MODELLING AND SIMULATION OF DRY ANAEROBIC FERMENTATION

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ABSTRACT
The paper is focused on mathematical modelling and computer simulation of the anaerobic fermentation mechanism for neutral or slightly acid and acid fermentation. 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 subsequent ones. Generally, the studied anaerobic fermentation processes progress in four stadiums, therefore a mathematical model of four-level decomposition is used. All mentioned processes were modeled through differential equations and computed and simulated in the MATLAB+SIMULINK environment.

INTRODUCTION

The necessity for alternative "green" energy from renewable resources has enhanced the role of environmental management of ecosystems. Today, anaerobic fermentation is widely accepted as a sound technology for many waste treatment applications, and novel reactor designs are being applied on a commercial scale. In spite of this acceptance, advances are still being made, and our developments are concentrating on the uses of small amount of biodegradable mass - especially for dry discontinuous fermentation processes.
Anaerobic fermentation is a biological process of organic mass decay which proceeds without oxygen (air). This process runs naturally in country e.g. in marshes, at the lake bottom but it is used also in different types of wastes (communal waste dump, cow and poultry manure, liquids from the agro-industries etc.). Mixed culture of microorganism in several steps decay organic mass during this process. A product of one microorganism group turns into substrate for the other group (Ahring, 2003).
The fermentation process can be divided 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 (CO2) and molecular hydrogen (H2).
- 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 - CH4. 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 N2, H2S, NH3, H2O, ethane and lower hydrocarbons. As a secondary product there is a stabilized anaerobic material (fermentation remainder, digestat, ferment) which is mostly exploited as a fertilizer material (Straka, 2003).
A fermentation processes usually run in large heated and mixed (stirred) tanks – fermentation reactors. It is a continuous or semicontinuous process. The tank size is given by quantity and quality of material, quantity of active biomass in the reactor and the desired time delay. These parameters significantly influence the production of biogas and quality of output materials.
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).

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Wet fermentation technology

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.

Dry fermentation technology

The technology of dry fermentation processes substrates about 30 - 35% of dry matter. It can be used for biomass production which is not possible to work up by wet fermentation (e.g. slurry, sawdust, straw, grass, foliage, leaf litter, wood waste). Generally, there are mesophilic conditions of anaerobic process; range of used reactionary temperatures is 32-38°C. The optimal pH is usually between 6.5 – 7.5. In principle, it is possible to divide out technologies on discontinuous (batch) and continuous one.
The discontinuous technology consists of several reaction chambers (metallic containers or bricked chambers) and a buffer stock. An anaerobic process is treated by the dosage of procedural liquids. For inoculation/vaccinations needs is exploited partly periodic injection of so-called percolate (material with content of suitable anaerobic cultures) and additions of fermentative remainder from previous cycle to the fresh substrate. From the investment and operational point of view discontinuous technologies are essentially less exacting than continuous ones.

THEORETICAL BACKGROUND

The simplest dynamic quantitative model of a complex fermentation process represents a set of four simple differential equations according to the following scheme:

$$c_1 \overset{k_1}{\rightarrow} c_2 \overset{k_2}{\rightarrow} c_3 \overset{k_3}{\rightarrow} c_4 \overset{k_4}{\rightarrow} c_5 \tag{1}$$

where k_1, k_2, k_3, k_4 are speed constants for each subsequent reaction.
Quantitative models of steady states are based on the mass and thermal balance of particular processes. It is necessary to emphasize that quantitative models rise from laws of mass and energy conservation equations. 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. The total anaerobic decomposition of the glucose as a product of the cellulose at usage of 100% substrate is possible to describe by the following formula:

$$C_6H_{12}O_6 \rightarrow 3CH_4 + 3CO_2 \tag{2}$$

According to the presented chemical equation from 1 kmol of 100% glucose can be obtained 6 kmol (134.4 m^3) of biogas (50% methane and 50% carbon dioxide) by anaerobic fermentation.
The quantitative description of the fermentation process depends on the idea of chemical mechanism of all four reactions - hydrolysis, acidogenesis, acetogenesis and methanogenesis. With the assumption that the source material is substrate, whose main biodegradable component forms cellulose, we can compile two basic mathematical models according the acidogenesis mechanism (Kodriková, 2004), (Kolomazník & Kodrikova, 2008).

Neutral or slightly acid fermentation

The butyric fermentation dominates When the pH value of reaction mixture is neutral or slightly acid. The complex mass balance of the chemical mechanism is then described by the following equations:

Hydrolysis: with speed constant = k_0

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

Acidogenesis: with speed constant = k_1

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

Acetogenesis: with speed constant = k_2

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

Methanogenesis: with speed constant = k_4

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

and with speed constant = k_3

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

The whole chemical status described by Equations (3) – (7) is illustrated by the following kinetic graph.

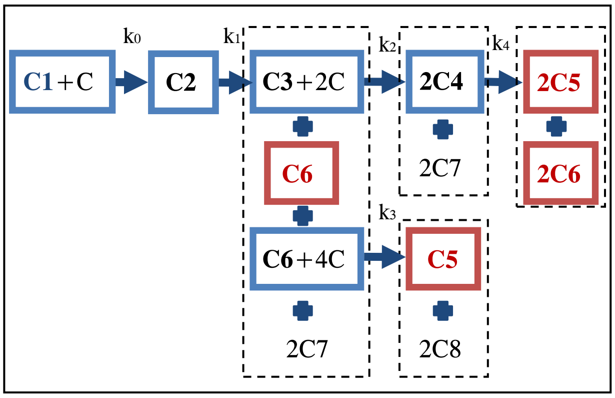

Figure 1: Kinetic graph of neutral or slightly acid fermentation

In Figure 1, abbreviations where C1 is cellulose, C2 is glucose, C3 is butyric acid, C4 is acetic acid, C5 is methane, C6 is carbon dioxide, C7 is hydrogen and C8 is water are used.

Acid fermentation

The lactic fermentation dominates for the lower (3-4) pH value of the reaction mixture. Then the complex mass balance of the chemical mechanism is described by the following equations:

Hydrolysis: with speed constant = k'_0

$$(C_6H_{12}O_5)_n + nH_2O =_n C_6H_{12}O_6 \qquad (8)$$

Acidogenesis: with speed constant = k'_1

$$C_6H_{12}O_6 = 2C_3H_6O_3 \qquad (9)$$

Acetogenesis: with speed constant = k'_2

$$2C_3H_6O_3 + 2H_2O = 2C_2H_4O_2 + 4H_2 + 2CO_2 \qquad (10)$$

Methanogenesis: with speed constant = k'_4

$$2C_2H_4O_2 = 2CH_4 + 2CO_2 \qquad (11)$$

and with speed constant = k'_3

$$CO_2 + 4H_2 = CH_4 + 2H_2O \qquad (12)$$

The whole chemical status described by Equations (8) – (12) is illustrated by the following kinetic graph.

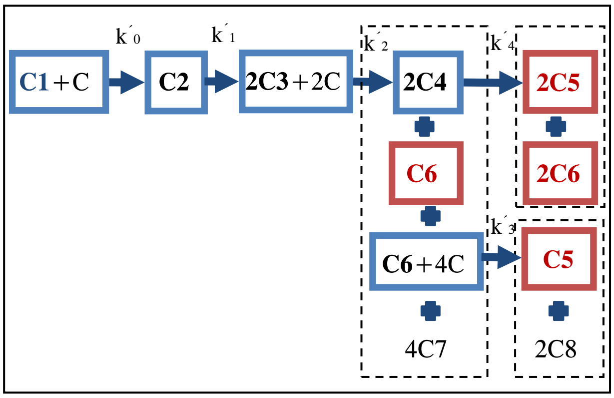

Figure 2: Kinetic graph of acid fermentation

In Figure 2, abbreviations where C1 is cellulose, C2 is glucose, C3 is is lactic acid, C4 is acetic acid, C5 is methane, C6 is carbon dioxide, C7 is hydrogen and C8 is water are used.

MATHEMATICAL MODEL

Now, the dynamic mathematical model can be summarized according to the mentioned chemical reactions, mechanisms and flows.

Neutral or slightly acid fermentation

The first set of differential equations describes the chemical processes shown in Figure 1 representing neutral and/or slightly acid fermentation:

$$\frac{dc_1}{dt} = -k_0c_1c_8 \qquad (13)$$
$$\frac{dc_2}{dt} = k_0c_1c_8 - k_1c_2 \qquad (14)$$
$$\frac{dc_3}{dt} = k_1c_2 - k_2c_3c_8^2 \qquad (15)$$
$$\frac{dc_4}{dt} = k_2c_3c_8^2 - k_4c_4 \qquad (16)$$
$$\frac{dc_5}{dt} = k_4c_4 + k_3c_6c_7^4 \qquad (17)$$
$$\frac{dc_6}{dt} = k_1c_2 + k_4c_4 - k_3c_6c_7^4 \qquad (18)$$
$$\frac{dc_7}{dt} = k_1c_2 + k_2c_3c_8^2 - k_3c_6c_7^4 \qquad (19)$$
$$\frac{dc_8}{dt} = -k_2c_3c_8^2 + k_3c_6c_7^4 \qquad (20)$$

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

Acid fermentation

The second dynamic mathematical model for the acid fermentation described previously and summarized in Figure 2 is presented by the set of the following differential equations:

$$\frac{dc_1}{dt} = -k'_0c_1c_8 \qquad (21)$$
$$\frac{dc_2}{dt} = k'_0c_1c_8 - k'_1c_2 \qquad (22)$$
$$\frac{dc_3}{dt} = k'_1c_2 - k'_2c_3^2 \qquad (23)$$
$$\frac{dc_4}{dt} = k'_2c_3^2c_8^2 - k'_2c_6^2 - k'_2c_7^4 - k'_4c_4^2 \qquad (24)$$
$$\frac{dc_5}{dt} = k'_4c_4^2 + k'_3c_6c_7^4 \qquad (25)$$
$$\frac{dc_6}{dt} = k'_2c_3^2c_8^2 + k'_4c_4^2 - k'_3c_6c_7^4 \qquad (26)$$
$$\frac{dc_7}{dt} = k'_2c_3^2c_8^2 - k'_3c_6c_7^4 \qquad (27)$$
$$\frac{dc_8}{dt} = -k'_0c_1c_8 - k'_2c_3^2c_8^2 + k'_3c_6c_7^4 \qquad (27)$$

where c_1, c_2, c_4, c_5, c_6, c_7 and c_8 represents the same sense as in Equations (13)-(20), c_3 represents lactic acid.

SIMULATIONS

Simulation experiments with dry fermentation of biomass has been provided in order to get the information about possibilities of its utilization for liquidation of biodegradable sorted communal waste dump. The results of simulations and obtained values are utilized for the design and development of technological reactors and plants.
As the fermenter we plan to use the ordinary commercial composter with some construction modifications. For this purpose we need to find out time behaviors of particular processes - time dependence of initial substances, intermediate and final products concentrations, their speed constants and so on.

Neutral or slightly acid fermentation

Experiment 1:

Speed constants were chosen as k_0=0.9, k_1=0.8, k_2=0.7, k_3=0.6, k_4=0.6.

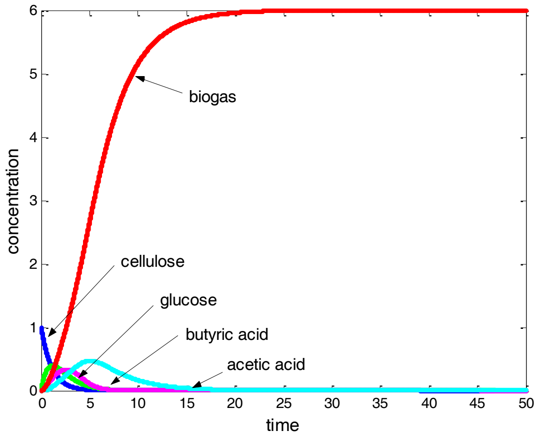

Figure 3: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.1.

Experiment 2:

Speed constants were chosen as k_0=0.9, k_1=0.8, k_2=0.7, k_3=0.2, k_4=0.2.

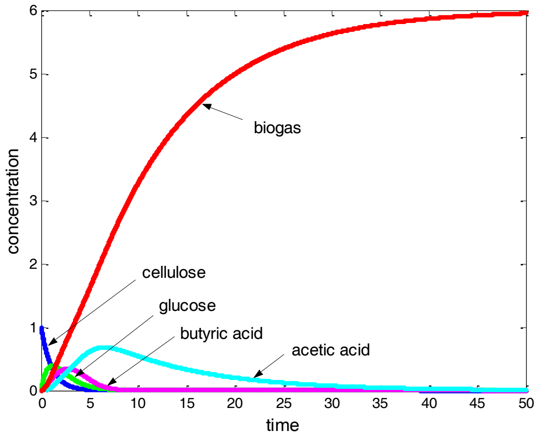

Figure 4: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.2.

Experiment 3:

Speed constants were chosen as k_0=0.9, k_1=0.8, k_2=0.7, k_3=0.6, k_4=0.2.

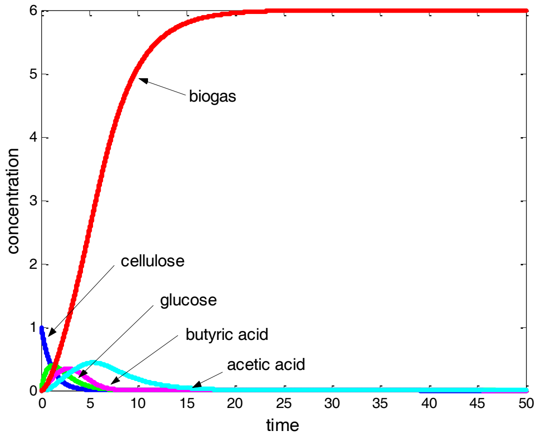

Figure 5: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.3.

Experiment 4:

Speed constants were chosen as k_0=0.9, k_1=0.8, k_2=0.7, k_3=0.2, k_4=0.6.

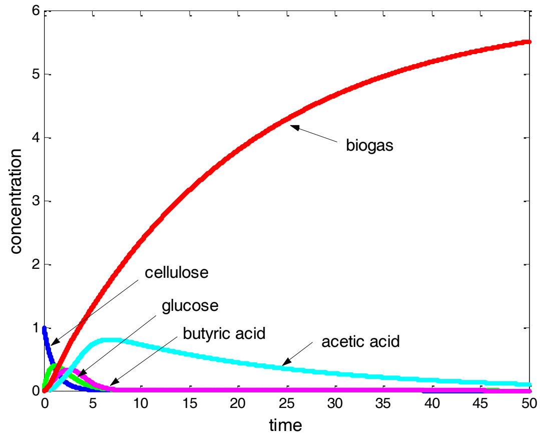

Figure 6: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.4.

Experiment 5:

Speed constants were chosen as k_0=0.6, k_1=0.5, k_2=0.4, k_3=0.3, k_4=0.2.

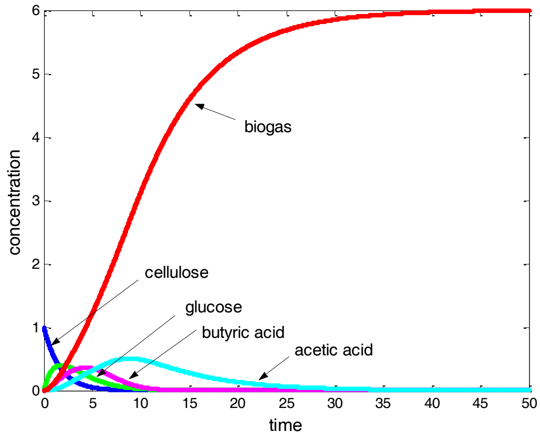

Figure 7: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.6.

Experiment 6:

Speed constants were chosen as k_0=0.2, k_1=0.3, k_2=0.4, k_3=0.5, k_4=0.6.

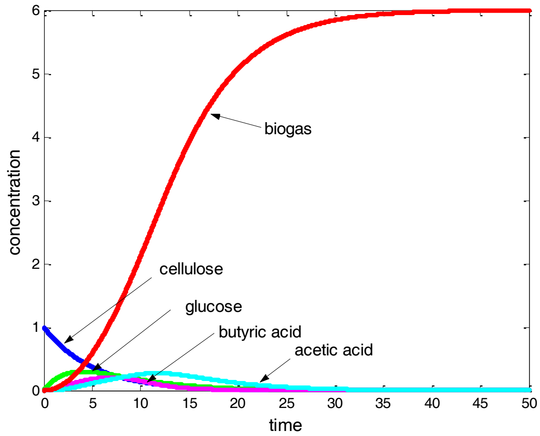

Figure 8: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.6.

Acid fermentation

Experiment 7:

Speed constants were chosen as $k'_0=0.9$, $k'_1=0.8$, $k'_2=0.7$, $k'_3=0.6$, $k'_4=0.6$.

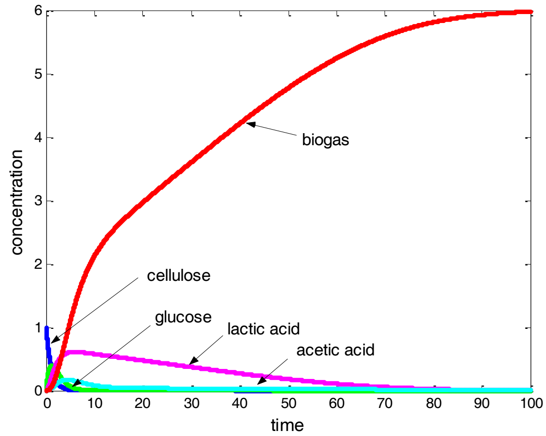

Figure 9: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.7.

Experiment 8:

Speed constants were chosen as $k'_0=0.9$, $k'_1=0.8$, $k'_2=0.7$, $k'_3=0.2$, $k'_4=0.2$.

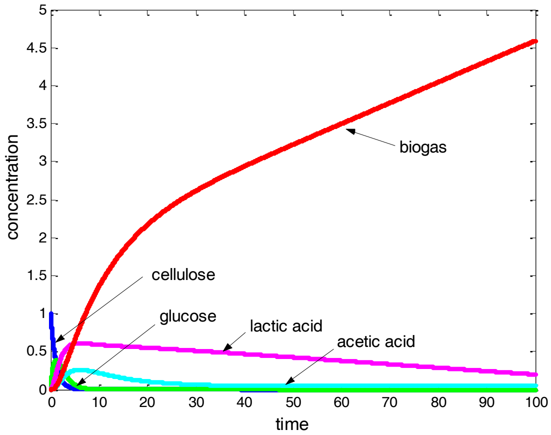

Figure 10: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.8.

Experiment 9:

Speed constants were chosen as $k'_0=0.9$, $k'_1=0.8$, $k'_2=0.7$, $k'_3=0.8$, $k'_4=0.8$.

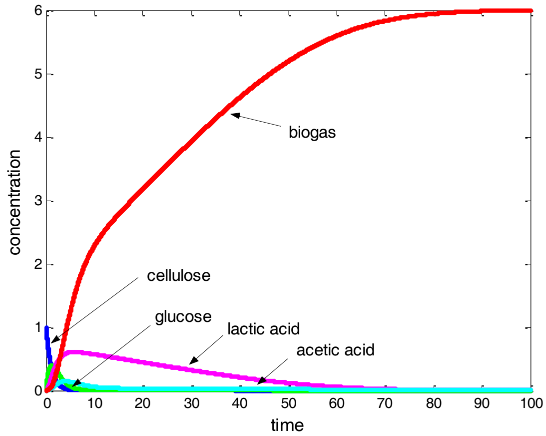

Figure 11: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.9.

Experiment 10:

Speed constants were chosen as $k'_0=0.9$, $k'_1=0.8$, $k'_2=0.7$, $k'_3=0.2$, $k'_4=0.8$.

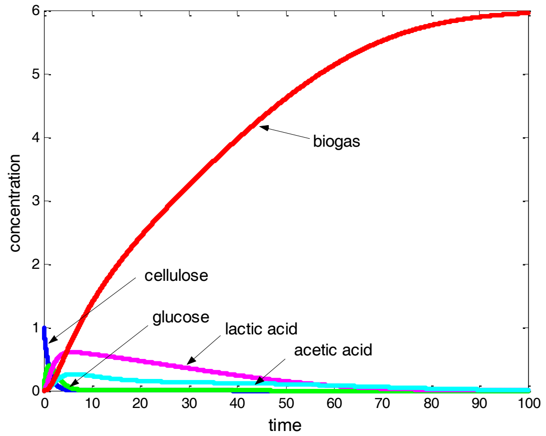

Figure 12: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.10.

Experiment 11:

Speed constants were chosen as $k'_0=0.5$, $k'_1=0.6$, $k'_2=0.7$, $k'_3=0.8$, $k'_4=0.9$.

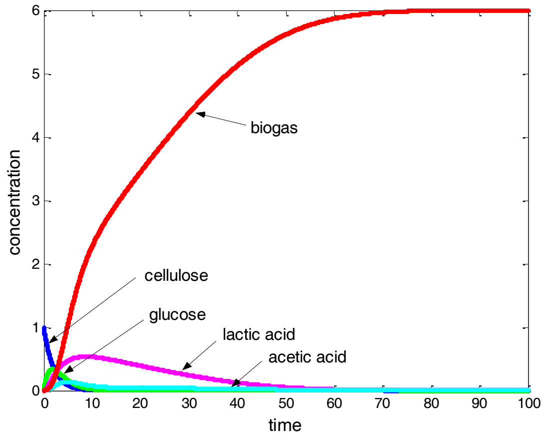

Figure 13: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.11.

Experiment 12:

Speed constants were chosen as $k'_0=0.2$, $k'_1=0.3$, $k'_2=0.4$, $k'_3=0.5$, $k'_4=0.6$.

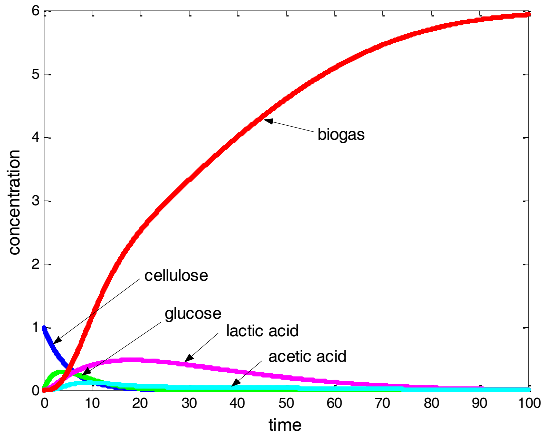

Figure 14: Time dependence of the initial substance, intermediate products and biogas concentration-Exp.10.

CONCLUSION

Biogas production combines the short-term economic needs of human communities with nature of conservation and the end of ecological degradation. This process producing alternative energy also generate other valuable materials as fertilizers, soil conditioners, animal and fish feed and so on. Further benefits of this technology can be seen also in e.g. odor problem reduction, microorganism pathogens control, water resources protection etc.

Deeper understanding and insight into special anaerobic technology is a key point for practical production of the biogas. This paper brings a look to the behavior of anaerobic decay of cellulose and its time progression under the various conditions. Mathematical models have been based only on the mass balance of particular processes. We have started from presumption that anaerobic reaction is exothermal and fermenter works without external heating. Temperature influence of reactions (interactions among microorganism) is partly hidden in speed constants. The obtained results and performed experiments demonstrate that the neutral or slightly acid fermentation is more fast (quick) than acid fermentation. The speed of fermentation depends on the activity of catalyzer which is used as an accelerator of chemical reactions. The presented figures and graphs disclose that the complex behavior of reactions is strongly influenced by the speed constants k_3 (resp. k'_3) and k_4 (resp. k'_4).

All analytical dynamic mathematical models were calculated and simulated in the MATLAB-SIMULINK environment.

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