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COMPUTER SIMULATION OF ANAEROBIC FERMENTATION

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Abstract: *The presented paper deals with mathematical modeling and computer simulation of the anaerobic fermentation mechanism. Degradation of organic substances to final products, methane and carbon dioxide, involves their coordinated metabolic cooperation. A product of one microorganism group turns into substrate for the other groups. Generally, anaerobic fermentation progress in four stadiums, therefore mathematical model of four-level decomposition is used. All computations and simulations were performed in the MATLAB+SIMULINK environment.*
Key words: *fermentation, anaerobic technologies, biogas, simulation*

1. INTRODUCTION

Anaerobic fermentation is biological process of organic mass decay which proceeds without oxygen (air). This process runs naturally in nature e.g. in marshes, at the lake bottom or communal waste dump. Mixed culture of microorganism in of several steps decay organic mass during this process. A product of one microorganism group turns into substrate for the other group. We can divide fermentation process into four main phases:

- Hydrolysis: by the activity of extracellular enzymes, macromolecular materials are outside the cell split into simpler organic substances, first of all fatty acids, alcohols, carbon dioxide (CO_2) and molecular hydrogen (H_2).
- Acidogenesis: products of hydrolysis are inside the cell rotted into simpler substances (acids, alcohols, carbon dioxide and molecular hydrogen). By the fermentation of these substances is generating mixture of products whose composition depends on initial substrate and reaction conditions. Under the low concentration of hydrogen is generating acetic acid. Under the higher concentration of hydrogen is generating lactic acid and alcohol. Another important factor is pH value of reaction mixture. When the pH is neutral or slightly acid it dominates the butyric fermentation and when the pH is more acid (3-4) it dominates lactic fermentation.
- Acetogenesis: in this step substances produced by acidogenesis are spread out into molecular hydrogen, carbon dioxide and acetic acid.
- Methanegenesis: it is the last stadium of the anaerobic decay when from the acetic acid, hydrogen and carbon dioxide rises methane - CH_4. This step is performing by methanogene microorganisms which are strictly anaerobic organism and oxygen is poison for them.

The main product of anaerobic fermentation of organic mass is biogas. Biogas is colorless gas consisting primarily of methane (approx. 60%) and carbon dioxide (approx. 40%). It is able to contain small quantities of N_2, H_2S, NH_3, H_2O, ethane and lower hydrocarbons. As a secondary product there is a stabilized anaerobic material (fermentation remainder, digestat, ferment) which is mostly exploited as fertilizer in current time.

Fermentation is usually running in large heated and mixed tanks – fermentation reactors. It is continuous or semicontinuous process. The tank size is given by quantity and quality of material, quantity of active biomass in reactor and desired time delay. These parameters significantly influence the production of biogas and quality of output material.

Most widely used technology of biogas production is so-called "wet fermentation", which processes substrates with resulting dry matter content <12%. Wet anaerobic fermentation proceeds in reserved vessels (fermenters/reactors). These vessels are heated on designed operational temperature and mixed.

Technology of dry fermentation processes substrates about 30 - 35% dry matter. Generally there are mesophilic applications of anaerobic process; range of used reactionary temperatures is 32-38°C. Optimal pH is approximately 6.5 – 7.5. In principle, it is possible to divide out technologies on discontinuous (batch) and continuous one.

In light of reactionary temperatures we can divide anaerobic processes, according to optimal temperature for microorganism to psychrophilic (5-30°C), mesophilic (30-40°C), thermophilic (45-60°C) and extremely thermophilic (up 60°C). Most common applications are processes mesophilic at temperature approximately 38°C (Froment & Bischotf, 1990).

2. MATHEMATICAL MODEL

The simplest dynamic quantitative model of complex fermentation process is set of four simple differential equations describing following scheme:

$$c_1 \xrightarrow{k_1} c_2 \xrightarrow{k_2} c_3 \xrightarrow{k_3} c_4 \xrightarrow{k_4} c_5 \qquad (1)$$

where k_1, k_2, k_3, k_4 are speed constants for each subsequent reactions.

Quantitative models of steady states are based on mass and thermal balance of particular processes. It is necessary to emphasize that quantitative models rise from laws of mass and energy preservation. Hydrolysis of the cellulose is described in a lot of publications e.g. (Swift, 1998), (Smith, 1998) we shall deal only with acidogenesis, acetogenesis and methanogenesis. Total anaerobic decomposition of the glucose as a product of the cellulose at usage of 100% substrate is possible describe by following formula:

$$C_6H_{12}O_6 \rightarrow 3CH_4 + 3CO_2 \qquad (2)$$

According the presented chemical equation we can obtain by anaerobic fermentation from 1 kmol of 100% glucose 6 kmol (134.4 m^3) of biogas (50% methane and 50% carbon dioxide).

Quantitative description of the fermentation process depends on the idea of chemical mechanism of all four reactions - hydrolysis, acidogenesis, acetogenesis and methanogenesis. On the assumption that the source material is substrate, whose main biodegradable component forms cellulose, we can compile two basic models according the acidogenesis mechanism (Kodriková, 2004), (Kolomazník & Kodrikova, 2008).

2.1 Neutral or slightly acid fermentation

When the pH is neutral or slightly acid it dominates the butyric fermentation. Complex chemical mechanism is described by the following equations:

Hydrolysis: speed constant = k_0

$$(C_6H_{12}O_5)_n + nH_2O =_n C_6H_{12}O_6 \tag{3}$$

Acidogenesis: speed constant = k_1

$$C_6H_{12}O_6 = C_4H_8O_4 + 2CO_2 + 2H_2 \tag{4}$$

Acetogenesis: speed constant = k_2

$$C_4H_8O_4 + 2H_2O = 2C_2H_4O_2 + 2H_2 \tag{5}$$

Methanogenesis: speed constant = k_4

$$2C_2H_4O_2 = 2CH_4 + 2CO_2 \tag{6}$$

speed constant = k_3

$$CO_2 + 4H_2 = CH_4 + 2H_2O \tag{7}$$

Dynamic mathematical model is presented by the set of differential equations:

$$\frac{dc_1}{dt} = -k_0 c_1 c_8 \tag{8}$$

$$\frac{dc_2}{dt} = k_0 c_1 c_8 - k_1 c_2 \tag{9}$$

$$\frac{dc_3}{dt} = k_1 c_2 - k_2 c_3 c_8^2 \tag{10}$$

$$\frac{dc_4}{dt} = k_2 c_3 c_8^2 - k_4 c_4 \tag{11}$$

$$\frac{dc_5}{dt} = k_4 c_4 + k_3 c_6 c_7^4 \tag{12}$$

$$\frac{dc_6}{dt} = k_1 c_2 + k_4 c_4 - k_3 c_6 c_7^4 \tag{13}$$

$$\frac{dc_7}{dt} = k_1 c_2 + k_2 c_3 c_8^2 - k_3 c_6 c_7^4 \tag{14}$$

$$\frac{dc_8}{dt} = -k_2 c_3 c_8^2 + k_3 c_6 c_7^4 \tag{15}$$

Where c_1 is cellulose, c_2 is glucose, c_3 is butyric acid, c_4 is acetic acid, c_5 is methane, c_6 is carbon dioxide, c_7 is hydrogen and c_8 is water.

2.1 Acid fermentation

When the pH is lower (3-4) it dominates lactic fermentation. Chemical mechanism is described by:

Hydrolysis: speed constant = k'$_0$

$$(C_6H_{12}O_5)_n + nH_2O =_n C_6H_{12}O_6 \tag{16}$$

Acidogenesis: speed constant = k'$_1$

$$C_6H_{12}O_6 = 2C_3H_6O_3 \tag{17}$$

Acetogenesis: speed constant = k'$_2$

$$2C_3H_6O_3 + 2H_2O = 2C_2H_4O_2 + 4H_2 + 2CO_2 \tag{18}$$

Methanogenesis: speed constant = k'$_4$

$$2C_2H_4O_2 = 2CH_4 + 2CO_2 \tag{19}$$

speed constant = k'$_3$

$$CO_2 + 4H_2 = CH_4 + 2H_2O \tag{20}$$

Dynamic mathematical model is presented by the set of differential equations:

$$\frac{dc_1}{dt} = -k_0 c_1 c_8 \tag{21}$$

$$\frac{dc_2}{dt} = k'_0 c_1 c_8 - k'_1 c_2 \tag{22}$$

$$\frac{dc_3}{dt} = k'_1 c_2 - k'_2 c_3 c_8^2 \tag{23}$$

$$\frac{dc_4}{dt} = k'_2 c_3 c_8^2 + k'_2 c_8 - k'_4 c_4 \tag{24}$$

$$\frac{dc_5}{dt} = k'_4 c_4 + k'_3 c_6 c_7^4 \tag{25}$$

$$\frac{dc_6}{dt} = k'_2 c_3 c_8^2 + k'_4 c_4 - k'_3 c_6 c_7^4 \tag{26}$$

$$\frac{dc_7}{dt} = k'_2 c_3 c_8 - k'_3 c_6 c_7^4 \tag{27}$$

$$\frac{dc_8}{dt} = -k'_0 c_1 c_8 - k'_2 c_3 c_8^2 + k'_3 c_6 c_7^4 \qquad (27)$$

Where c_1 is cellulose, c_2 is glucose, c_3 is lactic acid, c_4 is acetic acid, c_5 is methane, c_6 is carbon dioxide, c_7 is hydrogen and c_8 is water.

3. SIMULATIONS

For computations of differential equations and simulations we have used the MATLAB+SIMULINK environment.

3.1 Neutral or slightly acid fermentation

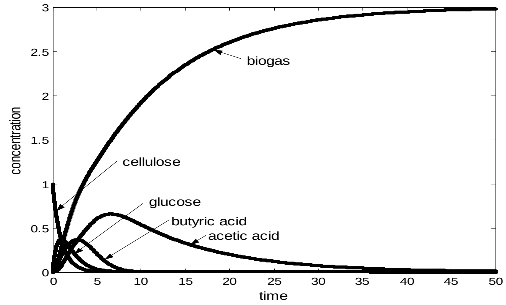

Fig. 1. Time dependence of the initial substance, intermediate products and product concentration

Speed constants were chosen as k_0=0.9, k_1=0.8, k_2=0.8, k_3=0.1, k_4=0.1.

3.2 Acid fermentation

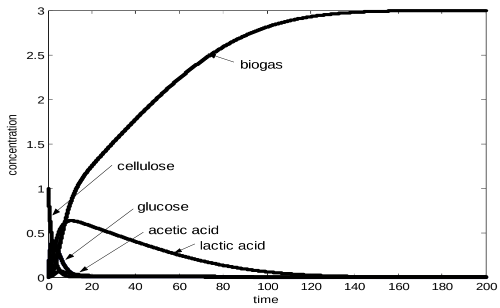

Fig. 2. Time dependence of initial substance, intermediate products and product concentration

Speed constants were chosen as k'$_0$=0.5, k'$_1$=0.4, k'$_2$=0.3, k'$_3$=0.6, k'$_4$=0.8.

4. CONCLUSION

To practical production of the biogas it's required to suggest special anaerobic technology and realize it in corresponding establishment. In this paper, the behavior of anaerobic decay of cellulose and its time progression are simulated using the MATLAB-SIMULINK environment.

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