СТОРІНКА МОЛОДОГО ВЧЕНОГО

УДК 628:519.87.

MODELING OF BIOGAS SIMULATION AT THE LANDFILL OF MUNICIPAL SOLID WASTE (MSW)

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Based on published data and theoretical notions of the processes in the body of the solid waste landfill, formulated an idea about the landfill as a biochemical reactor in which the interrelated processes of heat and mass flow in two-dimensional dense layer, through which the gas is filtered and internal sources of heat. The known mathematical model of biogas emissions at the site, suggested a more general mathematical model that takes into account the representation of a range of biochemical reactor. *Keywords:* municipal solid waste, ground, biodegradation, bioconversion.

Моделирование процессов образования биогаза на полигоне твердых бытовых отходов (ТБО). М.А. Бондарь. На основании известных литературных данных и теоретических представлениях о процессах в теле полигона твердых бытовых отходов, сформулировано представление о полигоне как о биохимическом реакторе, в котором протекают взаимосвязанные процессы тепломассопереноса в двухмерном плотном слое, через который фильтруется газ и с внутренними источниками тепловыделения. Проанализированы известные математические модели эмиссии биогаза на полигоне, предположена более общая математическая модель, учитывающая представление о полигоне как о биохимическом реакторе. *Ключевые слова:* полигон твердых бытовых отходов, биоразложение, биоконверсия.

Моделювання процесів утворення біогазу на полігоні твердих побутових відходів (ТПВ). М.О. Бондар. На підставі відомих літературних даних і теоретичних уявленнях про процеси в тілі полігону твердих побутових відходів, сформульовано уявлення про полігоні як про біохімічному реакторі, в якому протікають взаємозв'язані процеси тепломасопереносу в двомірному щільному шарі, через який фільтрується газ і з внутрішніми джерелами тепловиділення. Проаналізовано відомі математичні моделі емісії біогазу на полігоні, припущена більш загальна математична модель, що враховує уявлення про полігоні як про біохімічному реакторі. Ключові слова: полігон твердих побутових відходів, біорозпад, біоконверсія.

Under solid-state fermentation of solid waste that occurs in the body of the landfill and in the normal course of processes of all organisms work in concert. All intermediate products of alignment of one stage are processed by bacteria of other stage.

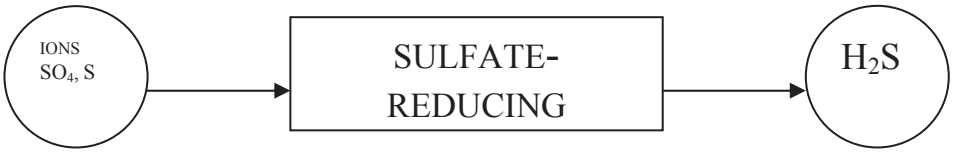
In general, during decomposition of the organic matter amount of the final products can be obtained according to the equation:

$$C_nH_aO_b + (n - a/4 + b/2)\ H_20 \rightarrow \rightarrow (n/2 + a/8 + b/4)\ C0_2 + (n/2 + +a/8 + b/4)\ CH_4 \quad (1)$$

In each case the yield of biogas depends on the composition of organic matter, process conditions, etc.

Biogas produced after the anaerobic decomposition of organic substances also contains ethane, propane, butane. It is assumed that they are formed by alkyl radicals with the transfer of coenzyme M. Apparently, the reaction between two molecules methyl-ComM catalyzed by appropriate enzymes lead to the synthesis of ethane. At influence of methyl- CoM and ethyl-CoM can form propane, etc.

The works [1-4] gives the vertical distribution of microbial processes in the interior of the landfill (dump). Analysis of the data indicates that the thickness of the landfill is (starting from the surface) aerobic zone ~1,25 m, then a transition zone ~1, 2 meters and down to the foundation pit anaerobic zone. In the first zone, there is flowing oxidation of organic and gaseous products and because of the microbial oxidation tails progressively mineralize partially complex multi carbon substances (proteins, lipids, polysaccharides) are exposed to enzymatic hydrolysis. The result of these organisms are formation of hydrogen, carbon dioxide, low molecular weight fatty acids, alcohols, etc. The second zone is characterized by the process and the denitrification of nitrate and nitrides to nitrogen gas and oxides. Central microbiological process, anaerobic zone, closing desintegration of organic components is a formation of methane. In this zone all of the above reactions and the process of sulfate reduction can be realized under the scheme:



In general, it is considered that stages of anaerobic the process in landfills thicker characterized as preparatory - 0.5 - 1 year of exponential - 10 years, stationary - 20 years, decaying - 30 years, biological inertness - 30 - 40 years. Analysis shows that the thickness of aforementioned zones and stages of operation depends on many factors. The main ones are: the composition and structure of wastes under recycling; porosity thickness, core temperature, content of light fatty acid, humidity of systems, the intensity of diffusion of gases through the thickness of the landfill.

Let us briefly consider the impact of these factors.

Usually in foreign practice tails of sorting, which consist of food waste - 60.4%, landscape debris - 4.31%, paper - 3.9%; tree - 1.55%; textiles - 1 , 38% plastic + leather + rubber - 2.5% organic screenings -5.86%, the rest inactive will be subjected to solid-phase fermentation. Organics cover 80,4% including composed nutrients N, P, K, C, Ca. A ratio of N: P is approximately

equal to 5:1, while the ratio of C: N: P ≈ 47:5:1. According to Spitz and McCarthy [5], such a ratio of nutrients meets the needs of methanogenic bacteria, and the empirical gross formula for anaerobic biomass can be written as $S_5N_9O_3N$.

Development of rapid anaerobic processes requires not only optimal conditions anaerobic biodegradation, but a high content of active biomass in a volume. Activity depends on the type of components that make up the tails (morphological structure) sort of the kinetic parameter, which determines the maximum degree of decomposition of each component in the real world, the amount of water and its distribution uniformity in size, the particle size of biodegradable ingredients. All the above factors are manifested in the total value of the factor of biodegradation, which is introduced in [6] and is recommended for use in calculating the methane potential. The value of the factor Bf biodegradation of the various components in the range:

- food waste - 0.83;
- park and garden debris - 0.25;
- paper - 0.2;
- wood - 0.22;
- plastic + leather + rubber - 0.22.

These values characterize the highest possible degree of biodegradation component in specific circumstances. The rate of decomposition of the individual components is also related to their chemical nature, for the calculation of the rate of decomposition is often used recommended by the Agency for Environmental Protection mathematical model of the United States, the so-called first-order decay model:

$$\frac{dC}{d\tau} = -k \cdot C, \qquad (3)$$

where C is the initial content of the substance;

$k = \frac{1}{\tau}$ (1/year) - the rate constant of decomposition.

The rate constant of decomposition may vary from 0.001 to 0.45 y^{-1}

Highest value k typical for food waste as in the initial stages of their degradation greatest yield of soluble compounds such as simple monosaccharides and amino acids. For the rest of the components are typical values close to the 0,001 $year^{-1}$. Therefore, the most important step, limiting the overall speed of decomposition of organic substances polygon is depolymerization of high-molecular compounds, primarily cellulose and plastics, which can be stretched up to 100 years. According to some reports [2-3], a little more than half of the cellulose-containing materials decompose for 100 years. Especially long substrates wherein the cellulose is encrusted with lignin, poorly controlled microbial degradation decompose. The same performance, but for the worse, and can be brought for plastics, rubber and leather. Based on the theoretical foundations of biochemistry [7], the anaerobic digestion of simple compounds (monosaccharides, amino acids) a significant amount of energy that accumulates in the part of high-energy bonds of ATP releases and partially dispersed in the form of heat. According to [7], quite a lot of energy (ΔG10 = - 196,9 kJ / mol) According to [7], is released quite a lot of energy (ΔG10 = - 196,9 kJ / mol), 30-35% of which goes to the biosynthesis of two molecules of ATP, and 65-70% dissipate as heat, 30-35% of which goes to the biosynthesis of two

molecules of ATP, and 65-70% is dissipated as heat.

Obviously, thanks to the temperature changes in the thickness of the polygon. Apparently, the activity begins to psychrophilic bacteria zone characterized by a temperature 15-20 ° C, then heating at least the thickness polygon, the period mesophilic zone - 20-40 ° C, and then the thermophilic - 50-60 ° C. The optimum temperature for mesophilic zone is 32-33 ° C, the thermophilic - 52-54 ° C. Obviously, to obtain a relatively uniform temperature over the layer thickness of the polygon are all readily degradable components should be evenly distributed over the volume (i.e., volume to be uniformly distributed heat sources). The second condition is obviously also has to be a smooth flow of substances on the surface of a solid, liquid and gaseous phases, which is a prerequisite for high activity of the reactions. Paper [8] argues that the absence of solid-state fermentation conditions for the attainment of those effects has led to the fact that solid state fermentation has not found wide application in industry (except for landfills). To achieve the second condition, but uniform distribution of the components, it is necessary that the thickness of the landfill has a relatively high porosity. It is a porous addition landfills and a large number of affordable organic microbes create the preconditions for the development of microbial processes in the volume of the landfill. Porosity depends on the size of the intensity of gas formation in wide layers of the landfill, the rate of diffusion of the gas flow to the upper layers and, consequently, the power of the aerobic zone and the duration of the preparatory period. All the above indicators will determine the period of exponential development and actual output range at maximum efficiency of biogas, as well as the mosaic of the landfill gas field.

Conditions of heat transfer in the landfill can affect the local hydrogen concentration and affect the kinetics of the bioconversion of fatty acids and the kinetics of the whole bioconversion [9]. Consequently, it can be assumed that a correlation between the presence of these acids and hydrogen partial pressure in the gas flow through the layer of body. From this standpoint, there is a need to maintain a certain porosity in the interior, since the intense gas diffusion (in the case of high porosity) is maintained relatively low hydrogen partial pressure in the gas flow needed for the bioconversion of fatty acids geteroatsetogennymi bacteria which can grow successfully only by cocultivation with methanogenic bacteria disposing hydrogen.

One of the above mentioned factors is system humidity. In the literature for solid-state fermentation systems we found no specific guidance on the interval humidity solid framework within which to carry out the process. It is only noted that the water in the system with the crystal form should be enough for the life of bacteria [8]. However, the practice of landfill operation and the values of the quantities of rainfall in the regions where the landfills are it can be roughly assumed that humidity should be at least 40-50%.

2. Analysis of mathematical models for estimating emissions of biogas at landfills and their modernization.

The development of the theoretical foundations of forecasting methods of biogas generation from the decomposition of municipal solid waste is a pre-

requisite for further progress in the field of waste treatment and disposal technology of MSW.

In the literature, there are several methods for estimating emissions of biogas, which is based on a stoichiometric approach [10.5, 7], the theory of transport phenomena of gases [11], the kinetics and dynamics of anaerobic processes [6].

Stoichiometric approach is based on the gross formula expansion of basic organic components - waste (see equation 1). In paper [10] the qualitative characteristics of the process, some of the empirical values are presented, the assessment on the specific model of heat and mass transfer is not given. For example, to calculate the amount of released methane Gτ for the recommended time τ is given by:

$$G_\tau = 1{,}868\ C_0\ (0{,}014\ T + 0{,}028)\ (1 - 10\ k\tau), \quad (4)$$

where C_0 is organic carbon;

T is a temperature in the landfill;

k is a constant of decomposition year^{-1} (see formula 3)

τ is a time, year.

There are a number of models based on the dynamics of anaerobic processes [11]

$$G_\tau = \sum i \cdot T_i \left[\frac{MP_0}{\tau} \cdot exp\left(-\frac{\tau_1}{\tau} \right) \right], \quad (5)$$

where Gτ is amount of methane, m 3 / year;

M is the mass of waste in a landfill cell, t;

i is the number of cells or charts;

τ is the degradation time in years;

τ1 is length biogas yield, the years;

MR_0 is methane potential of undecomposed waste m^3 / year.

Предложен также ряд мультиплетных моделей [12], объединяющих различные параметры:

We propose a number of multiplet models [12], bringing together the various parameters:

$$C_1 = \frac{\int W \cdot k^2 \cdot \tau \cdot e^{-k\tau}(\tau, T) \cdot p(T_b) \cdot \upsilon(T_b)}{q \cdot A}, \quad (6)$$

where W is the total weight of waste, t;

k is the expansion, year^{-1};

p (T_b) is possibility of time travel components from the surface to the base of the landfill;

Ci is concentration of i component;

q is the water flow through the thickness of the waste;

A is area of the base polygon;

T_b is time, year.

A common disadvantage of these models, including a model of the first order (formula 3) is to use of dependent parameters (rate constants, the values of the water flow, and the probability values, etc.) that can not be properly determined or measured. However, analysis of the model equations (3-12) leads to the conclusion that the findings made in the introduction, are true and are essential.

In paper [6], a model that, according to the authors, allows defining the maximum possible in the real degree of decomposition of the various components of MSW is suggested:

$$Q = (1 - w) * M_{в.п} \Sigma\ [L_{oi} \cdot X_i * B_f) * (1 - e^{-k\tau}), \quad (7)$$

where *w* is humidity;

$M_{в.п}$ is mass of wet waste;

L_{oi} is methane potential of dry waste for each component;

X_i is the proportion of biodegradable fractions;

B_f is the proportion of biodegradable fractions;

k is constant of decomposition;

τ is time equal to the difference between the current time and time τ_l, necessary for the establishment of anaerobic conditions.

However, the resulting model is uncertain parameters k and τ_l, which are, without a doubt, the functions of the body temperature in the range and nature of its distribution by volume. Therefore, for the calculation of the authors of [6] uses a sound empirical value of k and τ_l. Despite this, obtained in [6], a mathematical model is the most simple and involves the actual quantities in the calculation formula.

If we proceed from the concept of the landfill as a reactor in which the interrelated processes of heat and mass flow in two-dimensional dense layer (stationary) to filter out the gas flow, the analysis of these processes must be based on the presentation of the theory of heat and mass transfer in dense particulate layer [13-14]. However, most of the known methods [15,16] is based on the integral balance sheet ratios, based on the concept of the "amount of heat per ton of product", and not even the ability to correctly carry out a qualitative analysis of these laws. A number of studies [17] attempts to describe the processes of cooling and storage of food rich in a dense layer of field crops based on local patterns of heat and mass transfer in the bed. It does not take into account the transfer of heat and moisture in the direction of the normal rate of filtration of gas in the bed, the contact between the elements of the thermal conductivity of the layer, the heat of reaction and a number of other factors, which limits the application of the recommendations [17] for the case.

Therefore, it is advisable to consider the heat transfer in the dense layer mass height H through which diffuses in the direction Y gas (biogas) coming from the lower layer in a horizontal cross section of 2L and a depth considerably greater than 2L. Bed temperature at the initial time $T\tau_{00}$ differs from the temperature at the inlet of the $M_{вл}$, so in the time-dependent flow interrelated heat and mass transfer processes. And at constant parameters inlet gas temperature distribution and moisture content in the system tend to some steady-state (equilibrium). For a description of these processes two-component model of interpenetrating fluids (gas and solid) [18] can be taken. Each component is considered as a quasi-homogeneous medium characterized by effective transport coefficients, which differ in the longitudinal (Y) and transverse (X) direction. The effective thermal conductivity in the solid component consider conduction through the particles (elements of the layer), the contacts and the gas layer between them, the radiation, the gas component - conduction, radiation and convection component. Mass transfer resistance within the layer elements accept negligible. Heat and mass transfer between the solid and gas in the bed, as well as between the gas and the side surfaces of the reactor and a layer accounted for by appropriate thermal mass transfer coefficients. The heat generated as a result of biological processes in the layer is seen as a positive internal heat source in the solid component. Contribution heat biochemical process becomes noticeable in quasi-stationary conditions and increases as the velocity of gas through the filter layer. Vaporization considered as a heat sink on the surface of the solid

component. In accordance with the physical model of transient heat and mass transfer are described by the following system of differential equations obtained on the basis of the laws of conservation of energy and mass.

- energy for a solid and a gas layer components:

$$\begin{aligned}&(1-\varepsilon)\,p_T\cdot C_T\cdot\frac{\delta T_T}{\delta\tau}-\lambda_{Tx}\frac{\delta^2 T_T}{\delta x^2}-\lambda_{Ty}\frac{\delta^2 T_T}{\delta y^2}-\\&-\alpha\cdot\alpha_T\left(T_\Gamma-T_T\right)-p_T\left(1-\varepsilon\right)q_T\cdot exp\left(b\cdot T_T\right)+,\\&+\beta\cdot a_T\cdot q_\Pi\left[\int\left(T_T\right)-E\cdot d_\Gamma\right]=0\end{aligned}\qquad(8)$$

$$\varepsilon\cdot\rho_\Gamma\cdot C_{P\Gamma}\frac{\delta T_\Gamma}{\delta\tau}+C_{P\Gamma}\frac{\delta T_\Gamma}{\delta y}\cdot G-\lambda_{\Gamma x}\frac{\delta^2 T_\Gamma}{\delta y^2}+\alpha\cdot\alpha_T\left(T_\Gamma-T_T\right)=0\,,\qquad(9)$$

- mass transfer of the gas component layer::

$$\varepsilon\cdot p_\Gamma\frac{\delta d}{\delta\tau}+G\frac{\delta d}{\delta y}-p_\Gamma\cdot D_x\frac{\delta^2 d}{\delta x^2}-p_\Gamma\cdot D_y\frac{\delta^2 d}{\delta y^2}-\beta\cdot\alpha_T\left[\int\left(T_\Gamma\right)-E\cdot d\right]=0\,,\qquad(10)$$

- energy of the gas in the boundary layer of the reactor:

$$\rho_\Gamma\cdot C_{P\Gamma}\cdot L_3\frac{\delta T_3}{\delta\tau}+C_{P\Gamma}\cdot L_3\frac{\delta T_3}{\delta y}+\alpha_1\left(T_3-T_1\right)=0\,,\qquad(11)$$

- mass transfer of the gas into the clearance (3), - the boundary layer of the reactor:

$$\rho_\Gamma\cdot L_3\frac{\delta d_3}{\delta\tau}+C_3\cdot L_3\frac{\delta d_3}{\delta y}+\beta_1\left(d_3-d_1\right)=0\,,\qquad(12)$$

In equations 8-12 ε is porosity layer, the proportion of the section;

p_T, P_Γ~ density of the solid, gas;

C_T, C_Γ - specific heat of solid, gas at constant pressure;

λ- corresponding coefficients of thermal conductivity;

a_T - specific surface area, the proportion of the surface;

α - coefficient of heat transfer;

β - mass transfer coefficient;

b - coefficient;

f (T_T) - approximation of dependence of the equilibrium moisture content of the gas temperature;

E - coefficient;

d_T - a particle diameter of the solid component;

x, y - transverse and longitudinal coordinates;

d_Γ, d_3 - moisture content of the gas;

q_T - specific heat produced by a biological process;

$q_п$ - specific heat of vaporization;

τ- time;

T- temperature;

G - mass flow rate of gas through the layer.

In the case of uneven profile of the gas velocity through the layer with uniform porosity to the system 8-12 equation of continuity and the motion of the

gas in the layer should be added. Here we consider the case of a uniform velocity distribution over the cross section and constant porosity layer. This is due to the fact that the homogenizing and briquetting assumed tails sorting before storage.

Boundary conditions of system (8-12)

$$\begin{aligned}
&\tau=1; T_T=T_{00}; T_\Gamma=T_{\Gamma 00}; d=d_{00}; T_3=T_{00}; d_3=d_{300}\\
&y=0, 0\le x\le L; \frac{\delta T_T}{\delta y}=0; T_\Gamma=T_{\Gamma 0}(\tau); d=d_0(\tau);\\
&y=H; 0\le x\le L; -\lambda_{Ty}\frac{\delta T_T}{\delta y}=\alpha_2\cdot\alpha_{T2}(T_\Gamma-T_\Gamma);\\
&\frac{\delta T_\Gamma}{\delta y}=0; \frac{\delta d}{\delta y}=0;\\
&x=0; 0\le y\le H; \frac{\delta T_T}{\delta x}=0; \frac{\delta T_\Gamma}{\delta x}=0; \frac{\delta d}{\delta x}=0;\\
&x=0; 0\le y\le H; -\lambda_{Ty}\frac{\delta T_x}{\delta x}=\alpha_{T1}\cdot\alpha_{T2}(T_{T2}-T_3);\\
&-\lambda_{Ty}\frac{\delta T_\Gamma}{\delta x}=\alpha_{\Gamma 1}\cdot\alpha_{\Gamma 2}(T_{\Gamma 1}-T_3); -D_X\frac{\delta d}{\delta x}=\beta_1\cdot\alpha_{\Gamma 1}\left[\int(T_{T1}-E_{d3})\right];\\
&y=0; T_3=T_{30}(\tau)
\end{aligned} \quad , \quad (13)$$

Здесь индексы: 0 - нижняя граница; 1 - боковая граница (у стенки реактора); 2 - верхняя граница; 00 - начальное значение; *i*, *j* - number of grid point in the x,y; k- number of the step in the time coordinate.

When recording 8-13 exchange conditions considered identical in both side surfaces of the layer, heat release due to heat biochemical reaction accepted varying depending on CT exponentially [15] mass transfer on the surface of flowing waste relied on Dalton's law [9] equation 11,12 for gas at the reactor walls are written in the one-dimensional approximation.

To find the functions in equation 8-13 is used numerical method of finite differences [19]. In developing the methodology for calculating the system of equations was introduced a number of restrictions that have simplified its form:

1) side walls of the reactor and a layer of a wall envisaged heat and water resistant, and therefore excluded equation 11, 12;

2) thermal properties and characteristics of the layer components are taken independent of temperature;

3) members, taking into account the heat of biochemical reactions and f (TT), linearize the range of possible changes in the TT.

These assumptions are chosen based on the fact that a possible change in temperature ranges from 20 to 60°C. Change in temperature estimated from known relationships for exothermic reactions [20].

$$T=T_0+T_a x$$

$$T_a = \frac{(+\Delta H)\cdot(C_0 - C)}{C_{PT}\cdot p_T \cdot g}, \qquad (14)$$

where T_0 is initial temperature;;

T_a - adiabatic temperature;

x - degree of degradation of organic matter into simple systems;

$+\Delta H$- heat of reaction;

C_0,C- concentration of organics with $B_f > 0,5$

Then

$$k = k0\cdot e^{\frac{-E/R}{T_0 + T_a \cdot x}}, \qquad (15)$$

After selecting the finite difference schemes and writing tasks of difference equations 8-12 turn into a system of algebraic equations, which consists of three subsystems. This system can be solved by iterative method [21].

Thus, the equations 7-15 are complete mathematical model of the reactor-polygon in which the interrelated processes of heat and mass flow in a dense layer, through which the gas is filtered and internal sources of heat.

The presented model and calculation methods can be used to analyze the processes of heat and mass transfer in packed beds with internal heat source and the calculation of the emission of biogas in the design and operation of the landfill reactor.

The following report will present the experimental results and literature data confirming the adequacy of the proposed model.

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