; Tubular digester; OMW; OMSW; Thermophilic temperature

## 1. Introduction

Treatment and disposal of olive mill wastes and especially olive mill wastewaters (OMWs) represent one of the main environmental concerns of olive oil producing countries. These liquid wastes are acid influents containing low amount of ammonium nitrogen and heavily loaded with pollutants than ordinary domestic wastewaters (pH = 4.9; TCOD = 202 g/l and $NH_4^+$–N = 100 mg N/l) [1]. The high polluting activity of OMW is linked with high content of dissolved and particulate organic compounds such as sugars, carbohydrates, lipids, proteins, volatile fatty acids (VFA) and phenolic compounds (carbohydrates = 13.79 g/l; proteins = 3.95 g/l; lipids = 18 g/l and TVFA = 0.3 g/l) [2]. Furthermore OMW contains high concentration of potassium, calcium, magnesium, phosphate, chloride and other salts [3]. Applying anaerobic digestion either at mesophilic or thermophilic temperature to treat OMW without previous treatment is failed due to the previous mentioned characteristics of OMW. But, the co-digestion of OMW with other organic wastes containing high level of ammonium nitrogen such as piggery effluents and dairy wastewaters [2,4] or cattle manures [5] or olive mill solid wastes (OMSWs) [6], to compensate the lack in OMW, has proven their success in treating OMW by anaerobic digestion process because it does not require any addition of chemical substances which are not economically and environmentally desirable. Subsequently two multistep dynamic models have been developed to predict accurately gas flow, pH and VFA under different feed concentrations, to provide a guide line for operation and optimisation of anaerobic reactors and to improve understanding of the difficulties observed when

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doi:10.1016/j.cej.2007.10.024

**Nomenclature**

| | |
|---|---|
| COD | chemical oxygen demand |
| $CH_4$ | methane (%) |
| $CO_2$ | carbon dioxide (%) |
| DE | differential equations |
| HRT | hydraulic retention time (days) |
| LCFA | long chain fatty acids |
| $NH_4^+$–N | total ammonium nitrogen (mg N/l) |
| OMW | olive mill wastewater |
| OMSW | olive mill solid waste |
| OLR | organic loading rate (g COD/l/day) |
| ODE | ordinary differential equations |
| $PO_4^{3-}$–P | total mineral phosphate (mg P/l) |
| SCOD | soluble chemical oxygen demand (g COD/l) |
| TS | total solids (g/l) |
| TVS | total volatile solids (g/l) |
| TCOD | total chemical oxygen demand (g COD/l) |
| TVFA | total volatile fatty acids (g COD/l) |
| TK-N | total kjeldahl nitrogen (g/l) or (g/kg TS) |
| VFA | volatile fatty acids |

co-digesting OMW with other wastes. The first model is developed by Gavala et al. for the co-digestion of OMW, piggery effluents and dairy wastewaters in a continuous stirred tank (CSTR) and batch digesters [2,4]. This model considers four steps of degradation processes (hydrolysis, acidogenesis, acetogenesis and methanogenesis) and three bacterial groups (the acidogens, the acetogens and the acetoclastic methanogens).

It is assumed that OMW, piggery effluents and dairy wastewaters are mainly consisted of carbohydrates (soluble and insoluble), proteins (soluble and insoluble) and VFA. Besides, this model is based on batch kinetic experiments and is capable of predicting adequately the COD and VFA. But, it neither predicts pH and biogas composition nor takes into account the inhibitory effect by low pH values, high concentration of VFA and shortage in ammonium nitrogen. The second model, which is more sophisticated than the previous, is developed by Angelidaki et al. for the anaerobic co-digestion of OMW and cattle manures in a continuous stirred tank (CSTR) at thermophilic temperature [5]. The substrates (OMW and cattle manures) are described by their composition of basic organic components: carbohydrates, lipids, proteins, long chain fatty acids (LCFA), VFA and important inorganic components (ammonium, phosphate, cations and anions). Also, it is assumed that insoluble proteins and carbohydrates are lumped together and are stoichiometrically represented as glucose units with an amount of ammonia attached. The model considers four steps of degradation processes (hydrolysis, acidogenesis, acetogenesis and methanogenesis) and six bacterial groups (the glucose fermenting acidogens, lipolytic bacteria, LCFA degrading acetogens, propionate and butyrate degrading acetogens and acetoclastic methanogens). Equilibrium relationships of ammonia, carbon dioxide, and pH, as well as gas phase dynamics and temperature effects are included in the model. Furthermore, free ammonia inhibition of the acetoclastic step and acetate inhibition of the acetogenic steps are considered in the model. Volatile fatty acids (VFA) inhibition of the initial enzymatic hydrolytic step and inhibition caused by LCFA are also considered. This model is capable of predicting pH, VFA, methane flow and effluent $NH_4^+$ content and is used later as a basis to develop more sophisticated models [7].

Consequently, and to respond the increasing need for accurate modelling of anaerobic degradation of mixed complex wastes, in recent years, an intensive and fruitful collaboration between a number of international experts in anaerobic process analysis, modelling and simulation has succeeded in developing the most sophisticated dynamic model known as anaerobic digestion model No. 1 (ADM1) [8]. This model describes complex substrates by their general composition (carbohydrates, lipids, proteins, inerts, sugars, amino acids, LCFA, VFA, $CO_2$, $NH_4^+$, cations and anions). It predicts so many dynamic species (gas flow, $CH_4$, $CO_2$, $H_2$, $NH_4^+$, VFA, COD, alkalinity, etc.) and can serve as a tool to design full-scale industrial plants, to assist their operational management and to predict their process performance and behaviour over a range of design and operating conditions. Besides, it can be used either as a common basis for further development or as a common platform for dynamic simulation for a variety of anaerobic processes. Afterwards, many implementations of this powerful tool have been tested and proved their success in simulating the anaerobic digestion of several organic wastes such as: industrial wastewaters [9]; sludge from wastewater treatment plants [10,11]; sewage sludge [12]; black water from vacuum toilet [13]; olive mill solid wastes [14]. However, the ADM1 has never been applied by any researcher to simulate the anaerobic digestion of OMW either alone nor mixed with other solid wastes and mainly OMSW. So, taking into account the ADM1 potential advantages in modelling and continuing the research of ADM1 implementations for simulating the anaerobic digestion of more complex organic mixed substrates such as the mixture of OMW with OMSW, the main objective of the present work is to develop and implement the ADM1 for simulating the thermophilic anaerobic co-digestion of OMW with OMSW in a semi-continuous tubular reactor working under different operating conditions. Then, it will be calibrated and validated using some lab-scale data and experimental results from our previous work [6].

## 2. ADM1 theoretical background

### 2.1. Description and basic concepts

The ADM1 is a structured model that reflects the major processes that are involved in the conversion of complex organic substrates (polymers) into methane and carbon dioxide and inert by products. The model includes disintegration of complex solids (non biological step) into carbohydrates, proteins, lipids and inert substances (soluble and particulate inerts). Then, the first three products of disintegration are hydrolysed

(enzymatic step) to sugars, amino acids and LCFA, respectively. Afterwards, sugars and amino acids are fermented to produce VFA, hydrogen and carbon dioxide (acidogenesis). LCFA, propionate, butyrate and valerate are oxidized anaerobically to produce acetate, carbon dioxide and hydrogen (acetogenesis). Finally, methane is produced by both cleavage of acetate to methane (acetoclastic methanogenesis) and reduction of carbon dioxide by molecular hydrogen to produce methane (hydrogenotrophic methanogenesis). To address these mechanisms, the model employs state variables to describe the behaviour of soluble and particulate components submitted to anaerobic digestion. All organic species and molecular hydrogen are described in terms of chemical oxygen demand (COD). Nitrogenous species and inorganic carbon species are described in terms of their molar concentrations. Soluble components are those that can pass through microbial cellular walls and include the monomers of complex polymers (sugars, amino acids, LCFA), VFA (propionate, butyrate, valerate, acetate), hydrogen, methane and $CO_2$. Whereas, particulate species consist of either active biomass species or particulate substances that are incapable of directly passing through bacterial cell walls [11]. The microbial species that are considered in the model include sugar fermenters, amino acid fermenters, LCFA oxidizers, butyrate and valerate oxidizers, propionate oxidizers, acetoclastic methanogens and hydrogenotrophic methanogens.

Non-microbial particulate species include complex organics that either enter the process in the influent or that result from the death and decay of microbial species and the products of disintegration of the complex organics. This latter group consists of carbohydrates, proteins and lipids [11]. In addition to the organic species, the model addresses inorganic carbon (carbon dioxide and bicarbonate), nitrogenous species (ammonia and ammonium), anions and cations.

### 2.2. Growth kinetics

Substrates conversion processes are described by a number of kinetic expressions that describe the conversion rates in terms of substrate concentrations and rate constants. The disintegration of composite substrates and hydrolysis of carbohydrates, proteins and lipids are described by first order rate expressions. Monod-type growth kinetic expressions, with pH inhibition and non competitive inhibition by TVFA, free ammonia and hydrogen, are used as basis for all inter-cell biochemical reactions of substrates uptake in acidogenic and acetogenic steps. Endogenous decay processes are represented by first order kinetic expressions and dead biomass is maintained in the system as composite particulate material [8].

### 2.3. Basic equations

The original ADM1 is a set of 32 differential equations (DE) for modelling the rate change of concentrations of different species contained in liquid and gas phases as follows: 10 (DE) for soluble matter degradation processes and 2 (DE) for inorganic carbon (IC) and inorganic nitrogen (IN) modelling; 4 (DE) for particulate matter degradation processes; 8 (DE) for biomass concentrations modelling; 2 (DE) for cations and anions modelling and an additional 6 (DE) for acid–base reactions in order to describe the effect of physicochemical states, such as pH, upon the biochemical reactions. More details about the elaboration of these DE are presented in the IWA-ADM1 report of Batstone et al. [8] that was updated later by Rosen and Jeppsson [15].

### 2.4. Inhibition functions

In the ADM1 report of Batstone et al. [8], different inhibition functions were suggested with emphasis in modelling the effects

Table 1
Characteristics of the OMW and the sludge used in ADM1 as input main influent and initial conditions, respectively

| Parameters | Units | OMW initial characteristics | Sludge (initial characteristics) | Sludge after batch mode fermentation |
|---|---|---|---|---|
| pH | – | 7.5 ± 0.3 | 7.5 ± 0.2 | 7.5 ± 0.1 |
| TCOD | g COD/l | 130 ± 3.5 | 37.5 ± 0.5 | 20.56 ± 0.7 |
| SCOD | g COD/l | 80 ± 2.5 | 0.04 ± 0.005 | 1.72 ± 0.4 |
| Total carbohydrates | g COD/l | 35 ± 1.5 | 10.05 ± 0.3 | 0.7 |
| Total proteins | g COD/l | 14 ± 1.5 | 8.4 ± 0.2 | 0.8 |
| Total Lipids | g COD/l | 25 ± 1.5 | 2.03 ± 0.005 | 0.3 |
| Total Inerts | g COD/l | 26 ± 1.5 | 17 ± 0.25 | 19 |
| Sugars (monosaccharide) | g COD/l | 18 ± 1.5 | 0.015 ± 0.01 | 0.08 |
| Amino acids | g COD/l | 6.5 ± 1.5 | 0.0015 ± 0.001 | 0.05 |
| LCFA | g COD/l | 10 ± 1.5 | 0.0 ± 0.0 | 0.03 |
| Soluble inerts | g COD/l | 8 ± 1.5 | 0.0 ± 0.0 | 1.5 |
| Acetic acid | g COD/l | 7.5 ± 0.5 | 0.0 ± 0.0 | 0.02 |
| Propionic acid | g COD/l | 3.75 ± 0.5 | 0.0 ± 0.0 | 0.01 |
| Butyric acid | g COD/l | 4.85 ± 0.5 | 0.01 ± 0.002 | 0.01 |
| Valeric acid | g COD/l | 1.85 ± 0.5 | 0.01 ± 0.008 | 0.02 |
| Alkalinity | g $CaCO_3$/l | 3.8 ± 0.3 | 3.8 ± 0.35 | 3.4 ± 1.2 |
| Inorganic nitrogen (IN) | g N/l | 750 ± 55 | 1.3 ± 0.05 | 1.6 ± 0.15 |
| Inorganic carbon (IC) | mol/l | 0.074 ± 0.006 | 0.062 ± 0.006 | 0.054 |
| Anions | mol/l | 0.073 ± 0.003 | 0.091 ± 0.002 | 0.091 |
| Cations | mol/l | 0.464 ± 0.018 | 0.027 ± 0.004 | 0.027 |

(*) Each value is an average of three replicates. ± shows standard deviations among replicates.

of pH, insufficient nitrogen inhibition, hydrogen and free ammonia inhibition. The implemented inhibition functions used in the ADM1 kinetic rate equations for this work were those updated by Rosen and Jeppsson [15].

## 3. ADM1 implementation

### 3.1. Substrates definitions and hypothesis

According to the original ADM1 structure sludge, OMW and OMSW were represented by their main components. OMW (primary organic substrate) and the sludge (substrate used as inoculums at initial conditions) were represented as soluble substrates (sugars, amioacids, LCFA, VFA, soluble inerts, inorganic carbon, inorganic nitrogen, anions and cations) and particulates substrates (carbohydrates, proteins, lipids and particulate inerts) while the dry OMSW was represented as composites substrates. Phenol compounds and others contained in OMW and OMSW were assumed negligible due to the fact that they were not taken into account by the original ADM1. Tables 1 and 2 show the characteristics of OMW, OMSW and the sludge (before and after batch mode period) used to determine the steady-state input variables values and the the initial values of ADM1 steady-state variables respectively, for the ADM1 simulations of OMW mixed with OMSW. The concentrations of main cations (sodium, potassium, calcium, magnesium and manganese) and main anions (phosphate, chloride, sulphate and nitrate) contained in OMW and sludge are given in Table 3.

### 3.2. Suggested modification to ADM1

The inhibition factor $I_5$ applied to the rate of acetate uptake of the original ADM1 updated by Rosen and Jeppsson [15] was modified as follows:

$$I_5 = I_{\mathrm{pH,ac}}\, I_{\mathrm{IN,lim}}\, I_{\mathrm{NH_3}}\, I_{\mathrm{TVFA}} \quad (1)$$

Instead of its original expression:

$$I_5 = I_{\mathrm{pH,ac}}\, I_{\mathrm{IN,lim}}\, I_{\mathrm{NH_3}} \quad (2)$$

where $I_{\mathrm{TVFA}}$ is a non competitive function added to take into account the inhibition of methanogenic steps by TVFA and expressed as follows:

$$I_{\mathrm{TVFA}} = \frac{1}{1 + S_{\mathrm{TVFA}}/K_{\mathrm{I,TVFA}}} \quad (3)$$

This inhibition term was added to take into account and predict effectively the inhibition of methanogenic process by high TVFA concentration mainly at low HRT which is not predicted quite well by the original ADM1.

Table 2
Characteristics of OMSW used as co-substrate

| Parameters | Units | OMSW Average values |
|---|---|---|
| TS | % | 97 ± 2 |
| TVS | g/kg TS | 970 ± 0.5 |
| TCOD | g/kg TS | 1180 ± 2 |
| Carbohydrates | g/kg TS | 365 ± 10 |
| Total Lignin | g/kg TS | 450 ± 10 |
| Total Proteins | g/kg TS | 125 ± 5 |
| Total Lipids | g/kg TS | 110 ± 5 |
| Total polyphenols | g/kg TS | 23 ± 5 |
| TK-N | g N/kg TS | 20 ± 1.5 |

(*) Each value is an average of three replicates. ± shows standard deviations among replicates.

Table 3
Concentrations of main anions and cations in OMW and sludge

| Mineral Elements | Units | OMW | Sludge |
|---|---|---|---|
| Phosphate ($PO_4^{3-}$) | mg/l | 980 ± 20 | 1050 ± 5 |
| Chloride ($Cl^-$) | mg/l | 2230 ± 80 | 2000 ± 50 |
| Sulphate ($SO_4^{2-}$) | mg/l | 20 ± 5 | 2200 ± 70 |
| Nitrate ($NO_3^-$) | mg/l | 10 ± 5 | 20 ± 6 |
| Total anions | mol/l | 0.073 ± 0.003 | 0.091 ± 0.002 |
| Sodium ($Na^+$) | mg/l | 450 ± 20 | 210 ± 30 |
| Potassium ($K^+$) | mg/l | 3750 ± 500 | 240 ± 50 |
| Calcium ($Ca^{2+}$) | mg/l | 12950 ± 100 | 205 ± 25 |
| Magnesium ($Mg^{2+}$) | mg/l | 575 ± 40 | 125 ± 15 |
| Manganese ($Mn^+$) | mg/l | 80 ± 30 | 50 ± 10 |
| Total cations | mol/l | 0.464 ± 0.018 | 0.027 ± 0.004 |

(*) Each value is an average of three replicates. ± shows standard deviations among replicates.

### 3.3. ADM1 parameters

ADM1 parameters values (stoichiometric, physicochemical and kinetic parameters) were taken from the literature relative to the original ADM1 [8,15]. All physicochemical parameters values, such as equilibrium coefficients and constants were those of the original ADM1 without any modification. Also, most of the kinetic parameters and stoichiometric coefficients implied in the rate equation matrix were those of the original ADM1 without any modification due to the fact that they were considered fixed since they were generally known to have limited variability in anaerobic systems [8]. The modified stoichiometric parameters were determined according to the OMSW chemical composition as presented in Table 5. Whereas, the modified kinetic parameters were determined using optimisation methods after calibration with the experimental results of the thermophilic anaerobic co-digestion of OMW with OMSW.

### 3.4. Computational implementation

The set of ordinary differential equations of the ADM1 model was coded and implemented using Matlab 7.0 and integrated with the ODE15s solvers which solves stiff ODE systems as recommended by Rosen et al. [16].

### 3.5. Lab-scale experimental data

The experimental data against which the ADM1 simulations were compared were obtained from our previous work [6].

In fact, the anaerobic co-digestion experiments of OMW with OMSW under thermophilic conditions (55 °C) were carried out using three different influent concentrations composed of OMW

Table 4
Initial and estimated values of kinetic parameters

| Kinetic parameters | Names | Units | Initial values | Estimated values |
|---|---|---|---|---|
| $k_{dis}$ | Disintegration constant | $day^{-1}$ | 0.115 | 0.03 |
| $k_{hyd,Ch}$ | Carbohydrate hydrolysis constant | $day^{-1}$ | 0.35 | 0.35 |
| $k_{hyd,Pr}$ | Proteins hydrolysis constant | $day^{-1}$ | 0.20 | 0.20 |
| $k_{hyd,Li}$ | Lipids hydrolysis constant | $day^{-1}$ | 0.063 | 0.063 |
| $k_{m,ac}$ | Maximum uptake rate for acetate utilisers | $day^{-1}$ | 8 | 21.31 |
| $k_{m,pro}$ | Maximum uptake rate for propionate utilisers | $day^{-1}$ | 13 | 11 |
| $k_{m,But}$ | Maximum uptake rate for butyrate utilisers | $day^{-1}$ | 20 | 20 |
| $k_{S,ac}$ | Half saturation constant for acetate utilisers | kg COD/$m^3$ | 0.15 | 0.96 |
| $k_{S,pro}$ | Half saturation constant for propionate utilisers | kg COD/$m^3$ | 0.1 | 0.1 |
| $k_{S,But}$ | Half saturation constant for butyrate utilisers | kg COD/$m^3$ | 0.2 | 0.2 |
| $k_{I,TVFA}$ | TVFA inhibition constant for acetate utilisers | kg COD/$m^3$ | – | 1.932 |
| $k_{I,NH_3}$ | Ammonia inhibition constant for acetate utilisers | kmol/$m^3$ | 0.0018 | 0.00247 |

(43, 67 and 130 g COD/l) and OMSW in semi-continuous tubular digesters of 22 L volume. The amount of the dry OMSW was 56 g TS per litre of OMW. Alkalinity in the form of $Ca(OH)_2$ was added to all influents (5–25 g/l of OMW) to ensure a neutral medium (pH = 7.0–8.0) for the methanogenic bacteria growth. At the beginning of each run all the digesters were inoculated with 18 L of sludge from aerobic urban wastewaters plant (initial characteristics was given in Table 1) and set in batch mode with gradual increase of temperature from 37 to 55 °C (2 °C per day) during 10–15 days until the start-up of biogas production from the sludge. Then, in the run R1 to run R3 each digester was fed with an influent substrate concentration of 43 g COD/l at a HRT of 36, 24 and 12 days, respectively. In the run R4 to run R6, each digester was fed with an influent substrate concentration of 67 g COD/l at a HRT of 36, 24 and 12 days, respectively. Finally, in the run R7 to run R9 each digester was fed with an influent substrate concentration of 130 g COD/l at a HRT of 36, 24 and 12 days, respectively.

## 4. Results and discussion

### 4.1. Model calibration

Experimental results of the thermophilic anaerobic co-digestion of OMW (TCOD = 67g/l) and OMSW at a HRT of 36 days (corresponding to the run R4) were used to assist the model calibration. Initial values of hydrolysis parameters for carbohydrates, proteins and lipids were those suggested by Gavala and co-workers [14,17]. Whereas, all the other initial values of ADM1 parameters were those suggested by Batstone et al. [8] and Rosen and Jeppson [15]. Initial values of the model state variables were taken from the composition of sludge which was presented in Table 1.

Most of these initial values were obtained from simulating the inoculum sludge in batch mode during 10 days using the ADM1. The estimation procedure to identify the most sensitive parameters in this work (disintegration and hydrolysis constants; maximum specific uptake rates; half saturation values; inhibition factor to uptake and decay constants) to fit the model outputs to the set of experimental results was as following: the first step was to set the initial values to all the model parameters. Then an iterative method was applied in adjusting the most sensitive parameters until fitting the ADM1 outputs to the experimental results and especially gas flow, pH and TVFA because these parameters have great impact upon these frequently measured variables. In fact, disintegration rate constant was set initially to 0.115 $day^{-1}$ and the hydrolysis rate constants for carbohydrates, proteins and lipids were set initially to 0.35, 0.2 and 0.063 $day^{-1}$, respectively, as determined previously by Stamatelatou et al. who studied the anaerobic digestion of OMSW under mesophilic and thermophilic conditions [14]. Then an iterative procedure was applied in adjusting especially disintegration rate constant trough fitting the predicted gas flow to measured gas flow. Whereas the hydrolysis rate constants were let without change. The correlated parameters: maximum specific uptake rates ($K_m$) and half saturation values ($K_s$) for acetate, propionate and butyrate were estimated through ADM1 fitting to TVFA experimental data. TVFA and ammonia inhibition parameters for acetate bacteria were adjusted to predict the digester failure at short HRT. The modified stoichiometric parameters were

Table 5
Initial and estimated values of stoichiometric parameters

| Stoichiometric parameters | Names | Units | Original ADM1 suggested values | Estimated values |
|---|---|---|---|---|
| $f_{SI\,Xc}$ | Soluble inert fraction in OMSW | – | 0.1 | 0 |
| $f_{XI\,Xc}$ | Particulate inert fraction in OMSW | – | 0.2 | 0.36 |
| $f_{ch\,Xc}$ | Carbohydrates fraction in OMSW | – | 0.2 | 0.37 |
| $f_{pr\,Xc}$ | Proteins fraction in OMSW | – | 0.2 | 0.13 |
| $f_{li\,Xc}$ | Lipids fraction in OMSW | – | 0.3 | 0.11 |
| $N_{Xc}$ | Nitrogen content in OMSW | kmole N/kg COD | 0.0376/14 | 0.0167/14 |
| $N_I$ | Nitrogen content in inert substrates of OMSW | kmole N/kg COD | 0.06/14 | 0.00 |

determined according to the OMSW chemical composition. Many other parameters were applied without any optimisation. Estimated parameters values having the greatest impact upon the model outputs and fitting better the experimental results are given in Tables 4 and 5. Fig. 1 shows the measured and simulated results of gas flow, methane and carbon dioxide contents, pH and TVFA after model calibration.

As can be seen the biogas flow was predicted quite well at steady-state period while at the transient sate period we observe some deviations between measurements and simulation which may due to cumulative errors in estimating initial steady-state

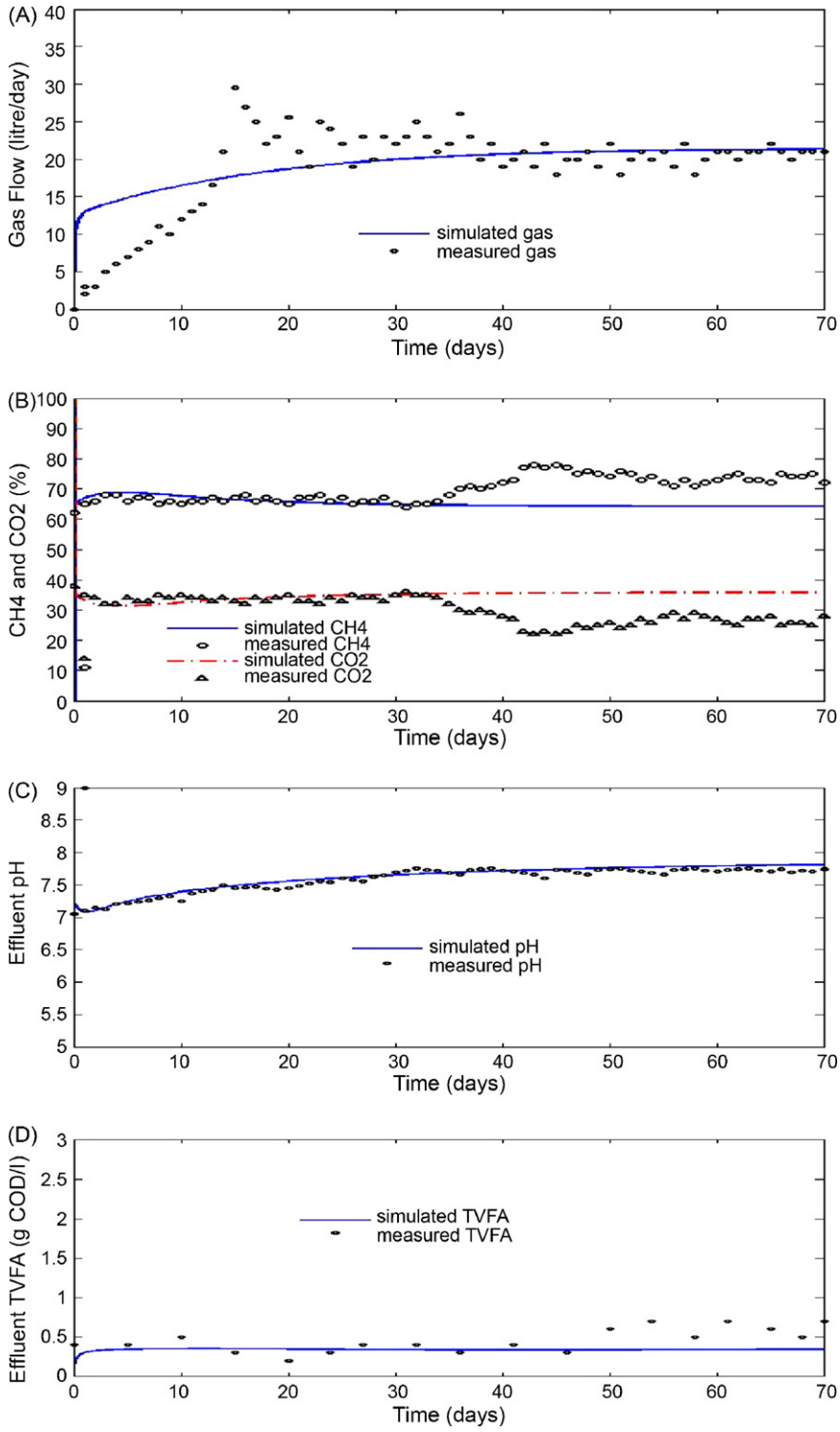


Fig. 1. Comparison between the simulations and the experimental results of the run R4 after the parameters calibration: (A) gas flow; (B) $CH_4$ and $CO_2$; (C) effluent pH and (D) effluent TVFA.

variables and input feed data of the ADM1. Also to the simplifying assumptions made on basic organic composition of OMW and OMSW. As well as to some structural weak points of ADM1 that have been recently addressed by some researchers [18,19]. For methane and carbon dioxide contents the model predictions were much accurate in transient state period than in steady-state period which presented some deviations about 7% with experimental results. Finally pH and TVFA measurements were well replicated by the ADM1 in both transient and steady-state periods.

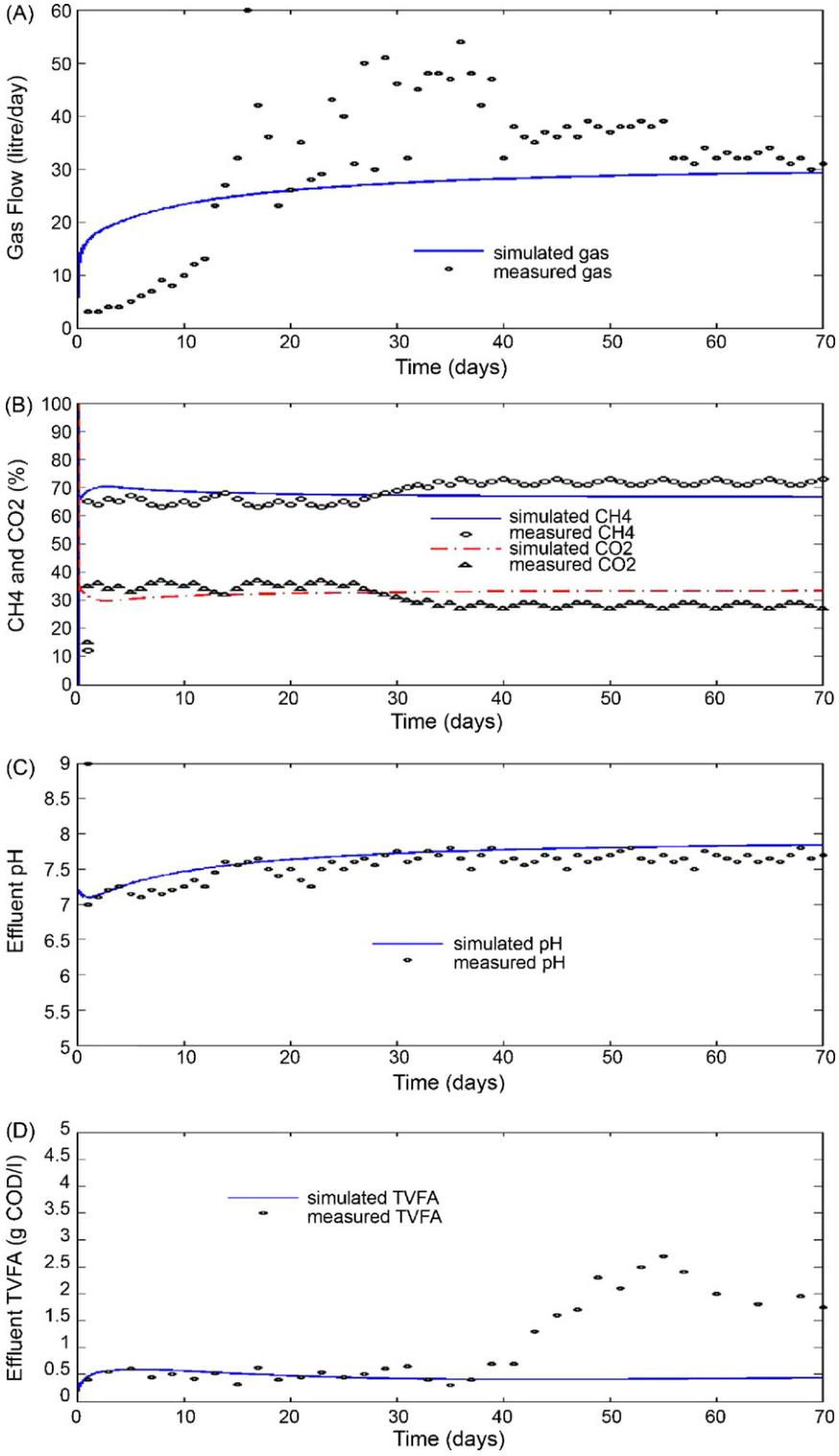


Fig. 2. Validation of simulations with the experimental results of the run R5: (A) gas flow; (B) $CH_4$ and $CO_2$; (C) effluent pH and (D) effluent TVFA.

### 4.2. Model validation

To asses the quality of the optimised parameters and their applicability, the calibrated model was validated on three quite different scenarios by comparison with some experimental results of our previous work [6] applying the same previously optimised parameters to achieve reasonable predictions under variable experimental conditions. In the first scenario the model was validated with the experiments R5 and R6 corresponded to an influent TCOD concentration of 67 g COD/l digested at a HRT of 24 and 12 days, respectively. In the second scenario the model was validated further with the experiments R1 and R2 corresponded to an influent TCOD concentration of 43 g COD/l digested at a HRT of 36 and 24 days, respectively. Finally in the third scenario the model was validated with the experiments R7 and R8 corresponded to an influent TCOD concentration

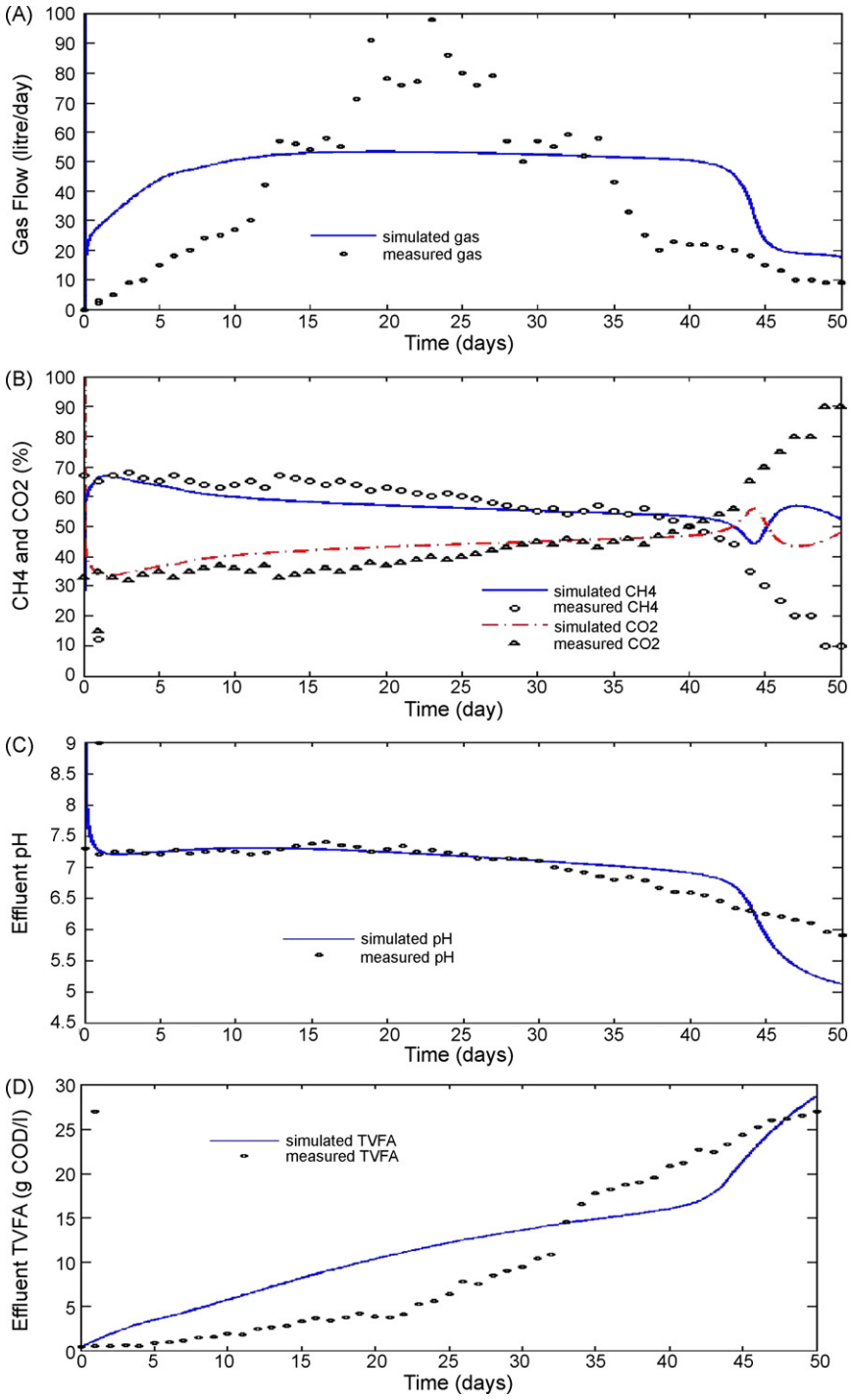


Fig. 3. Validation of simulations with the experimental results of the run R6: (A) gas flow; (B) $CH_4$ and $CO_2$; (C) effluent pH and (D) effluent TVFA.

of 130 g COD/l digested at a HRT of 36 and 24 days, respectively. The developed model could simulate the performance and the behaviour of tubular digester treating in co-digestion OMW with OMSW under different thermophilic conditions and simulations results were comparable to the measurements, as shown below.

#### 4.2.1. Simulation results of scenario one: medium feed concentration

Figs. 2 and 3 show measured and simulated results of gas flows, methane and carbon dioxide percentages, pH and TVFA of the runs R5 and R6, respectively. As can be seen from Fig. 2: pH, methane and carbon dioxide contents were predicted

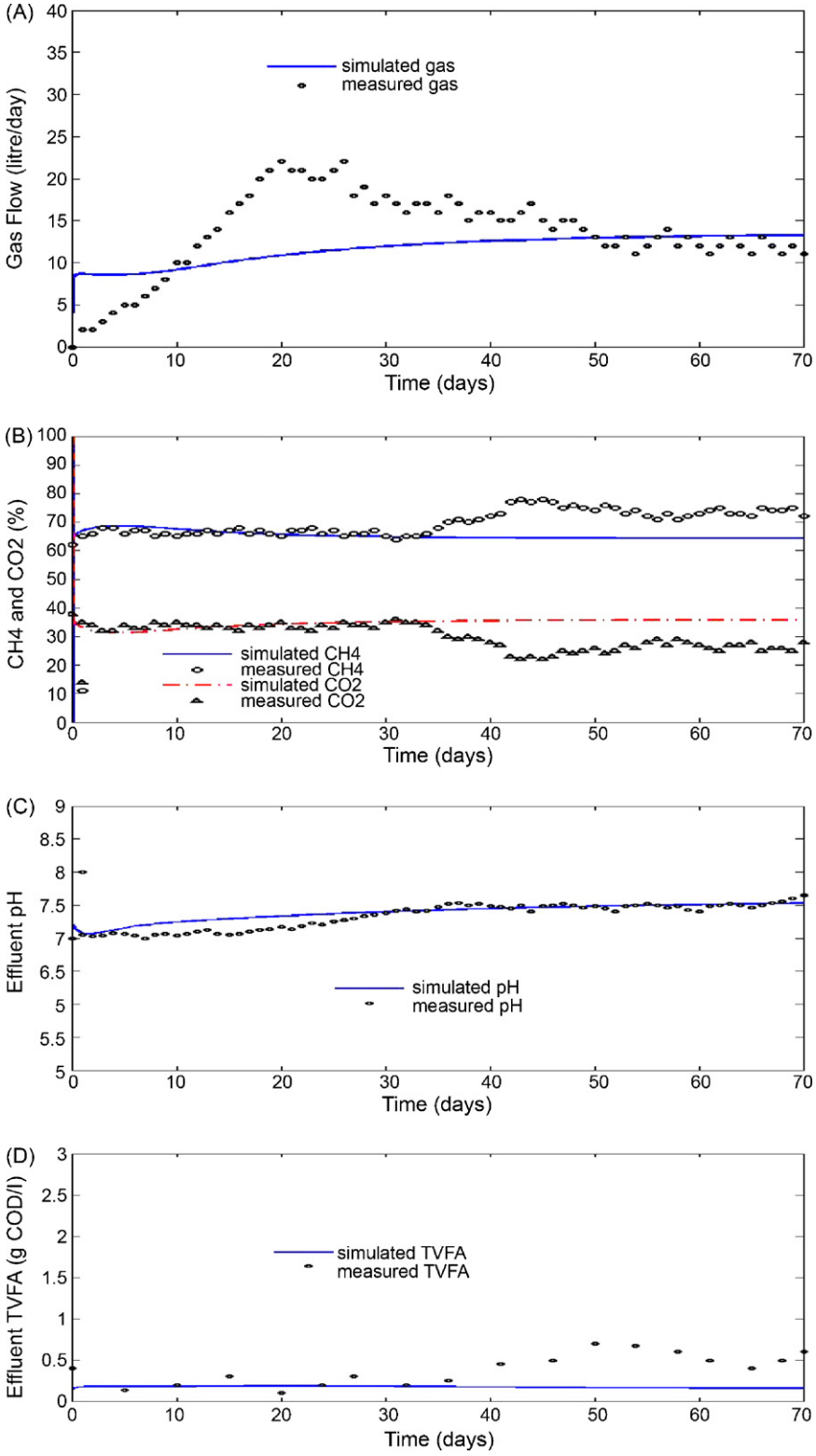


Fig. 4. Validation of simulations with the experimental results of the run R1: (A) gas flow; (B) $CH_4$ and $CO_2$; (C) effluent pH and (D) effluent TVFA.

with high accuracy at both transient and steady-states periods. Also, TVFA were predicted accurately at transient state period but they showed some deviations at steady-state period (about 2 g COD/l). However, gas flow was over predicted at transient sate period and under predicted at steady-state period. Deviations between simulation and gas flow measurements were about 20 L/day at transient state period and about 2 L/day at the end of steady-state period. From Fig. 3 it can be seen that pH, methane and carbon dioxide contents were well predicted at transient state period but they revealed some deviations with experimen-

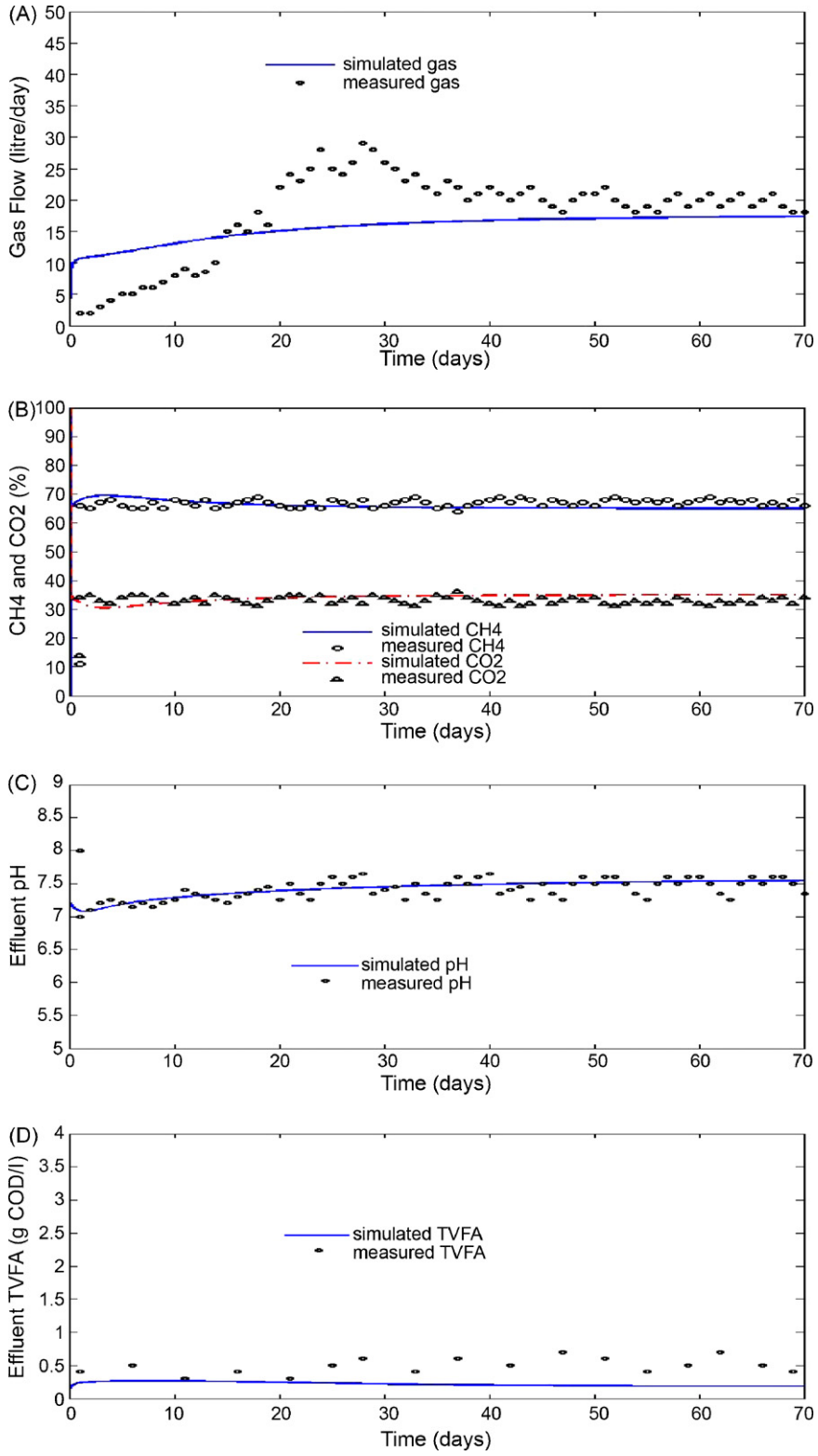


Fig. 5. Validation of simulations with the experimental results of the run R2: (A) gas flow; (B) $CH_4$ and $CO_2$; (C) effluent pH and (D) effluent TVFA.

tal results at the decline period of biogas production. Besides, the model failed to predict the pick of gas flow and succeeded in predicting biogas decline. In fact, gas flow was over predicted at the beginning of transient state period and under predicted from 10th to 35th day, whereas, the decline of biogas production observed from the 35th day was well predicted by the model. Also, TVFA were over predicted with an average deviation about 6 g COD/l at transient state period and under predicted with deviation about 3 g COD/l at digester failure period. These last results were due to the weakness of the ADM1 in predicting gas flow and TVFA at short HRT and digester failure as mentioned by Parker Wayne [11].

#### 4.2.2. Simulation results of scenario two: low feed concentration

Figs. 4 and 5 show measured and simulated results of gas flows, methane and carbon dioxide percentages, pH and TVFA for low feed concentration of the runs R1 and R2, respectively.

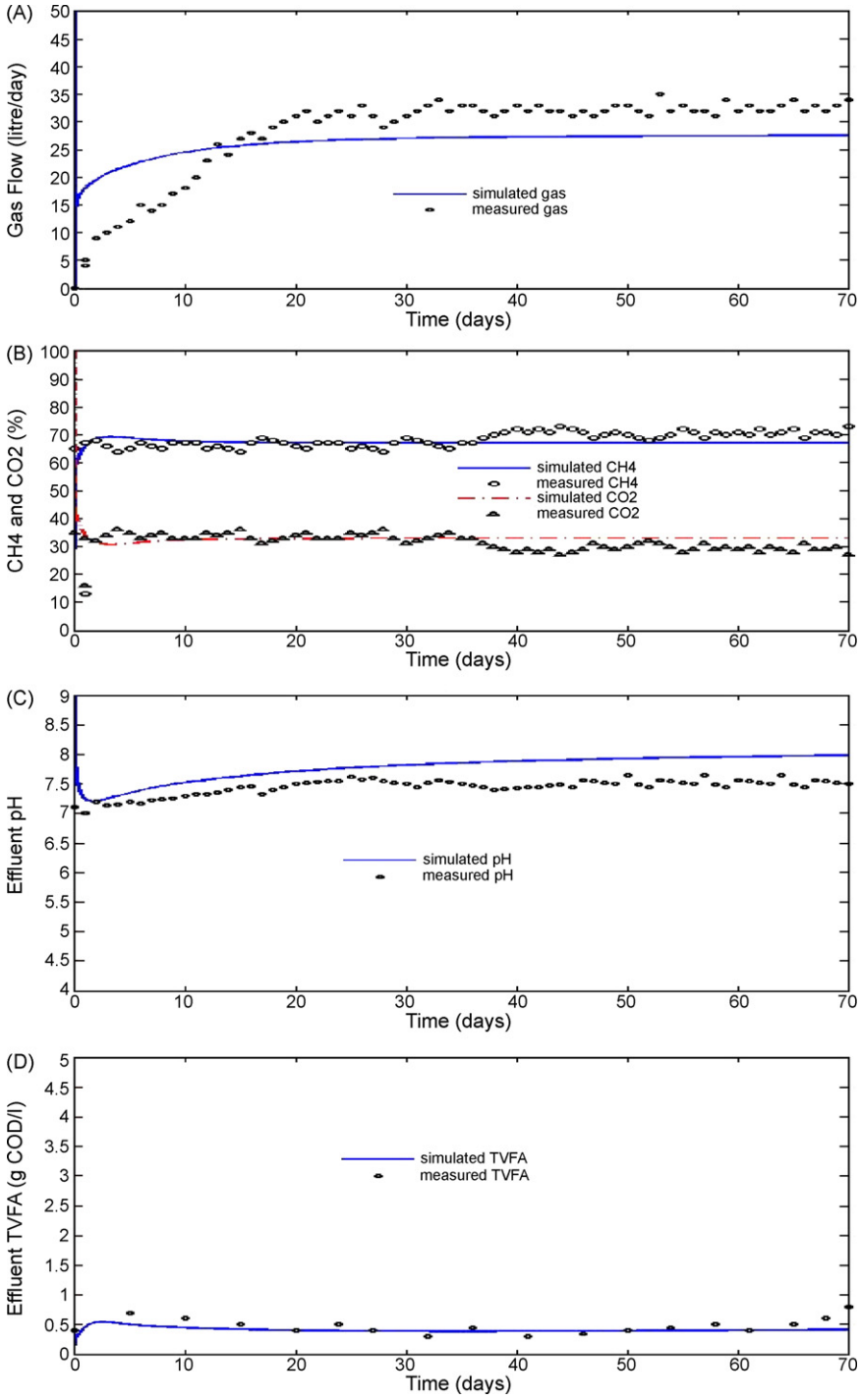


Fig. 6. Validation of simulations with the experimental results of the run R7: (A) gas flow; (B) $CH_4$ and $CO_2$; (C) effluent pH and (D) effluent TVFA.

As can be seen experimental results of pH and TVFA were predicted accurately by the ADM1 for the two runs R1 and R2.

Whereas, methane and carbon dioxide contents were well predicted in run R2 at both transient and steady-states periods than in run R1 which presented some deviations of about 10% at steady-state period. Finally, gas flows in both runs R1 and R2 were replicated with reasonable accuracy at steady-state periods while at the transient periods they were predicted with some deviations about 7 L/day.

#### *4.2.3. Simulation results of scenario three: high feed concentration*

Figs. 6 and 7 show measured and simulated results of gas flows, methane and carbon dioxide percentages, pH and TVFA for high feed concentration fermented at HRTs of 36 and 24 days (Runs R7 and R8). As can be seen experimental results of methane and carbon dioxide contents were quite well predicted at both transient and steady-state periods for the two runs R7 and R8. Also, TVFA measurements were well predicted in the

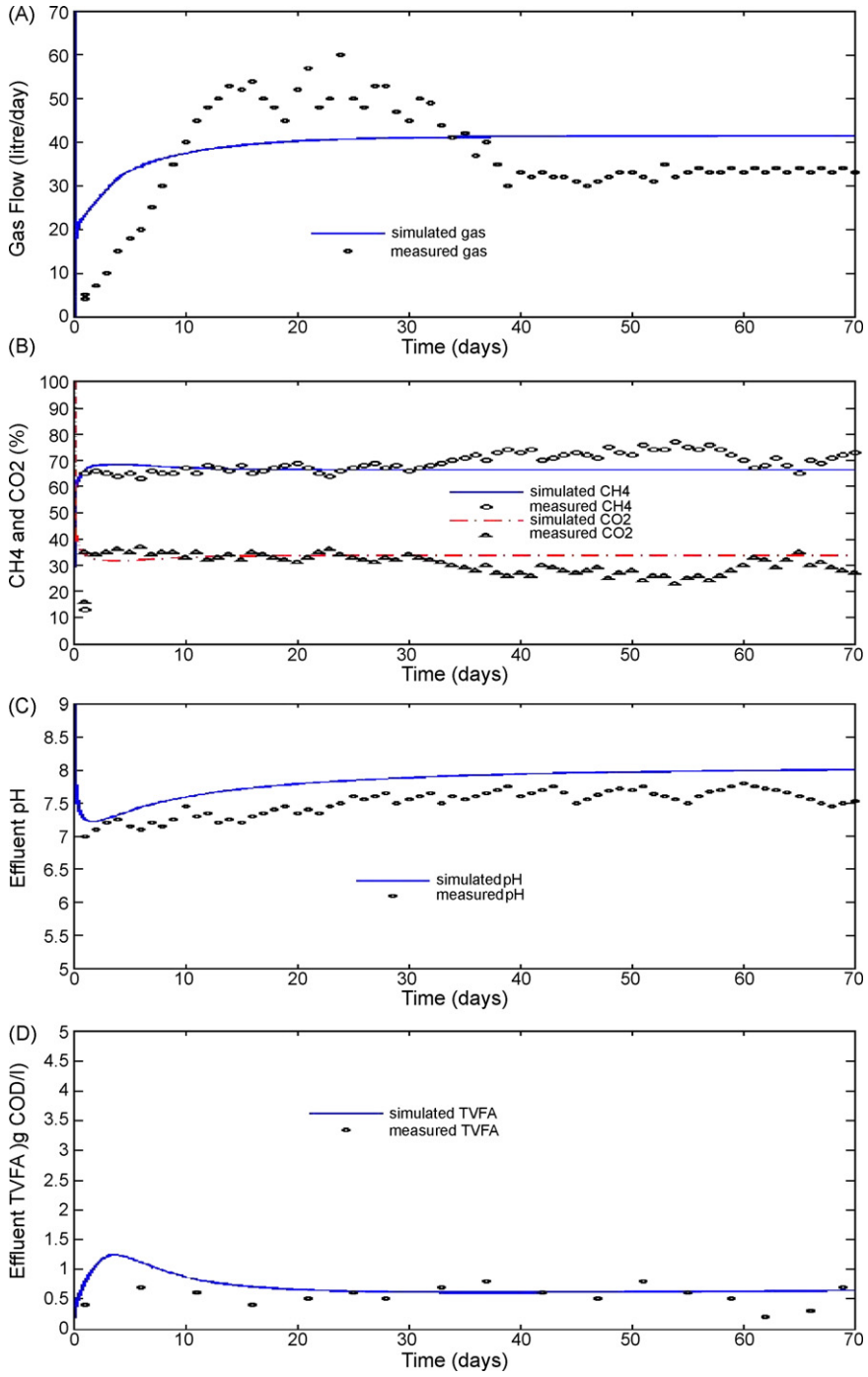


Fig. 7. Validation of simulations with the experimental results of the run R8: (A) gas flow; (B) $CH_4$ and $CO_2$; (C) effluent pH and (D) effluent TVFA.

both runs R7 and R8 but for the run R8 the prediction revealed minor deviations about 0.2–0.5 g COD/l at transient state period. Whereas, gas flow values at steady-state period were under predicted in the run R7 (with deviation about 5 L/day) and over predicted in the run R8 (with deviation about 7 L/day). Finally, pH measurements in both runs of this scenario were predicted with slight deviations about 0.2–0.5 at both transient and steady-state periods. The inconsistencies between simulations of gas flow and experimental results especially for the run R8 may due to the drawbacks of the ADM1 in taking into account the correlation of the most sensitive parameters such as hydrolysis constants with feed concentration and HRT as mentioned by Gavala et al. in their work [17]. Moreover, the discrepancy between pH simulations and pH measurements at both runs R7 and R8 were due to the limitations of this model in taking into account the possible increasing of both cations and anions concentrations inside the reactor especially by the hydrolysis of OMSW.

## 5. Conclusions

This study has demonstrated that the modified ADM1 model could adequately simulate the steady-state behaviour of anaerobic semi-continuous tubular digesters treating in co-digestion OMW with OMSW under different operating conditions at thermophilic temperature and could tolerate the change in both feed concentrations and HRTs with the same calibrated parameters. In fact, gas flow was predicted quite well at steady-state periods for different feed concentrations digested at HRTs of 24 and 36 days. While, for methane and carbon dioxide the predictions of experimental trials in most cases were with reasonable accuracy at both steady-state and transient periods. Besides, pH measurements were predicted with high accuracy for different feed concentrations digested at HRTs of 36, 24 and 12 days which may due to a good estimation of influent cations and anions concentrations. Nevertheless and despite the reasonable accuracy in predicting the most experimental results with different feed concentrations at HRTs of 36 and 24 days, some remarkable deviations between measurements and model simulations were observed firstly with gas flows at transient periods of all runs also with feed concentration of 130 g COD/l digested at a HRT of 24 days and with feed concentration of 67 g COD/l digested at a HRT of 12 days; secondly with TVFA, pH, $CH_4$ and $CO_2$ contents at digester failure period at a HRT of 12 days. These inconsistencies between simulations and experimental results were due to the identification difficulties and validity of all the most sensitive ADM1 parameters for different OLRs which were the major drawbacks for ADM1 applications. In fact, ADM1 differential equations were non linear equations and it was complicated to optimise all the sensitive parameters by adjusting ADM1 outputs with all main experimental results simultaneously without making some discrepancy by any parameters identification method as mentioned by previous researchers that have implemented the ADM1 with other wastes such as: Parker Wayne [11], who found several discrepancies between simulations and measurements; Shang et al. [12] who found good agreement between ADM1 output and measured data but with a 10% over prediction of gas flow. Furthermore, some parameters such as gas transfer coefficient may correlate with reactor configuration [10] and other parameters such as hydrolysis constants may correlate with feed concentrations and HRTs but this dependency was not taken into account by the ADM1. Finally, the fundamentals of the model are generally valid and it can be used for designing full-scale industrial plant to manage the thermophilic anaerobic co-digestion of OMW with OMSW and to assist its behaviour under different operating conditions.

## Acknowledgements

The authors wish to express their gratitude and thanks to Dr. Jeppsson Ulf and Dr. Rosen Christian (Department of Industrial Electrical Engineering and Automation, Lund university, Sweden), to Dr. Steyer Jean Philippe (INRA—Narbonne, Montpellier, France) and to Dr. Damien Batstone (advanced wastewater management centre, Queensland University, Australia) for their kind and excellent help with documents related to ADM1. Also the authors express their thanks to Pr. Mokhtar Zarrouk and all technical staffs of olive oil laboratory in the Biotechnology centre at INRST and Pr. Abdelhafidh Nafti from Food industrial High School of Tunis for their kind and excellent helps with some experimental work of this study.

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