II. BIOAUTOMATICS AND BIOINFORMATICS

MATHEMATICAL MODELLING OF A TWO-STAGE ANAEROBIC DIGESTION PROCESS WITH HYDROGEN AND METHANE PRODUCTION USING ADM1

Milen Borisov, Dencho Denchev, Ivan Simeonov

Abstract: The aim of this study is to implement a mathematical model to simulate the dynamic behaviour of a two-stage anaerobic digestion process for simultaneous production of hydrogen and methane. The process is carried out in two connected continuously stirred bioreactors. The proposed model is developed by reducing the well known IWA Anaerobic Digester Model No 1 (ADM1). In the present study the original model concept was adapted and applied to replicate a two-stage process. The proposed model involves 13 ODEs for the 1st stage and 7 ODEs for the 2nd stage. The numerical coefficient values in the model are taken from specified literature and adapted to the case of wheat straw AD. Important input-output static characteristics and existence of maxima of the input-output static characteristics concerning the biohydrogen and biomethane production in function of the control variable (dilution rate) are presented. Supposing that both bioreactors are operating nearby these maxima the optimal ratio of the working volumes was obtained. Numerical simulations using a specially elaborated web-based software environment are presented to demonstrate the dynamic behavior of the model solutions.

Keywords: anaerobic two-stage digestion; hydrogen and methane production; mathematical model; ADM1, static characteristics, simulation

1. INTRODUCTION

Anaerobic digestion (AD) of organic wastes has become a very attractive biotechnology during last years, mainly in the field of the renewable energy sources and biofuels. However, this biotechnology is very useful for depollution of highly polluted with organics wasted waters and municipal wastes. It is known that more than 95% of working industrial biogas plants operate with the so called continuously stirred tank bioreactors (CSTRs).

AD is a multi-step biotechnological process with hydrogen (H_2) as a non-accumulating intermediate product (Ahring, 2003; Deublein, 2008). Recently, the interest in H_2 production through AD, also known as dark fermentative H_2 production, has increased (Guo et al., 2010; Pakarinen et al., 2011; Ruggeri, et al, 2015). This is due to the fact that the rates of H_2 production are rather high and a variety of feedstock can be used as a substrate. In traditional AD, H_2 is not detected as it is consumed immediately e. g. by hydrogenotrophic methanogens to produce methane CH_4 and carbon dioxide CO_2 (Gerardi, 2003). On the other hand, H_2 can be produced separately by engineering the process conditions. However, the main limitation of dark fermentative H_2 production is the rather low energy recovery. In order to completely utilize the organic acids produced during dark fermentation and improve the over-all energy conversion efficiency, a two-stage AD (TSAD) concept consisting of hydrogenic process followed by methanogenic process has been suggested (Pakarinen et al., 2011).

A lot of models describing separately the fermentative hydrogen production (Nasr et al., 2013; Wang et al., 2009) and the AD for methane production (Batstone et al., 2002; Dochain, 2001; Simeonov, 2010) are known. However, only few models of TSAD processes are known (Simeonov, 2016; Borisov et al., 2016). In (Blumensaat and Keller, 2005) modelling of TSAD using the IWA Anaerobic Digestion Model No 1 (ADM1) is presented. However, the described AD process is not real TSAD process because methane is obtained from both of bioreactors. Volumes of bioreactors are presented different on a figure but without discussing the ratio between them. In (Simeonov and Stoyanov, 2007) experimental studies of co-digestion of mixtures of milk whey and wasted activated sludge in a TSAD process and modelling of this process is presented, however methane is obtained from both of bioreactors.

In this paper a new mathematical model describing the process of simultaneous H_2 and CH_4 production from organic wastes in a cascade of two CSTRs is presented. The proposed model is developed by reducing the universal but very complicated Anaerobic Digester Model № 1 (ADM1) basic structure elaborated by the IWA, (Batstone et al., 2002).

The aim of this study is, as well, to investigate the input-output static characteristics and to shows existence of maxima with respect to hydrogen and methane. This fact is important for the practical applications and will be further used in optimising the bioreactors to achieve maximal production of both

hydrogen and methane. The model also allows finding the optimal ratio between the volumes of the two bioreactors subject to the same optimisation goal.

2. PROCESS DESCRIBTION

The application of a TSAD process for simultaneous H_2 and CH_4 production has been proposed as a promising technology for better process performance and higher energy yields as compared to the traditional one-stage CH_4 production process. In the two-stage AD system, relatively fast growing acidogens and H_2 producing microorganisms are developed in the first-stage hydrogenic bioreactor (with working volume V_1) and are involved in the production of volatile fatty acids (VFA) and H_2. On the other hand, the slow growing acetogens and methanogens are developed in the second-stage methanogenic bioreactor (with working volume V_2) in which the produced VFA are further converted to CH_4 and CO_2. Scheme of TSAD is shown on Fig. 1.

It is known that in the TSAD H_2 + CH_4 system the energy yields are up to 43% more, as compared to the traditional one-stage CH_4 production process (Schievano et al., 2014; Ruggeri, et al, 2015).

In the TSAD system relatively fast growing acidogens and H_2 producing microorganisms are grown in the first-stage, the hydrogenic bioreactor (BR1 with working volume V_1). They are involved in the production of volatile fatty acids (VFAs) and H_2. On the other hand, the slow growing acetogens and methanogens are grown in the second stage, the methanogenic bioreactor (BR_2 with working volume V_2) in which the produced VFAs are further converted to CH_4 and CO_2.

The biochemical processes in the first bioreactor (BR1) include (Table 1) disintegration of organic wastes (composites), hydrolysis (of carbohydrates, proteins and lipids), acidogenesis (from sugars and amino acids) and acetogenesis from LCFA with hydrogen production.

Acetogenesis (from valerate, butyrate and propionate) and the methane production from acetate (methanogenesis) is separated in the second bioreactor (BR2) (Table 2).

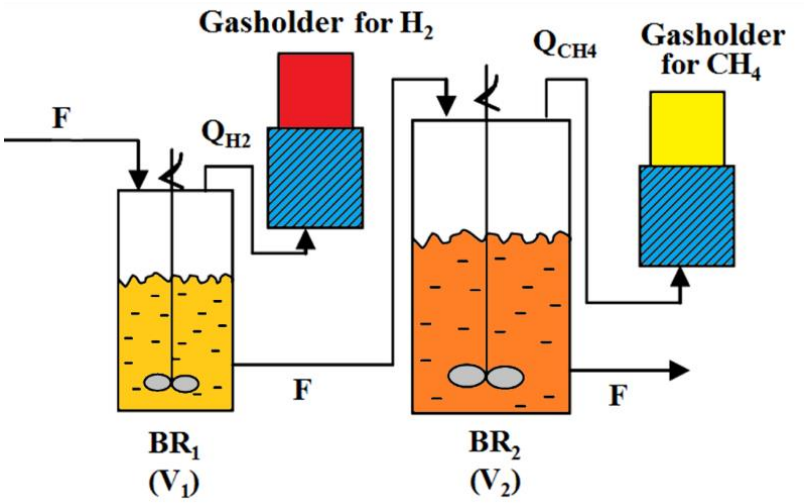

Fig. 1. Scheme of TSAD with production of hydrogen (H_2) and methane (CH_4)

Assume that the volumes V_1 and V_2 of the bioreactors are constant. Let F_1 and F_2 be the inflows in the first and second bioreactor respectively and let $F_1 = F_2 = F$ be valid. It is well known that the dilution rates D_1 and D_2 are defined as:

$$D_1 = \frac{F}{V_1} \text{ and } D_2 = \frac{F}{V_2}. \quad (1)$$

After some transformations it was obtained:

$$\gamma = \frac{V_1}{V_2} = \frac{D_2}{D_1}. \quad (2)$$

It is known that the volume V_2 of the second bioreactor for methane production is larger than the volume V_1 of the first bioreactor. Therefore, $\gamma < 1$ should be valid. Later on, in the paper we shall determine the constant γ using the proposed model equations and one idea for maximal energy production.

In (Denchev et al., 2016) experimental studies in laboratory scale of our team are presented. AD of lignocellulosic waste (wheat straw) in single and two-stage processes with production of hydrogen through the acidogenic phase and of methane through the methanogenic phase is studied. As a

result, the total amount of energy that is produced in the single-stage methanogenic process is 34% less compared to a two-staged one. This difference comes from both: hydrogen released – about 17%, together with the increased amount of methane - about 13%.

Table 1. Biochemical processes in BR1

	Process in BR1 (H2)	Process reaction
1	Disintegration of composites	$X_c \Rightarrow X_{ch} + X_{pr} + X_{li}$
2	Hydrolysis of carbohydrates	$X_{ch} \Rightarrow S_{su}$
3	Hydrolysis of proteins	$X_{pr} \Rightarrow S_{aa}$
4	Hydrolysis of lipids	$X_{li} \Rightarrow S_{su} + S_{fa}$
5	Acidogenesis from sugars	$S_{su} \overset{X_{suaa}}{\Longrightarrow} S_{ac} + S_{bu} + S_{pro} + S_{h2}$
6	Acidogenesis from amino acids	$S_{aa} \overset{X_{suaa}}{\Longrightarrow} S_{ac} + S_{va} + S_{bu} + S_{pro} + S_{h2}$
7	Acetogenesis from LCFA (Long Chan Fatty Acids)	$S_{fa} \overset{X_{fa}}{\Longrightarrow} S_{ac} + S_{h2}$

Table 2. Biochemical processes in BR2

	Process in BR2 (CH4)	Process reaction
1	Acetogenesis from valerate	$S_{va} \overset{X_{c4}}{\Longrightarrow} S_{pro} + S_{ac}$
2	Acetogenesis from butyrate	$S_{bu} \overset{X_{c4}}{\Longrightarrow} S_{ac}$
3	Acetogenesis from propionate	$S_{pro} \overset{X_{pro}}{\Longrightarrow} S_{ac}$
4	Methanogenesis form acetate	$S_{ac} \overset{X_{ac}}{\Longrightarrow} S_{ch4}$

3. PROCESS MODEL

The model is derived on the basis of the ADM1 basic structure as well as on our experience with TSAD process with hydrogen and methane production (Denchev et al., 2016). The following assumptions have been accepted:

- Balance equations of the hydrogen and methane in the liquid phases have been neglected because they are practically not dissolved in liquids.
- Hydrogenotrophic bacteria do not exist in this process.
- Equations describing balances of inorganic components and some biochemical equations have been neglected in view of simplifying the model.
- The very important parameter *pH* is not included in the model, however *pH* is kept in the interval 5.0−5.5 in the first bioreactor, and in the interval 6.5 − 8.5 in the second bioreactor.
- The biochemical processes in BR1 include disintegration of organic wastes (composites), hydrolysis (of carbohydrates, proteins and lipids), acidogenesis (from sugars and amino acids) and acetogenesis from LCFA with hydrogen production. These processes are omitted in BR2.
- Acetogenesis (from valerate, butyrate and propionate) and the methane production from acetate (methanogenesis) are separated in the BR2.

Following the above presented assumptions, the dynamics in the BR1 is described by the following set of 13 nonlinear ordinary differential equations (ODEs):

$$\frac{d}{dt}S_{su,RH_2}(t) = D_{RH_2}\left(S_{su,RH_2,in} - S_{su,RH_2}\right) + k_{hyd,ch}\,X_{ch,RH_2} + f_{su,li}\,k_{hud,li}\,X_{li,RH_2} - k_{m,suaa}\frac{S_{su,RH_2}X_{suaa,RH_2}}{K_{S,suaa}+S_{su,RH_2}}\,\frac{S_{su,RH_2}}{S_{su,RH_2}+S_{aa,RH_2}} \quad (3)$$

$$\frac{d}{dt}S_{aa,RH_2}(t) = D_{RH_2}\left(S_{aa,RH_2,in} - S_{aa,RH_2}\right) + k_{hyd,pr}\,X_{pr,RH_2} - \frac{S_{aa,RH_2}X_{suaa,RH_2}}{K_{S,suaa}+S_{aa,RH_2}}\,\frac{k_{m,suaa}S_{aa,RH_2}}{S_{su,RH_2}+S_{aa,RH_2}} \quad (4)$$

$$\frac{d}{dt}S_{fa,RH_2}(t) = D_{RH_2}\left(S_{fa,RH_2,in} - S_{fa,RH_2}\right) + f_{fa,li}\,k_{hud,li}\,X_{li,RH_2} - k_{m,fa}\frac{S_{fa,RH_2}X_{fa,RH_2}}{K_{S,fa}+S_{fa,RH_2}} \quad (5)$$

$$\frac{d}{dt}S_{va,RH_2}(t) = D_{RH_2}\left(S_{va,RH_2,in} - S_{va,RH_2}\right) + \left(1 - Y_{suaa}\right) f_{va,aa}\, k_{m,suaa} \frac{S_{aa,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{aa,RH_2}} \quad (6)$$

$$\frac{d}{dt}S_{bu,RH_2}(t) = D_{RH_2}\left(S_{bu,RH_2,in} - S_{bu,RH_2}\right) + \left(1 - Y_{suaa}\right) k_{m,suaa} \left(\frac{S_{su,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{su,RH_2}} \frac{f_{bu,su} S_{su,RH_2}}{S_{su,RH_2} + S_{aa,RH_2}} + \frac{S_{aa,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{aa,RH_2}} \frac{f_{bu,aa} S_{aa,RH_2}}{S_{su,RH_2} + S_{aa,RH_2}}\right) \quad (7)$$

$$\frac{d}{dt}S_{pro,RH_2}(t) = D_{RH_2}\left(S_{pro,RH_2,in} - S_{pro,RH_2}\right) + \left(1 - Y_{suaa}\right) k_{m,suaa} \left(\frac{S_{su,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{su,RH_2}} \frac{f_{pro,su} S_{su,RH_2}}{S_{su,RH_2} + S_{aa,RH_2}} + \frac{S_{aa,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{aa,RH_2}} \frac{f_{pro,aa} S_{aa,RH_2}}{S_{su,RH_2} + S_{aa,RH_2}}\right) \quad (8)$$

$$\frac{d}{dt}S_{ac,RH_2}(t) = D_{RH_2}\left(S_{ac,RH_2,in} - S_{ac,RH_2}\right) + \left(1 - Y_{fa}\right) 0.7\, k_{m,fa} \frac{S_{fa,RH_2}}{K_{S,fa} + S_{fa,RH_2}} X_{fa,RH_2}\, v + \left(1 - Y_{suaa}\right) k_{m,suaa} \left(\frac{S_{su,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{su,RH_2}} \frac{f_{ac,su} S_{su,RH_2}}{S_{su,RH_2} + S_{aa,RH_2}} + \frac{S_{aa,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{aa,RH_2}} \frac{f_{ac,aa} S_{aa,RH_2}}{S_{su,RH_2} + S_{aa,RH_2}}\right) \quad (9)$$

$$\frac{d}{dt}X_{c,RH_2}(t) = D_{RH_2}\left(X_{c,RH_2,in} - X_{c,RH_2}\right) - k_{dis}\, X_{c,RH_2} \quad (10)$$

$$\frac{d}{dt}X_{ch,RH_2}(t) = D_{RH_2}\left(X_{ch,RH_2,in} - X_{ch,RH_2}\right) + f_{ch,xc}\, k_{dis}\, X_{c,RH_2} - k_{hyd,ch}\, X_{ch,RH_2} \quad (11)$$

$$\frac{d}{dt}X_{pr,RH_2}(t) = D_{RH_2}\left(X_{pr,RH_2,in} - X_{pr,RH_2}\right) + f_{pr,xc}\, k_{dis}\, X_{c,RH_2} - k_{hyd,pr}\, X_{pr,RH_2} \quad (12)$$

$$\frac{d}{dt}X_{li,RH_2}(t) = D_{RH_2}\left(X_{li,RH_2,in} - X_{li,RH_2}\right) + f_{li,xc}\, k_{dis}\, X_{c,RH_2} - k_{hyd,li}\, X_{li,RH_2} \quad (13)$$

$$\frac{d}{dt}X_{suaa,RH_2}(t) = D_{RH_2}\left(X_{suaa,RH_2,in} - X_{suaa,RH_2}\right) Y_{suaa}\, k_{m,suaa} \left(\frac{S_{su,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{su,RH_2}} \frac{S_{su,RH_2}}{S_{su,RH_2} + S_{aa,RH_2}} + \frac{S_{aa,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{aa,RH_2}} \frac{S_{aa,RH_2}}{S_{su,RH_2} + S_{aa,RH_2}}\right) \quad (14)$$

$$\frac{d}{dt}X_{fa,RH_2}(t) = D_{RH_2}\left(X_{fa,RH_2,in} - X_{fa,RH_2}\right) + Y_{fa}\, k_{m,fa} \frac{S_{fa,RH_2} X_{fa,RH_2}}{K_{S,fa} + S_{fa,RH_2}} \quad (15)$$

$$Q_{h2}(t) = Y_{h2,su}\, k_{m,suaa} \frac{S_{su,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{su,RH_2}} \frac{S_{su,RH_2}}{S_{su,RH_2} + S_{aa,RH_2}} + Y_{h2,aa}\, k_{m,suaa} \frac{S_{aa,RH_2} X_{suaa,RH_2}}{K_{S,suaa} + S_{aa,RH_2}} \frac{S_{aa,RH_2}}{S_{su,RH_2} + S_{aa,RH_2}} + Y_{h2,fa}\, k_{m,fa} \frac{S_{fa,RH_2} X_{fa,RH_2}}{K_{S,fa} + S_{fa,RH_2}} \quad (16)$$

The algebraic equation (16) describes the hydrogen formation in the gaseous phase of BR1. The dynamics of the process in BR2 is described by the following set of 7 ODEs:

$$\frac{d}{dt}S_{va,RCH_4}(t) = D_{RCH_4}\left(S_{va,RCH_4,in} - S_{va,RCH_4}\right) - k_{m,c4} \frac{S_{va,RCH_4} X_{c4,RCH_4}}{K_{S,c4} + S_{va,RCH_4}} \frac{S_{va,RCH_4}}{S_{bu,RCH_4} + S_{va,RCH_4}} \quad (17)$$

$$\frac{d}{dt}S_{bu,RCH_4}(t) = D_{RCH_4}\left(S_{bu,RCH_4,in} - S_{bu,RCH_4}\right) - k_{m,c4} \frac{S_{bu,RCH_4} X_{c4,RCH_4}}{K_{S,c4} + S_{bu,RCH_4}} \frac{S_{bu,RCH_4}}{S_{bu,RCH_4} + S_{va,RCH_4}} \quad (18)$$

$$\frac{d}{dt}S_{pro,RCH_4}(t) = D_{RCH_4}\left(S_{pro,RCH_4,in} - S_{pro,RCH_4}\right) + \left(1 - Y_{c4}\right) 0.54\, k_{m,c4} \frac{S_{va,RCH_4} X_{c4,RCH_4}}{K_{S,c4} + S_{va,RCH_4}} \frac{S_{va,RCH_4}}{S_{bu,RCH_4} + S_{va,RCH_4}} - k_{m,pro} \frac{S_{pro,RCH_4} X_{pro,RCH_4}}{K_{S,pro} + S_{pro,RCH_4}} \quad (19)$$

$$\frac{d}{dt}S_{ac,RCH_4}(t) = D_{RCH_4}\left(S_{ac,RCH_4,in} - S_{ac,RCH_4}\right) + \left(1 - Y_{c4}\right) k_{m,c4} \left(0.31 \frac{S_{va,RCH_4} X_{c4,RCH_4}}{K_{S,c4} + S_{va,RCH_4}} \frac{S_{va,RCH_4}}{S_{bu,RCH_4} + S_{va,RCH_4}} + 0.8 \frac{S_{bu,RCH_4} X_{c4,RCH_4}}{K_{S,c4} + S_{bu,RCH_4}} \frac{S_{bu,RCH_4}}{S_{bu,RCH_4} + S_{va,RCH_4}}\right) + \left(1 - Y_{pro}\right) 0.57\, k_{m,pro} \frac{S_{pro,RCH_4} X_{pro,RCH_4}}{K_{S,pro} + S_{pro,RCH_4}} - Y_{ac}\, k_{m,ac} \frac{S_{ac,RCH_4} X_{ac,RCH_4}}{K_{S,ac} + S_{ac,RCH_4}} \quad (20)$$

$$\frac{d}{dt}X_{c4,RCH_4}(t) = D_{RCH_4}\left(0 - X_{c4,RCH_4}\right) + Y_{c4}\, k_{m,c4}\, \frac{S_{va,RCH_4} X_{c4,RCH_4}}{K_{S,c4}+S_{va,RCH_4}}\, \frac{S_{va,RCH_4}}{S_{bu,RCH_4}+S_{va,RCH_4}} + Y_{c4}\, k_{m,c4}\, \frac{S_{bu,RCH_4} X_{c4,RCH_4}}{K_{S,c4}+S_{bu,RCH_4}}\, \frac{S_{bu,RCH_4}}{S_{bu,RCH_4}+S_{va,RCH_4}} \quad (21)$$

$$\frac{d}{dt}X_{pro,RCH_4}(t) = D_{RCH_4}\left(0 - X_{pro,RCH_4}\right) + Y_{pro}\, k_{m,pro}\, \frac{S_{pro,RCH_4} X_{pro,RCH_4}}{K_{S,pro}+S_{pro,RCH_4}} \quad (22)$$

$$\frac{d}{dt}X_{ac,RCH_4}(t) = D_{RCH_4}\left(0 - X_{ac,RCH_4}\right) + k_{m,ac}\, \frac{S_{ac,RCH_4} X_{ac,RCH_4}}{K_{S,ac}+S_{ac,RCH_4}} \quad (23)$$

$$Q_{ch4}(t) = Y_{ch4,ac}\, k_{m,ac}\, \frac{S_{ac,RCH_4} X_{ac,RCH_4}}{K_{S,ac}+S_{ac,RCH_4}} \quad (24)$$

The algebraic equation (24) describes the methane formation in the gaseous phase of BR2, where:

$S_{va,RCH_4,in} = S_{va,RH_2}$, $S_{bu,RCH_4,in} = S_{bu,RH_2}$, $S_{pro,RCH_4,in} = S_{pro,RH_2}$.

The definitions of the phase variables and parameters in the equations (3)–(24) are given in Table 3 and Table 4, respectively. The coefficient values in the right column of Table 4 are taken from (Rosen et al., 2006). In the model variables and parameters, the subscripts *h*2 and *ch*4 indicate hydrogen (H_2) and methane (CH_4) respectively.

Table 3. Phase variables

Eq.	Variable	Component	Processes
(1)	S_{su,RH_2}	Monosaccharides	+ hydrolysis of (carbohydrates, lipids) - uptake of sugar
(2)	S_{aa,RH_2}	Amino acids (AA)	+ hydrolysis of proteins - uptake of amino acid
(3)	S_{fa,RH_2}	Fatty acids (LCFA)	+ hydrolysis of lipids - uptake of LCFA
(4)	S_{va,RH_2}	Total valerate	+ uptake of amino acids
(5)	S_{bu,RH_2}	Total butyrate	+ uptake of (sugar, amino acids)
(6)	S_{pro,RH_2}	Total propionate	+ uptake of (sugar, amino acids)
(7)	S_{ac,RH_2}	Total acetate	+ uptake of (sugar, amino acids, LCFA)
(8)	X_{c,RH_2}	Composites	- disintegration of composites
(9)	X_{ch,RH_2}	Carbohydrates	+ disintegration of composites - hydrolysis of carbohydrates
(10)	X_{pr,RH_2}	Proteins	+ disintegration of composites - hydrolysis of proteins
(11)	X_{li,RH_2}	Lipids	+ disintegration of composites - hydrolysis of lipids
(12)	X_{suaa,RH_2}	Sugar and AA degraders	+ uptake of (sugar, amino acids)
(13)	X_{fa,RH_2}	LCFA degraders	+ uptake of LFCA
(14)	Q_{h2}	Hydrogen gas	stripping of hydrogen
(15)	S_{va,RCH_4}	Total valerate (Va)	– uptake of valerate
(16)	S_{bu,RCH_4}	Total butyrate (Bu)	– uptake of butyrate
(17)	S_{pro,RCH_4}	Total propionate	+ uptake of valerate - uptake of propionate
(18)	S_{ac,RCH_4}	Total acetate	+ uptake of (valerate, butyrate, propionate) – acetate
(19)	X_{c4,RCH_4}	Va and Bu degraders	+ uptake of (valerate, butyrate)
(20)	X_{pro,RCH_4}	Propionate degraders	+ uptake of propionate
(21)	X_{ac,RCH_4}	Acetate degraders	+ uptake of acetate
(22)	Q_{ch4}	Methane gas	stripping of methane

Table 4. Parameters values

Parameter	Definition of the model parameters	Values
$S_{su,RH_2,in}$	input concentration of S_{su,RH_2} [gCOC/L]	0.01
$S_{aa,RH_2,in}$	input concentration of S_{aa,RH_2} [gCOC/L]	0.001
$S_{fa,RH_2,in}$	input concentration of S_{fa,RH_2} [gCOC/L]	0.001
$S_{va,RH_2,in}$	input concentration of S_{va,RH_2} [gCOC/L]	0.0
$S_{bu,RH_2,in}$	input concentration of S_{bu,RH_2} [gCOC/L]	0.0
$S_{pro,RH_2,in}$	input concentration of S_{pro,RH_2} [gCOC/L]	0.0
$S_{ac,RH_2,in}$	input concentration of S_{ac,RH_2} [gCOC/L]	0.0
$X_{c,RH_2,in}$	input concentration of X_{c,RH_2} [gCOC/L]	50.0
$X_{ch,RH_2,in}$	input concentration of X_{ch,RH_2} [gCOC/L]	0.0
$X_{pr,RH_2,in}$	input concentration of X_{pr,RH_2} [gCOC/L]	0.0
$X_{li,RH_2,in}$	input concentration of X_{li,RH_2} [gCOC/L]	0.0
$X_{suaa,RH_2,in}$	input concentration of X_{suaa,RH_2} [gCOC/L]	0.0
$X_{fa,RH_2,in}$	input concentration of X_{fa,RH_2} [gCOC/L]	0.0
$f_{ch,xc}$	stoichiometric parameter [–]	0.2
$f_{pr,xc}$	stoichiometric parameter [–]	0.2
$f_{li,xc}$	stoichiometric parameter [–]	0.3
$f_{su,li}$	stoichiometric parameter [–]	0.05
$f_{fa,li}$	stoichiometric parameter [–]	0.95
$f_{ac,su}$	stoichiometric parameter [–]	0.41
$f_{ac,aa}$	stoichiometric parameter [–]	0.4
$f_{bu,su}$	stoichiometric parameter [–]	0.13
$f_{pro,su}$	stoichiometric parameter [–]	0.27
$f_{va,aa}$	stoichiometric parameter [–]	0.23
$f_{bu,aa}$	stoichiometric parameter [–]	0.26
$f_{pro,aa}$	stoichiometric parameter [–]	0.05
Y_{suaa}	stoichiometric parameter [–]	0.1
Y_{ac}	stoichiometric parameter [–]	27.3
Y_{fa}	stoichiometric parameter [–]	0.06
$Y_{h2,su}$	physicochemical parameter [L^2/g]	0.7
$Y_{h2,aa}$	physicochemical parameter [L^2/g]	0.7
$Y_{h2,fa}$	physicochemical parameter [L^2/g]	0.7
$Y_{ch4,ac}$	physicochemical parameter [L^2/g]	75
k_{dis}	biochemical parameter [h^{-1}]	0.0208
$k_{hyd,ch}$	biochemical parameter [h^{-1}]	0.417
$k_{hyd,pr}$	biochemical parameter [h^{-1}]	0.417
$k_{hyd,li}$	biochemical parameter [h^{-1}]	0.417
$k_{m,suaa}$	biochemical parameter [h^{-1}]	1.25
$k_{s,suaa}$	biochemical parameter [h^{-1}]	0.5
$k_{m,fa}$	biochemical parameter [h^{-1}]	0.15
$k_{m,ca}$	biochemical parameter [h^{-1}]	0.0167
$k_{s,fa}$	biochemical parameter [h^{-1}]	0.67
$k_{s,ac}$	biochemical parameter [h^{-1}]	0.4
$k_{m,c4}$	biochemical parameter [h^{-1}]	0.833
$K_{S,c4}$	biochemical parameter [g/L]	0.2
$k_{m,pro}$	biochemical parameter [h^{-1}]	0.542
$K_{S,pro}$	biochemical parameter [g/L]	0.1

4. INPUT OUTPUT STATIC CHARACTERISTICS

The function $Q_{h2}(D_1)$ depends on the input D_1 and is called input-output static characteristic with respect to the hydrogen production. Fig. 2 presents the graph of the input-output static characteristic for three value of the parameter $X_c^{(in)} = X_{c,RH_2,in}$. From this figure is evident that $Q_{h2}(D_1)$ is unimodal with respect to D_1 in the admissible interval for D_1 and there exist a unique (admissible) point $D_{1,\max}$, such that $Q_{h2}(D_1)$ possesses maximum $Q_{h2,\max}$ ($Q_{h2,\max} = Q_{h2}(D_{1,\max})$), $Q_{h2}(D_1)$ is strongly increasing if $D_1 \leq D_{1,\max}$ and $Q_{h2}(D_1)$ is strongly decreasing if $D_1 > D_{1,\max}$.

Using the methane flow rate Q_{ch4} we compute the input-output static characteristic on the set of all steady states, namely: $Q_{ch4} = Q_{ch4}(D_1, D_2)$.

Fig. 3 visualizes the graph of $Q_{ch4}(D_{1,\max}, D_2)$; the latter is a unimodal function, taking its maximum at $D_{2,\max}$; $Q_{ch4,\max} = Q_{ch4}(D_{1,\max}, D_{2,\max})$.

Using the presentation (2) we define and compute the constant γ and in this way the relationship between the volumes V_1 and V_2 of the two bioreactors (Table 5).

For simulations the average value (from the last column) $\gamma = 0.253$ was adopted (the volume of BR2 is about 4 times bigger than those of BR1).

5. SIMULATION STUDIES

Fig. 4 and Fig. 5 present the time evolution of the outputs $Q_{h2}(t)$ and $Q_{ch4}(t)$, respectively, $X_c^{(in)}$ takes values from Table 6 for $D_1 = 0.025 = \text{const}$.

Fig. 6 to Fig. 11 present the time evolution of the other variable of the model solutions, where $X_c^{(in)}$ takes values from Table 6 for $D_1 = 0.025$, $\gamma = 0.253$.

Table 5. Values for the constant γ for different values of X_c^((in))

$X_c^{(in)}$ [g/L]	$D_{1,sup}$ [1/h]	$D_{1,max}$ [1/h]	$Q_{1,max}$ [L/h]	$D_{2,sup}$ [1/h]	$D_{2,max}$ [1/h]	$Q_{2,max}$ [L/h]	γ
40	0.089	0.041	0.132	0.0145	0.0106	0.0608	0.258
50	0.093	0.044	0.169	0.0150	0.0111	0.0774	0.252
60	0.097	0.046	0.206	0.0153	0.0115	0.0953	0.249

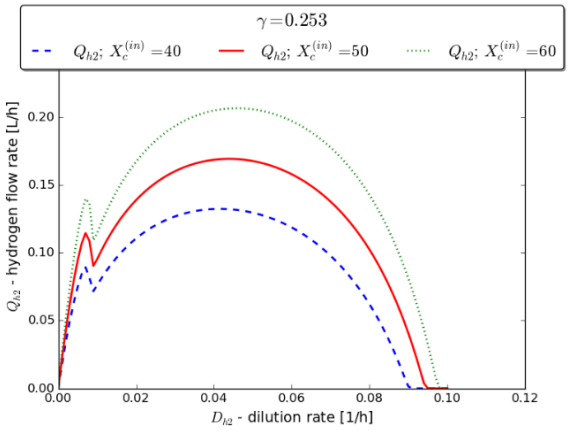

Fig. 2. Input-output static characteristics for BR1

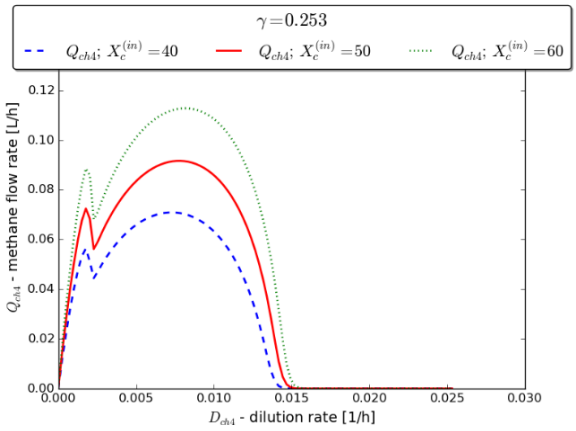

Fig. 3. Input-output static characteristics for BR2

Table 6. Values of $X_c^{(in)}$ for $D_1 = 0.025 = \text{const.}$, $D_2 = \gamma D_1$, where $\gamma = 0.253$

Time	**[h]**	**0−1000**	**1000−2000**	**2000−3000**	**3000−4000**
$X_c^{(in)}$	[g/l]	50	40	60	50

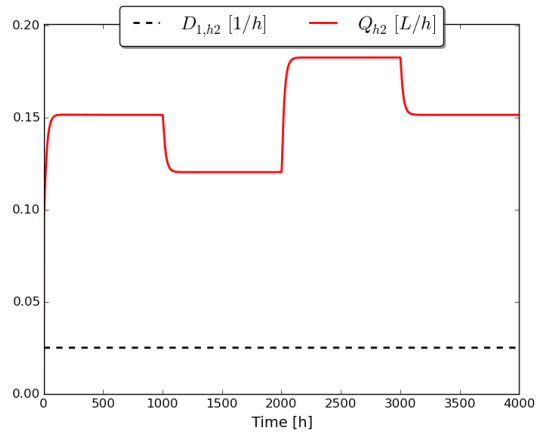

Fig. 4

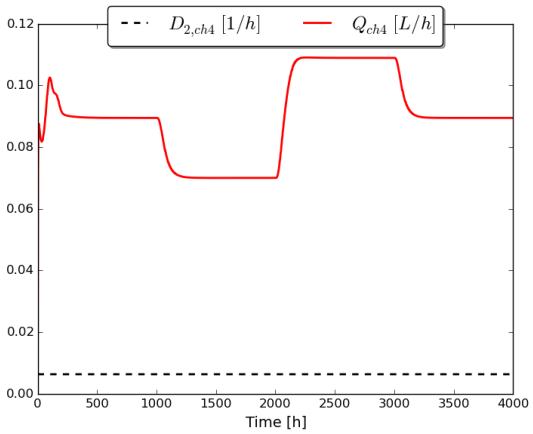

Fig. 5

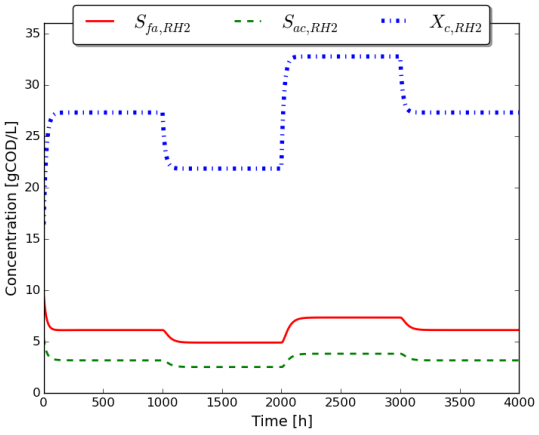

Fig. 6

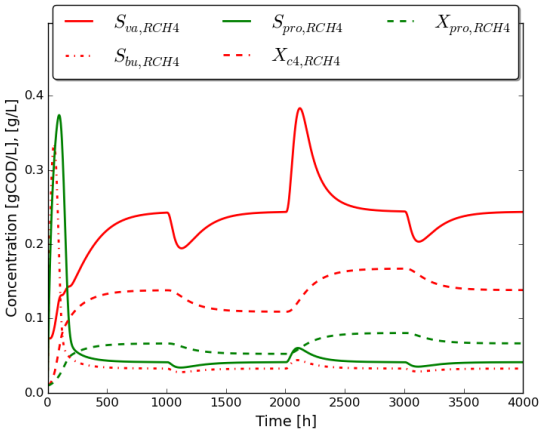

Fig. 7

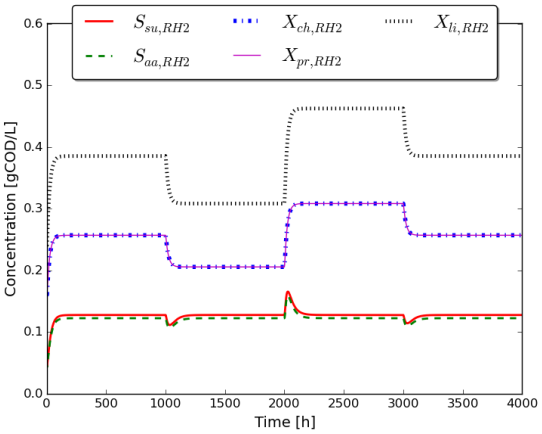

Fig. 8

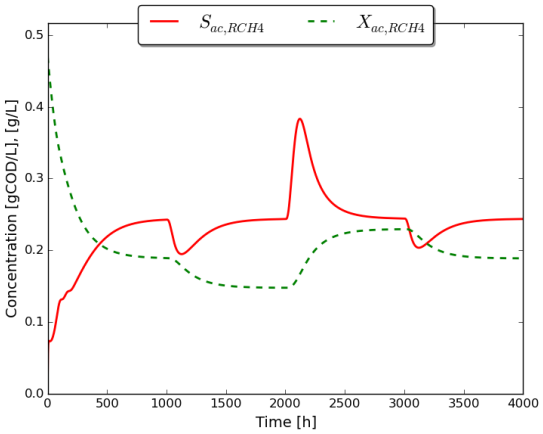

Fig. 9

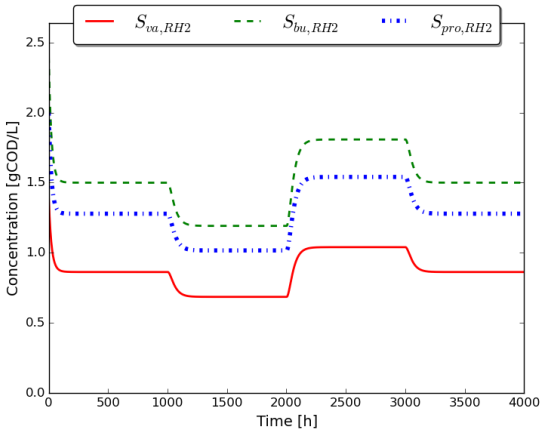

Fig. 10

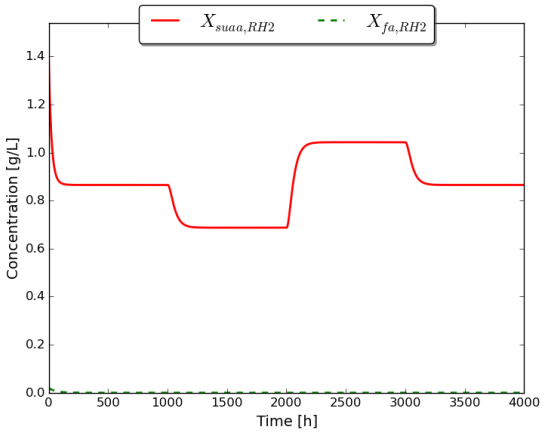

Fig. 11

Fig. 12 to Fig. 19 present the time evolution of the model solutions, where D_1 takes values from Table 7 for $X_c^{(in)}$= 50 = const., γ = 0.253.

Table 7. Step changes of D_1 with $D_2 = \gamma D_1$, $X_c^{(in)}$= 50 = const. (γ = 0.253, K = 1/ $\gamma \approx$ 3.95)

Time	**[h]**	**0 − 1000**	**1000−2000**	**2000−3000**	**3000−4000**	**4000−5000**	**5000−8000**
D_1	[1/*h*]	0.01	0.015	0.02	0.025	0.035	0.1

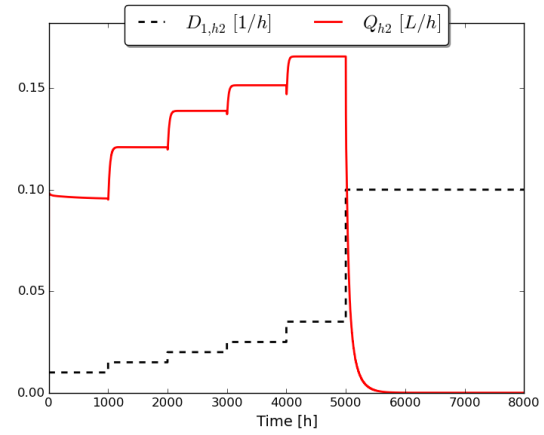

Fig. 12

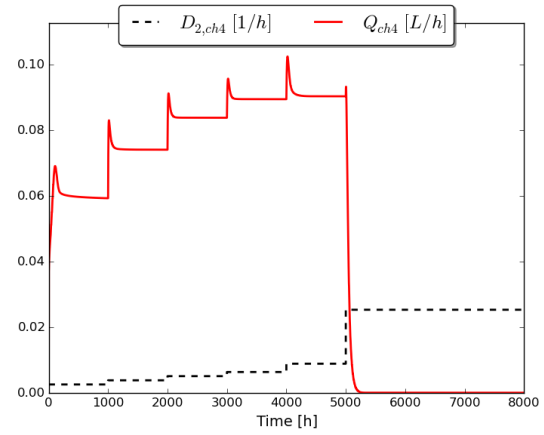

Fig. 13

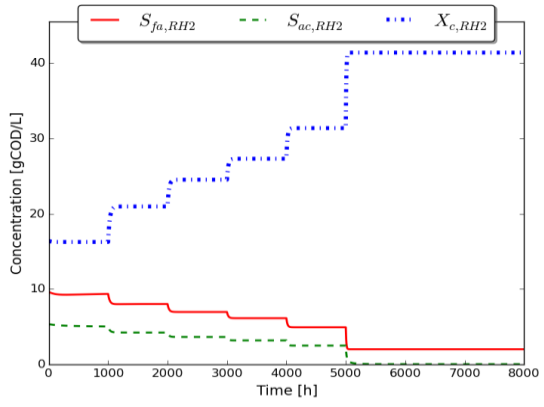

Fig. 14

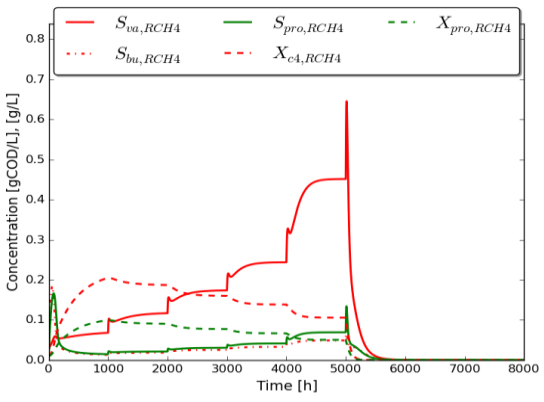

Fig. 15

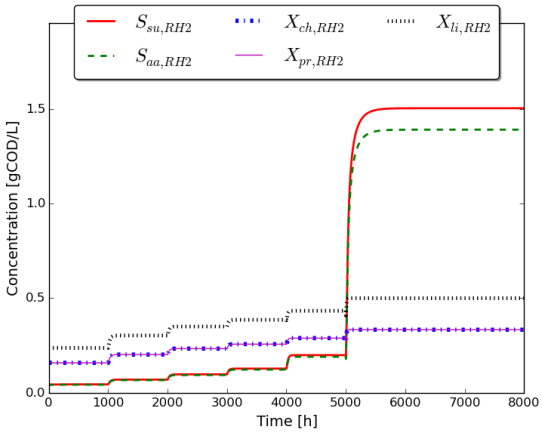

Fig. 16

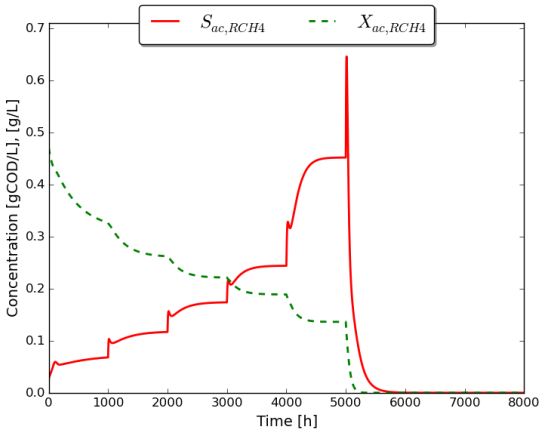

Fig. 17

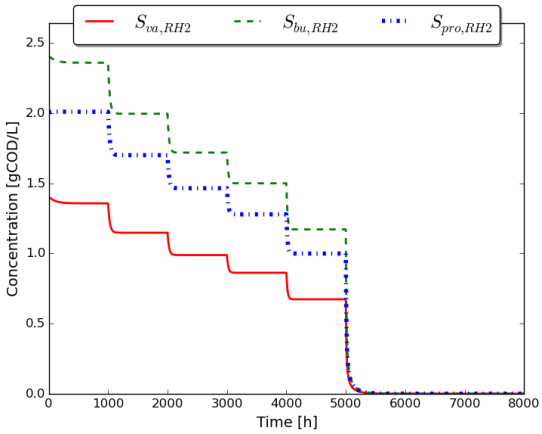

Fig. 18

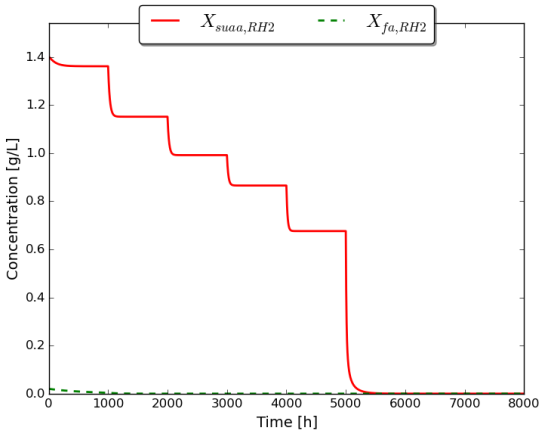

Fig. 19

6. CONCLUSION

In this paper a new mathematical model is proposed. This model describes the process of simultaneous production of hydrogen and methane by AD of organic wastes in a cascade of two CSTR bioreactors with different volumes. The proposed model is developed by reducing the universal but very complicated ADM1. The investigation of the input-output static characteristics Q_{h2} and Q_{ch4} shows existence of maxima with respect to hydrogen and methane. This fact is important for the practical applications and will be further used in optimising the bioreactors to achieve maximal production of either hydrogen and methane. The model also allows finding the optimal ratio between the volumes (V_1 and V_2) of the two bioreactors subject to the same optimisation goal.

Currently two-phase AD of lignocellulosic waste (wheat straw) with hydrogen and methane production in laboratory conditions are in experimental studies using some theoretical results obtained with the above presented model.

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Milen Borisov

Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
Bl. 8, Georgi Bonchev Str.
Sofia, 1113, Bulgaria

Address for correspondence:
Ivan Simeonov
e-mail: issim@microbio.bas.bg

Dencho Denchev, Ivan Simeonov

Institute of Microbiology
Bulgarian Academy of Sciences
Bl. 26, G. Bonchev Str.
Sofia, 1113, Bulgaria