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IFAC-PapersOnLine 49-26 (2016) 231–238

Mathematical Modelling of Anaerobic Digestion with Hydrogen and Methane Production ⋆

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Abstract: We propose a new mathematical model describing a biotechnological process of simultaneous production of hydrogen and methane by anaerobic digestion. The process is carried out in two connected continuously stirred bioreactors. The proposed model is developed by reducing the well known Anaerobic Digester Model No 1 (ADM1). The mathematical analysis of the model involves computation of equilibrium points, investigation of their local stability with respect to practically important input parameters, existence of maxima of the input-output static characteristics. Numerical simulations using a specially elaborated web-based software environment are presented to demonstrate the dynamic behavior of the model solutions.

Keywords: Biotechnological process; Hydrogen and methane production; Mathematical Model; Equilibrium points; Dynamics.

1. INTRODUCTION

Anaerobic digestion (AD) is a multi-step biotechnological process (Figure 1) with hydrogen (H_2) as a non-accumulating intermediate product (see e. g. Ahring (2003), Deublein (2008)). Recently, the interest in H_2 production through AD, also known as dark fermentative H_2 production, has increased (cf. Guo et al. (2010), Pakarinen et al. (2011)). 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 (cf. 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 overall energy conversion efficiency, a two-stage AD concept consisting of hydrogenic process followed by methanogenic process has been suggested (see e. g. Pakarinen et al. (2011)).

A lot of models describing separately the fermentative hydrogen production (see e. g. Nasr et al. (2013), Wang et al. (2009)) and the AD for methane production (see e. g. Batstone et al. (2002), Dochain (2001), Simeonov (2010)) are known. However, models of the two-stage AD process producing simultaneously H_2 and CH_4 are not known.

In this paper we present a new mathematical model describing the process of simultaneous H_2 and CH_4 production by AD of organic wastes in a cascade of two continuously stirred bioreactors. The biochemical processes in the first bioreactor include disintegration of organic wastes, hydrolysis and acidogenesis with hydrogen production. The methane production from acetate (methanogenesis) is separated in the second bioreactor. The proposed model is developed by reducing the well known Anaerobic Digester Model No 1 (ADM1) basic structure elaborated by the International Water Association (IWA), see Batstone et al. (2002).

The paper is organized in the following way. Section 2 is devoted to process description. Section 3 presents the mathematical model of the dynamic processes in the two bioreactors. The equilibrium points of the model are computed in Section 4 and their local stability is investigated in the next Section 5. Section 6 is devoted to investigations of input-output static characteristics with respect to H_2

⋆ This research has been partially supported by the Bulgarian Science Fund under contract No. DFNI–E02/13. The work of the second author has been partially supported by Sofia University "St Kl. Ohridski" under contract No. 58/06.04.2016.

2405-8963
Peer review under responsibility of International Federation of Automatic Control.
10.1016/j.ifacol.2016.12.131

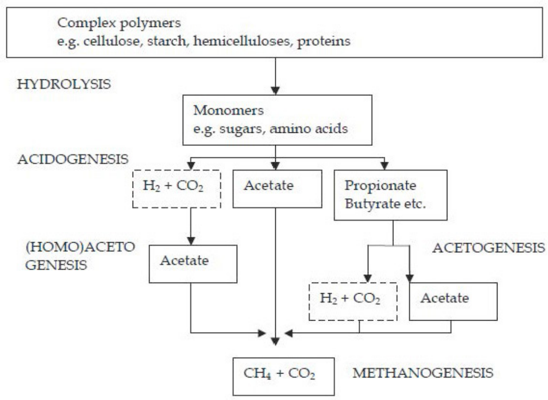

Fig. 1. Biochemical scheme of the AD

and CH_4 production; in particular existence of maxima is shown, which is important for the applications. Numerical simulations are presented in Section 7 as illustration of the theoretical results. The last Section 8 presents some concluding remarks and ideas for future studies.

2. PROCESS DESCRIPTION

The application of a two-stage AD process for sequential H_2 and CH_4 production (Figure 2) 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.

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

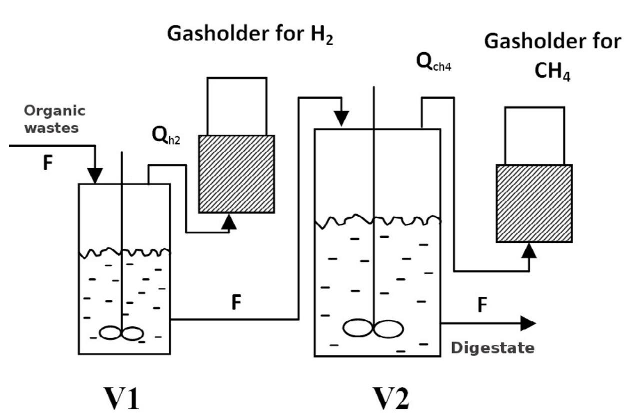

Fig. 2. Two-phases process of AD with production of hydrogen (H_2) and methane (CH_4)

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

$$D_1 = \frac{F}{V_1}, \quad D_2 = \frac{F}{V_2}.$$

Then

$$D_2 = \frac{V_1}{V_2} D_1 := \gamma D_1 \quad \text{within} \quad \gamma := \frac{V_1}{V_2}. \tag{1}$$

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.

3. MODEL DESCRIPTION

In this section we present the mathematical model describing the process of simultaneous H_2 and CH_4 production by AD of organic wastes in a cascade of two continuously stirred bioreactors. The model is derived on the basis of the ADM1 basic structure as well as on our experience with the two-phase AD process with hydrogen and methane production, see Denchev et al. (2016). The following assumptions have been accepted:

- The slow acetogenesis phase has been omitted and consequently in the second bioreactor only methanogenesis occurs.
- 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.

Following the above assumptions, the dynamics in the first bioreactor is described by the following set of 10 nonlinear ordinary differential equations

$$\frac{d}{dt}S_{su}(t) = D_1(S_{su}^{in} - S_{su}) + k_{hyd,ch}X_{ch} + f_{su,li}k_{hyd,li}X_{li} - \mu_{suaa,su}X_{suaa} \tag{2}$$

$$\frac{d}{dt}S_{aa}(t) = D_1(S_{aa}^{in} - S_{aa}) + k_{hyd,pr}X_{pr} - \mu_{suaa,aa}X_{suaa} \tag{3}$$

$$\frac{d}{dt}S_{fa}(t) = D_1(S_{fa}^{in} - S_{fa}) + f_{fa,li}k_{hyd,li}X_{li} - \mu_{fa}X_{fa} \tag{4}$$

$$\frac{d}{dt}S_{ac}(t) = -D_1S_{ac} + (1 - Y_{suaa})f_{ac,su}\mu_{suaa,su}X_{suaa} + (1 - Y_{suaa})f_{ac,aa}\mu_{suaa,aa}X_{suaa} + 0.7\,(1 - Y_{fa})\mu_{fa}X_{fa} \tag{5}$$