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Mathematical model of biochemical decomposition of organic in landfill *

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Abstract

The purpose of this paper is the description of the mathematical model of biochemical decomposition of landfill's organic components and to use it for analyzing the waste management decision in the landfills. From the mathematical point of view the model proposed in the paper represents the system of differential equations in partial derivatives. It allows to take into account the key parameters influencing on gas capacity and to carry out the forecasting and management of the modelled process.

1 Introduction

During the latest decade the volume of solid waste generation has essentially increased. This fact is connected with abrupt consumption rise, which is observed in industrial countries. According to the data from [1] the flow of solid waste, which is annually forthcoming into biosphere, has reached almost geological scale and amounts approximately 400 million tons per year. The permanently growing quantity of waste products has a sharp effect on global geochemical cycles of a lot of elements containing in organic chemistry, in particular organic carbon. So, the weight of this element forthcoming into an environment with waste products, makes approximately 85 million tones in one year while the general natural inflow of carbon into a soil cover of a planet makes only 41.4 million tons per one year.

One of the basic ways of solid waste removal all over the world remains its burial in the near-surface geological environment. In these

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conditions the waste products are exposed to intensive biochemical decomposition which causes in particular landfill gas generation. The issues of biogas forthcoming into the natural environment form negative effects of both local and global character.

From the other hand various research organizations in many countries of the world are actively engaged in the search of alternative sources of energy. There are many nonconventional energy sources: solar, wind, the heat of underground sources, the tidal energy in the seas and oceans etc. An energy source of anthropogenic character is of great importance now. It is the biogas received from organic components of household waste. By various expert estimations the organic components make $\sim 70\%$ of all waste products. Thus, usual dumps of waste are the powerful biological reactors capable to make the valuable energy carrier – biogas – within decades.

Practically in all industrially advanced countries, and also in many developing ones there are national programs of getting the biogas as a result of decomposition of organic substances and its further use.

The interest to biogas usage has increased in connection with the increase of prices for energy carriers. Biogas is formed of organic constituents of waste products at their decomposition by microorganisms. The process of decomposition proceeds in two stages: at presence of oxygen there is an aerobic process, and after an exhaustion of oxygen in deeper layers (oxygen-free) the anaerobic stage begins. Biogas evolved by microorganisms contains $\sim 60\%$ of methane and may be used on a place as low-calorie fuel, or may be processed into high-calorific gas and used for needs of gas supply.

Positive experience on biogas creation and use is received in many countries of the world. So, in USA the general number of municipal dumps has increased from 19.000 in 1985 up to 23.000 in 1995. Thus the share of dumps with the tonnage of waste more than 1 million tons has increased from 9% up to 23%. It is essential from the point of view of economy of biogas usage. The calculations of economic efficiency of biogas usage carried out in 1982 for dumps with various volumes of stored waste, show that for volumes more than 1 million tons the use of biogas becomes profitable. In Moldova, taking into

account the lower wages of workers and the world prices for gas, it is economically expedient to maintain dumps with the smaller contents of waste products.

As the researches show, biogas spreads in the thickness of the stored waste products mainly in horizontal direction (at presence of insulating layers). The issue of biogas from a surface into atmosphere is determined by a number of factors. If the top layer of a dump is insufficiently dense then the evolved gas is mixed up with atmospheric air. At good condensation or at presence of a tight covering of a surface the biogas is concentrated and evolved basically on slopes and on the limited sites of a surface.

Two kinds of degassing of dumps are applied to practical use of biogas:

1. passive degassing which is carried out due to the own pressure in thickness of a dump;

2. active degassing which is carried out with the help of special devices for extraction of gas.

Passive degassing is seldom applied to get biogas because of its low efficiency. The increased requirements for prevention of uncontrollable issue of gas into an atmosphere are made to the means of active degassing.

The process of organic components decomposition consists of three stages. At the first of them in the presence of great amount of oxygen the complex of organic molecules is decomposed in aerobic way. After the termination of access of oxygen the second phase - a fermentation and glycolysis - comes into effect. When the free oxygen biochemically becomes completely exhausted, the most prolonged stage - the stage of anaerobic decomposition - begins. The duration of this stage, i.e. the speed of organic chemistry decomposition, characterizes the "ageing" of a dump. After the complete decomposition of organic chemistry the active processes of biogas issue are stopping. The dump becomes ecologically inert.

The speed of organic chemistry decomposition depends on the great number of different factors: humidity, temperature, parameter of acid-

ity pH, specific gravity of waste, contents of organic chemistry etc. The functional dependencies of decomposition speed on the factors enumerated above, are unknown today. So it is impossible to calculate the decomposition speed directly. By accumulation the experimental data, which describe the microorganisms activity, it will be possible to calculate directly the decomposition speed, taking into account all these factors [4].

2 The mathematical model. Basic conceptions

In the given work an attempt to describe influence of temperature, humidity, density and other parameters on the process of decomposition of organic chemistry by methods of mathematical modelling is made.

The quantity of the evolved biogas, and also the speed of the gas generation process are determined by the conditions of the environment which have been usual in concrete dump body. The humidity, temperature, composition of organic fractions concern the number of parameters rendering essential influence on decomposition of organic chemistry. Their complex influence is reflected in the following kinetics equation of the first order for the gas generation reaction [1]:

$$V = Mqe^{-kt} \tag{1}$$

- V – quantity of biogas (m^3), formed in time t (years);
- M – weight of waste products (ton);
- q – specific gas potential (m^3/ton);
- k – a constant of speed of gas generation reaction (1/year).

In practice, various modifications of the formula (1) are applied for the forecasting of gas generation [6]. Their basic distinction is reduced to the quantity of fractions of the solid waste organic substance included into consideration. These fractions essentially differ in their physical-chemical properties and terms of biochemical decomposition. So, "fast" fractions decay during 2-4 years, and the slower ones - during decades.

In the work [2] the mathematical equation for an estimation of issue of biogas in England, for the period from 1970 till 2000 is given. It is

based on model of National Physical Laboratory (NPL). The NPL's model allows carrying out an estimation of issue of biogas depending on the row of the determining factors, which are based on statistical processing of data, received for this period of time. From the mathematical point of view this model (NPL) represents the polynomial of the 4th degree, which depends on time and which approximates the process of biogas issue during the period of time mentioned above.

The model proposed by the author enables to take into consideration the internal intercommunications between those factors (temperature, humidity, organic chemistry contents, density, temperature conductivity of the environment etc), on which the process of biogas issue in the dump body depends. From the mathematical point of view all these parameters are being interconnected and are being written down in a form of a system of differential equations in partial derivatives [3]. The solution of this system with corresponding initial and boundary conditions allows to carry out the forecasting and management of the concrete dump.

At the given stage of researches the influence of the following factors is investigated:

- contents of organic chemistry in waste products;
- density of substance;
- quantity of humidity;
- influence of seasonal difference of temperatures;
- account of reaction's exothermicity;
- account of influence of anaerobic and aerobic stages of organic chemistry decomposition;
- influence of development prehistory of processes, occurring in the dump.

2.1 The temperature effects modelling

For the description of the process of heat distribution along time and depth of the dump (taking into account the fact that the reactions are exothermic) the equation of heat conductivity is used.

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(\lambda(T)\frac{\partial T}{\partial z}\right) + Q(z). \tag{2}$$

This equation is of parabolic type and if dependencies $\lambda(T)$ and $Q(z)$ are known, then it is possible to solve the equation (2) numerically. Parameters $\lambda(T)$ and $Q(z)$ are the functional dependencies on temperature, humidity, depth and other parameters of environment.

$\lambda(T)$ may be received at numerical approximation of experimental data (see sec. 2.2). $Q(z)$ is determined by the quantity of decomposed organic chemistry (see sec.2.3).

Initial and boundary conditions. Initial conditions of a problem may be given through distribution of temperature along depth in an initial period of time $t = 0$:

$$T(z, 0) = T_0(z) \tag{3}$$

and through distribution of humidity along depth:

$$W(z, 0) = W_0(z) \tag{4}$$

In practice, naturally, it is difficult to define functions $T_0(z)$ by experimental way.

The initial temperature distribution doesn't influence essentially on the realization of calculations. After several iterations the influence of boundary conditions and the exothermicity of occurring reactions become much more essential. That is why for the beginning of calculations in the proposed model we can select linear approximation of the temperature between boundary conditions on the surface and on the bottom of the dump.

For setting the initial distribution of humidity the experimental data are to be used, which are to be got for modelled solid waste landfill (see subsec.2.2).

The problem becomes a little bit more complicated in the case of lamination of environment. Modern technologies of the waste burial on the solid waste landfills need the alternation of the waste by the layers of insulating material (sand, clay, gravel). That's why the account of multi-layerness is introduced into the mathematical model. Corresponding boundary conditions are set on these layers. Moreover, the insulating material doesn't take part in the biochemical reactions, what is taken into account in the model too.

The iterative process converges in this case too, however to get necessary accuracy it needs more iterations. As boundary conditions the conditions of the 1-st, 2-nd or the 3-rd sort may be used. From the physical point of view the boundary conditions of the 2-nd sort are more correct as they describe behavior of a stream of heat at the boundaries. It is supposed that the temperature changes along space are proportional to the difference of temperatures between organic chemistry and high boundary l_i of insulating material (see equation (5)), and between low boundary l_{i+1} of insulating material and organic chemistry (see equation (6)):

$$\frac{\partial T}{\partial z} = k_1(T - T_{l_i}), z = l_i \tag{5}$$

$$\frac{\partial T}{\partial z} = k_2(T - T_{l_{i+1}}), z = l_{i+1}, \tag{6}$$

where

- T_{l_i} and $T_{l_{i+1}}$ are the corresponding temperatures of the researched layer;
- k_1 and k_2 are the coefficients of temperature conductivity, which are determined experimentally.

The equations (2) - (6) represent the initial-boundary problem in partial derivatives.

The formulated problem is solved with the help of formalities, based on the finite difference method. The solution is sought in the area $R : [0 \leq z \leq l, t > 0]$ with initial and boundary conditions (3) - (6).

Let us for determination of numerical solution to substitute the area R of continuous change of arguments of the function sought T for

a finite array of the points, lying in this area. Let us call this array by difference mesh, the points themselves – by nodes, and the function which is determined in any way on this array – by mesh function:

$$R_{h,k} : [(z_j = jh,\ j = 0, 1, 2, \ldots, J),\ t_n = n\tau,\ n = 0, 1, 2, \ldots].$$

In every node (x_j, t_n) of the difference mesh the numerical solution $T(x_j, t_n)$, which approximates $T(x, t)$ with assigned initial and boundary conditions, is sought.

Let us denote $T(x_j, t_n) = v_j^n$. Then we can represent the initial equation (2) on the assigned mesh R as a system of algebraic equations (7):

$$\frac{v_j^{n+1} - v_j^n}{\tau} =$$
$$= \frac{1}{h}\left[a_{j+1}(v_j^{n+1})\frac{v_{j+1}^{n+1} - v_j^{n+1}}{h} - a_j(v_j^{n+1})\frac{v_j^{n+1} - v_{j-1}^{n+1}}{h}\right] + Q(v_j^{n+1}), \quad (7)$$

where τ is the step by time, h is the step by space.

This system of equations realizes the well-known implicit Laason scheme. The parameter a_j allows the approximation of the dependence λ on temperature.

With the help of expansion of the equations system (7) into Taylor's series in the neighbourhood of the difference mesh node we can show that this scheme is the coordinated one. The calculations carried out on sequentially refining mesh showed that the scheme is steady for the examined mathematical problem. This difference scheme is of the 2nd order of accuracy along time and space as well.

2.2 Data for initial and boundary conditions

To model the natural conditions arising during the waste products storage the seasonal changes of temperature on the landfill surface (high boundary conditions) and the temperature at the landfill bottom (low boundary conditions) are considered. For simplicity the harmonious

fluctuations in limits from T_{min} up to T_{max} may be used, where T_{min} is the minimal value of temperature in winter, T_{max} is the maximal temperature in summer. As well the real data or synoptic forecasting if they are, may be used. So, the information about seasonal temperature changes is one of the model parameters, which represents the high boundary condition of the model. Then, the practice shows, that irrespective of seasonal temperature fluctuations on the surface the temperature at the depth greater than 15m remains constant and equal to 12°C. This value is a model's parameter, representing low boundary condition. If there is a thermoisolation on the bottom of the dump, then it is necessary to use the corresponding boundary condition.

It is necessary to determine the initial conditions for the model (humidity, coefficient of temperature conductivity, organic chemistry contents etc.) experimentally for the modelled solid waste landfill.

As these experimental data have a large dispersion, it is necessary to process them statistically and then to approximate.

Thus, for example the corresponding experimental data were got at the Academy of the Municipal Services of K.D.Pamfilov for landfills of Brateevo and Timohovo (Russia, Moscow)[7].

For definition of change of a thermal capacity on humidity the sample was dried up and weighed in a dry condition on analytical scales such as ADV-200 with accuracy of 0.001. Humidity on weight was lead up to required value by addition of necessary amount of water to within 0.5%. The thermal capacity of a sample was measured at various values of humidity. Definition of change of heat conductivity on humidity was carried out similarly the definition of change of a thermal capacity. To define the density the humidity of the samples, taken from a dump, was brought up to the required value by the same way, as at measurement of a thermal capacity. Then an ampoule with strictly fixed volume was filled up with the received substance. The substance necessary for filling of the ampoule was weighed. The density of samples was determined with accuracy of 0.3 %.

The data were processed statistically to reduce the errors of the experiment. Besides that the experimental data were processed by the least-squares method [5]. The polynomial dependencies were used

as approximating functions. The dependencies received were used as initial data for distribution of humidity, density, coefficients of thermal conductivity and thermal capacity along depth.

2.3 The quantity of decomposed organic chemistry calculation

Let us consider that organic chemistry decomposition runs with "average" speed which is determining experimentally [4]. The reducing of organic chemistry mass in the waste as the dump age increasing we can describe in the following way. Let M be the general initial waste mass, m_0 – organic chemistry mass at the moment of time $t = 0$. The ratio $T_{0c} = m_{c0}/M_0$ determines the part of organic chemistry in the fresh waste. The residual organic chemistry mass by the moment of time t can be calculated by the formula:

$$m_c = M_{c0} \exp(-t/r) = T_{0c} M_0 \exp(-t/r), \tag{8}$$

where $r = t^*/\ln 2$; t^* – period of time necessary for the decomposition of half of the carbon amount. Having differentiated the equation (8) along time, we will get the speed of the organic chemistry decomposition:

$$\dot{m}_c = \frac{M_{c0} \exp(-t/r)}{r}. \tag{9}$$

The humidity contents and the temperature influence this speed. As it was mentioned above, the most favorable humidity value for vital functions of microorganisms and hence for organic chemistry decomposition is 60%. The temperature range, favorable for evolution of methanogenic bacteria, is $12 - 60°C$. Out of this range at the temperature near $0°C$ or greater than $80°C$ the bacteria activity stops and the decomposition speed becomes equal to 0. Let us consider that at the most favorable conditions, i.e. at the temperature $36°C$ and the humidity 60%, the decomposition speed increases (along humidity – with coefficient 1.25, along temperature– with coefficient 1.2) relatively standard speed, determined in (9).

Let us introduce two functions $g = g(W)$ and $f = f(T)$ that depend on humidity and temperature in the following way:

$$g = \frac{1.25}{\left(1 + \frac{W-60}{13}\right)^4}, \tag{10}$$

$$f = \frac{1.2}{\left(1 + \frac{T-36}{10}\right)^4}. \tag{11}$$

Let us multiply (9) by (10) and (11). Then we will get:

$$\dot{m}_c = \frac{m_{c0} \exp(-t/r)}{r}\, g(W)\, f(T). \tag{12}$$

Thus we can calculate quantity of the organic chemistry decomposed during any period of time.

Heat quantity, issuing at organic chemistry decomposition, depends on the type of reaction. There is oxygen at the depth of 2 meters, so the decomposition runs as the result of aerobic reaction:

$CO_2 + H_2O \rightarrow$ with heat issue at the amount of 2822 kJ/mol.

There is no oxygen at the depth greater than 2 meters, so the decomposition runs as the result of anaerobic reaction:

$CO_2 + CH_4 \rightarrow$ with heat issue at the amount of 393 kJ/mol.

Using these values recalculated into kkal/kg, we can find heat quantity, issued during the decomposition process at the necessary period of time. The value got will be used as $Q(z)$ by solving the heat conductivity equation (2).

Then, if we will know the quantity of the decomposed organic chemistry, we will be able to calculate the quantity of biogas generated during any period of time.

3 Conclusions

The mathematical model constructed on the basis of the factors influencing on the decomposition of organic chemistry and on manufacture of biogas allows to carry out necessary calculations and to predict behavior of the modelled system.

On the basis of the proposed mathematical model the algorithm for creation of computer programm is built. It is necessary to use as initial parameters the following:

- experimental data, got from the concrete solid waste landfill, for which the numerical modelling is intended to make;
- climatic conditions on the surface – the seasonal changes of temperature (real and assumed);
- humidity changes (natural or artificially produced).

As the result of the programm work the following will be got:

- temperature values inside the body of the dump at any moment of time;
- quantity of generated biogas at any moment of time;
- quantity of residuary biomass at any moment of time;
- time necessary for total organic chemistry decomposition at the modelled conditions.

So, the model's parameters management allows to forecast and control the behavior of the modelled dump.

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