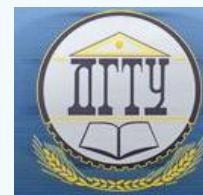


ИНФОРМАТИКА, ВЫЧИСЛИТЕЛЬНАЯ ТЕХНИКА И УПРАВЛЕНИЕ INFORMATION TECHNOLOGY, COMPUTER SCIENCE, AND MANAGEMENT



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Optimization of two-stage methanogenesis regime based on the Pontryagin's maximum principle *

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Оптимизация двухстадийного режима метаногенеза на основе принципа максимума Понтрягина ***

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Introduction. The solution to the problem of optimal control of the biogas process under its conversion in two digesters is considered. The work objectives are to propose a mathematical model of this process and to develop an optimal control algorithm.

Materials and Methods. The developed mathematical model describes the biomethanation from animal waste through the downstream processing of the substrate in two digesters. Cases of the same and different temperature media (mesophilic and thermophilic) are considered. An optimal control problem is defined as a Lagrange problem for this model. Its modifiers are the rates of substrate entry into the digesters. The algorithm for solving this problem is proposed; it is based on the numerical implementation of the Pontryagin maximum principle. When optimizing, a hybrid genetic algorithm was used with an additional search in the neighborhood of the best solution through the conjugate gradient method.

Research Results. A new mathematical model is developed. It describes the biomethanation during the downstream processing of the substrate in two digesters. A numerical algorithm for solving an optimal control problem is proposed and software-implemented. The numerical studies have shown that the biogas production rate is nearly twice as high for a thermophilic medium as for a mesophilic one. It is established that the downstream processing of the substrate in two digesters with the same temperature medium allows the biogas production rate to be doubled. If the temperature media in the digesters are different, then in the first of them, the mesophilic medium should be used, and in the second - the thermophilic medium. At this, the biogas formation rate is somewhat lower compared to the case when there is a mesophilic medium in each of the digesters; however, the degree of the substrate processing is by 10–15% higher.

Введение. Статья посвящена решению задачи оптимального управления процессом получения биогаза при непрерывном режиме его переработки в двух метантенках. Цели работы: представить математическую модель данного процесса и разработать алгоритм выбора оптимального управления.

Материалы и методы. Созданная математическая модель описывает получение биогаза из отходов животноводства при последовательной переработке субстрата в двух метантенках. Рассматриваются случаи одинаковых и различных температурных сред (мезофильной и термофильной). Для данной модели сформулирована задача оптимального управления в виде задачи Лагранжа. Ее управляющими параметрами являются скорости поступления субстрата в метантенки. Предложен алгоритм решения данной задачи, основанный на чис

ленной реализации принципа максимума Понтрягина. При оптимизации применялся гибридный генетический алгоритм с дополнительным поиском в окрестности лучшего решения методом сопряженных градиентов.

Результаты исследования. Разработана новая математическая модель, описывающая процесс получения биогаза при последовательной переработке субстрата в двух метантенках. Предложен и программно реализован численный алгоритм решения задачи оптимального управления. Численные исследования показали, что для термофильной среды скорость образования биогаза практически вдвое выше, чем для мезофильной. Установлено, что последовательная переработка субстрата в двух метантенках с одинаковыми температурными средами позволяет вдвое увеличить скорость образования биогаза. Если температурные среды в метантенках различны, то в первом из них следует использовать мезофильную среду, а во втором — термофильную. При этом скорость образования биогаза несколько ниже по сравнению со случаем, когда в каждом из метантенков мезофильная среда, однако степень переработки субстрата выше на 10–15 %.

* The research is done within the frame of the independent R&D.

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Discussion and Conclusions. The results obtained can be used for the calculation and design of biogas plants, as well as in the development of appropriate software.

Keywords: methanogenesis, biogas, digester, animal waste treatment, mathematical model, differential equation system, numerical solution, optimization methods, optimal control, Pontryagin's maximum principle.

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Обсуждение и заключения. Полученные результаты могут быть использованы для расчета и конструирования биогазовых установок, а также при разработке соответствующего программного обеспечения.

Ключевые слова: метаногенез, биогаз, метантенк, переработка отходов животноводства, математическая модель, система дифференциальных уравнений, численное решение, методы оптимизации, оптимальное управление, принцип максимума Понтрягина.

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Introduction. When livestock enterprises, in particular, poultry farms, pig farms, cattle farms, are operated, a large amount of waste is generated. As a result of their fermentation in special tanks (digesters), fuel gas (biogas) and valuable organic fertilizers can be obtained [1]. This process is called methanogenesis. It can occur under the periodic and continuous delivery of the substrate. In the first case, the digester is filled once and emptied completely upon completion of the fermentation. In the second case, two processes occur simultaneously and continuously: the supply of the substrate and the removal of its processed portion.

Usually, mesophilic medium (at a temperature of 25–38° C) or thermophilic (45–60° C) is used for methanogenesis. The optimum temperature for the mesophilic medium is 37° C, for the thermophilic medium, it is 56° C. The fermentation time for these media is 25 and 12 days, respectively.

The economic efficiency of biogas production depends on various factors: type and quantity of raw materials, climatic conditions [2], etc. In addition, the rate of substrate input into the digester affects significantly the biomethanation. This parameter value depends on the volume of the digester and the type of raw materials. To find the optimal value of the specified magnitude, it is required to solve an optimal control problem.

Under the continuous mode of fermentation, the substrate does not have time to go through full processing. To increase the biogas production, it is necessary to use two digesters so that the substrate is sequentially processed in each of them. Various aspects of this process are studied in [3, 4], and its technical implementations are reflected in the patents [5–7].

In the papers on the mathematical simulation of methanogenesis, for example [8, 9], the search for optimal control is not presented or its asymptotic value is found [10–12]. An analytical solution to the optimal control problem is obtained in [13]. However, the mathematical model described there differs significantly from that presented in this paper. The numerical method proposed here for solving an optimal control problem is applicable to a wide class of models.

Materials and Methods. The scheme of downstream processing of the substrate is shown in Fig. 1.

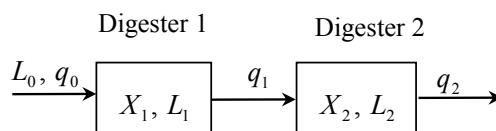


Fig. 1. Scheme of two-stage mode of methanogenesis

Assume L_0 is the concentration of nutrients in the substrate fed to the first digester (kg/m³); L_1 and L_2 are the concentration of nutrients in the substrate for the first and second digesters, respectively (kg/m³); X_1 and X_2 are the concentration of methane-producing bacteria in the first and second digesters (kg/m³); Q_1 is the volume of the substrate in the first digester (m³), Q_2 - in the second one; q_0 is the rate of the substrate input in the first digester (m³/day),

$q_1 = \frac{dQ_1}{dt}$ and $q_2 = \frac{dQ_2}{dt}$ are the rate of substrate delivery from the first and second digesters, respectively.

Losses of the substrate do not occur, therefore

$$q_0 = q_1 = q_2 = q.$$

The value of q_0 is determined by the volume of waste, the quantity and capacity of the biogas plants.

Relative rates of substrate input for the digesters are:

$$u_1 = \frac{1}{Q_1} \cdot \frac{dQ_1}{dt} = \frac{q_1}{Q_1} \text{ and } u_2 = \frac{1}{Q_2} \cdot \frac{dQ_2}{dt} = \frac{q_2}{Q_2}.$$

Substrate volumes in the digesters are equal to

$$Q_1 = \frac{q}{u_1} \text{ and } Q_2 = \frac{q}{u_2} = \frac{u_1 Q_1}{u_2}.$$

To describe methanogenesis during downstream processing of the substrate, a mathematical model based on the mathematical model of the population dynamics of methane-producing bacteria for a one-stage methanogenesis mode is used [11, 14]:

$$\begin{cases} \frac{dX_1}{dt} = \left(\frac{\mu_{mg1}L_1}{a_1 + L_1} - \frac{\mu_{md1}b_1}{b_1 + L_1} - u_1 \right) \cdot X_1, \\ \frac{dL_1}{dt} = u_1 \cdot (L_0 - L_1) - \frac{\beta_1 \mu_{mg1} L_1 X_1}{a_1 + L_1}, \\ \frac{dX_2}{dt} = \lambda u_2 X_1 + \left(\frac{\mu_{mg2}L_2}{a_2 + L_2} - \frac{\mu_{md2}b_2}{b_2 + L_2} - u_2 \right) \cdot X_2, \\ \frac{dL_2}{dt} = u_2 \cdot (L_1 - L_2) - \frac{\beta_2 \mu_{mg2} L_2 X_2}{a_2 + L_2}. \end{cases} \quad (1)$$

Here, the subscripts of the variables (X_i, L_i) and parameters ($\mu_{mg\ i}, \mu_{md\ i}, a_i, b_i, \beta_i, u_i$) correspond to the number of the digester $i \in \{1, 2\}$. The model parameters are $\mu_{mg\ i}$ and $\mu_{md\ i}$, the maximum possible relative rates of growth and dieoff of bacteria, respectively (day^{-1}); β_i is dimensionless coefficient of the substrate absorption; a_i and b_i are empirical coefficients (m^3/kg); λ is parameter equal to zero if the temperature media in the digesters are different, and equal to one if these media are the same.

Values of the model parameters are determined in accordance with the selected temperature regime of the methanogenesis (mesophilic or thermophilic). If temperature media in the digesters are the same, then $\mu_{mg1} = \mu_{mg2} = \mu_{mg}$, $\mu_{md1} = \mu_{md2} = \mu_{md}$, etc.

The initial conditions are:

$$X_1(0) = X_2(0) = X_0, \quad L_1(0) = L_2(0) = L_0,$$

where X_0 is a natural concentration of methane-producing bacteria in the feedstock; L_0 is equal to the concentration of nutrients in the unprocessed substrate.

The model (1) is built on the assumption that the digesters maintain an optimal and constant process temperature. If the temperature media are different, then, when the substrate is fed from one digester to another, heating or cooling to the temperature in the second digester should occur.

The rate of biogas production (m^3/day) in the i -th digester is equal to

$$w_i = \frac{\gamma_i \mu_{mg\ i} L_i X_i}{a_i + L_i},$$

where γ_i is the coefficient characterizing the rate of conversion of substrate nutrients into biogas ($\text{m}^3 \cdot \text{m}^3/\text{kg}$).

To obtain the optimal control problem, it is necessary to supplement the system of equations (1) with the criterion functional

$$V = \int_0^T \left(\frac{\gamma_1 \mu_{mg1} L_1 X_1}{a_1 + L_1} + \frac{\gamma_2 \mu_{mg2} L_2 X_2}{a_2 + L_2} \right) dt \rightarrow \max, \quad (2)$$

that determine the total biogas yield from 1 m^3 of the substrate in the first and second digesters over time T . The optimized parameters of the problem are relative rates of the substrate delivery into the digesters u_1 and u_2 in the system of equations (1).

The systems (1) - (2) are Lagrange problems. In general case of the optimal control problem, there is a system of differential equations of the form:

$$\frac{dx}{dt} = f(x(t), u(t), t), \quad t \in [0, T], \quad x \in R^n, \quad u \in R^k, \quad (3)$$

its initial conditions are:

$$x(0) = x_0.$$

It is required to find the optimal control $u(t)$ delivering a maximum to the criterion functional

$$J = \int_0^T F_0(x(t), u(t), t) dt \rightarrow \max. \quad (4)$$

For the numerical solution to the problem, a difference grid with nodes $t_0 = 0, t_1, t_2, \dots, t_i, t_{i+1}, \dots, t_q = T$ with the constant step $h = t_{i+1} - t_i$ is introduced on the interval $[0, T]$ [15].

The numerical solution to the system of differential equations (3) is carried out through the fourth-order Runge-Kutta method:

$$\begin{aligned} x_{i+1} &= x_i + \frac{h}{6} \cdot (k_1 + 2k_2 + 2k_3 + k_4), \quad i = \overline{0, q-1}, \\ k_1 &= f(x_i, u_i, t_i), \\ k_2 &= f\left(x_i + \frac{h}{2} \cdot k_1, u_i, t_i + \frac{h}{2}\right), \\ k_3 &= f\left(x_i + \frac{h}{2} \cdot k_2, u_i, t_i + \frac{h}{2}\right), \quad k_3 = f\left(x_i + \frac{h}{2} \cdot k_2, u_i, t_i + \frac{h}{2}\right), \\ k_4 &= f(x_i + h \cdot k_3, u_i, t_i + h). \end{aligned} \quad (5)$$

To solve the problem, it is convenient to introduce qk -dimensional full control vector $U = (u_i), i = \overline{1, q}$. In this case, the difference approximation of the criterion functional (4) is the expression:

$$J = J(U) = \sum_{i=0}^q F_0(x_i, u_i, t_i) \cdot h \rightarrow \max. \quad (6)$$

The problem is solved in the sequence given below.

- 1) Set the full control vector U .
- 2) The initial system of differential equations (3) is solved numerically using the relations (5), and the value of the criterion functional (4) is calculated using the difference approximation (6).
- 3) The system of adjoint equations is numerically integrated (in the direction “from right to left”) according to the relations:

$$\begin{aligned} p_i &= p_{i+1} + h \cdot \frac{\partial F_0}{\partial x_i} + G_i^T \cdot p_{i+1} \cdot h, \quad i = \overline{1, q-1}, \\ p_q &= 0. \end{aligned} \quad (7)$$

Here, $p = p(t)$ are dual variables of the Pontryagin maximum principle; $G_i = \left(\frac{\partial f(x_i, u_i, t_i)}{\partial x_i} \right)$ is Jacobi matrix composed for the system (3).

- 4) The optimization process is performed by vector U . In this paper, the genetic algorithm with real coding and an additional search in the neighborhood of the best solution through the conjugate gradient method was used as the optimization method.

For the considered problem of methanogenesis optimization, the vector of phase variables is equal to $x = \text{colon}(X_1, L_1, X_2, L_2)$, the control vector is equal to $u = \text{colon}(u_1, u_2)$, and the Jacobi matrix has the form:

$$G = \begin{pmatrix} \frac{\mu_{mg1}L_1}{a_1 + L_1} - \frac{\mu_{md1}b_1}{b_1 + L_1} - u_1 & \frac{a_1\mu_{mg1}X_1}{(a_1 + L_1)^2} + \frac{b_1\mu_{md1}X_1}{(b_1 + L_1)^2} & 0 & 0 \\ -\frac{\beta_1\mu_{mg1}L_1}{a_1 + L_1} & -u_1 - \frac{\beta_1a_1\mu_{mg1}X_1}{(a_1 + L_1)^2} & 0 & 0 \\ \lambda u_2 & 0 & \frac{\mu_{mg2}L_2}{a_2 + L_2} - \frac{\mu_{md2}b_2}{b_2 + L_2} - u_2 & \frac{a_2\mu_{mg2}X_2}{(a_2 + L_2)^2} + \frac{b_2\mu_{md2}X_2}{(b_2 + L_2)^2} \\ 0 & u_2 & -\frac{\beta_2\mu_{mg2}L_2}{a_2 + L_2} & -u_2 - \frac{\beta_2a_2\mu_{mg2}X_2}{(a_2 + L_2)^2} \end{pmatrix}.$$

Research Results. The theoretical values of the variables found as a result of the numerical solution to the system of differential equations of the mathematical model of methanogenesis are recorded. The deviations of the specified values from the experimental values with respect to the vector of parameters [10, 16] (Table 1) are considered. The parameter values of the methanogenesis model are estimated through minimizing the sum of squares of these deviations.

Table 1

Estimates of methanogenesis model parameters for mesophilic / thermophilic media

Coefficient	Source of raw materials		
	Poultry factories	Pig farms	Cattle farms
μ_{mg}	0.482 / 0.821	0.346 / 0.783	0.297 / 0.563
μ_{md}	0.353 / 0.528	0.291 / 0.423	0.254 / 0.351
a	34.781 / 43.875	7.242 / 21.653	5.013 / 8.733
b	116.457 / 14.674	37.347 / 9.278	18.722 / 5.455
β	2.344 / 3.189	1.495 / 2.084	1.413 / 1.983
γ	1.463 / 1.963	1.373 / 1.907	1.299 / 1.813

The following methods for processing the substrate are considered.

I. A single digester is used.

II. Two digesters are used with the downstream processing of the substrate, in which temperature media coincide.

At this, two options of the medium are possible for each digester: mesophilic or thermophilic (Table 2).

Table 2

Optimal methanogenesis parameters

Characteristics	Source of raw materials		
	Poultry factories	Pig farms	Cattle farms
I. One digester with mesophilic / thermophilic medium			
u^* , day ⁻¹	0.149 / 0.402	0.128 / 0.341	0.112 / 0.268
w^* , m ³ / day	7.25 / 24.51	3.58 / 10.76	1.81 / 5.42
L^* / L_0 , %	56 / 43	51 / 38	52 / 41
II. Two digesters with mesophilic / thermophilic medium in each			
u_1^* , day ⁻¹	0.168 / 0.432	0.144 / 0.362	0.117 / 0.287
u_2^* , day ⁻¹	0.491 / 2.448	0.412 / 1.858	0.367 / 1.424
w^* , m ³ / day	15.19 / 50.21	7.79 / 22.19	3.85 / 10.92
L_2^* / L_0 , %	45 / 35	38 / 33	38 / 33
III. Two digesters, in the first - mesophilic, in the second - thermophilic medium / in the first - thermophilic, in the second - mesophilic medium			
u_1^* , day ⁻¹	0.149 / 0.402	0.128 / 0.341	0.112 / 0.268
u_2^* , day ⁻¹	0.312 / 0.051	0.222 / 0.059	0.183 / 0.051
w^* , m ³ / day	15.35 / 25.12	6.61 / 11.42	3.26 / 5.42
L_2^* / L_0 , %	30 / 34	29 / 35	26 / 32

Here, u^* are the optimal values of the relative rate of the substrate delivery; w^* is the corresponding daily average biogas yield; $\frac{L^*}{L_0}$ is the completeness of the processing of substrate nutrients.

Graphs of the biogas production rate are shown in Fig. 2.

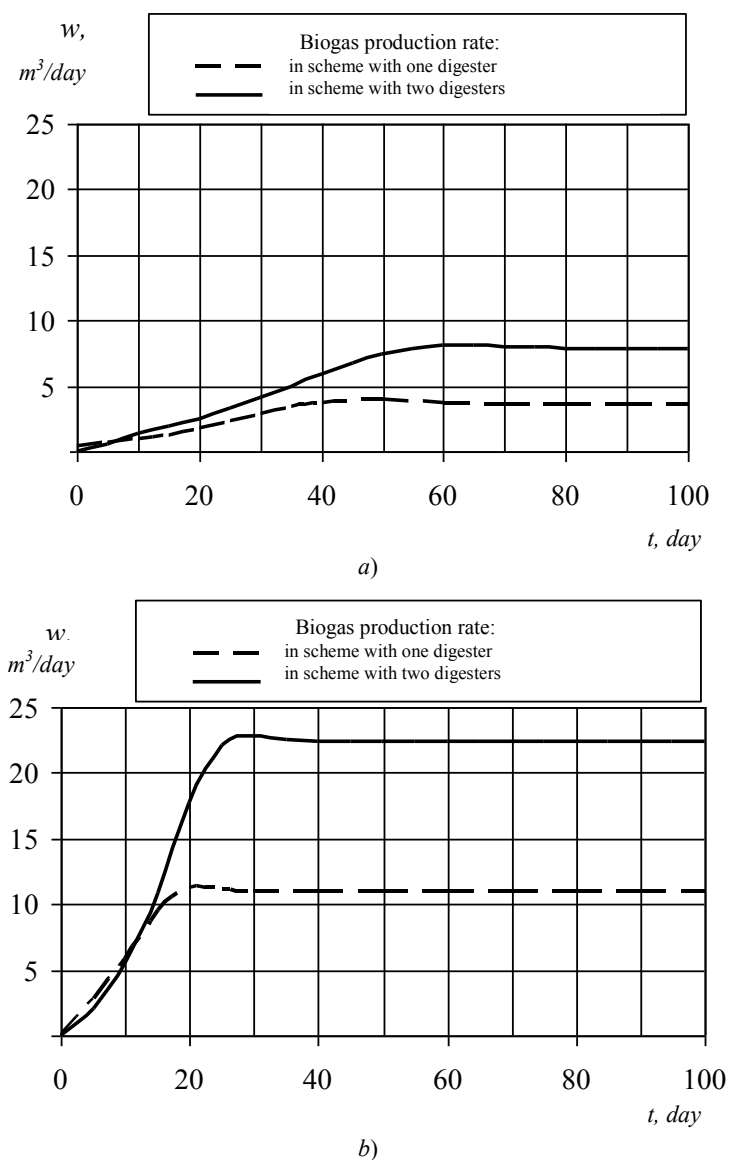


Fig. 2. Biogas production rate when using waste of pig farms for two digesters with mesophilic (a) and thermophilic (b) medium in each

III. Two digesters are used with downstream processing of the substrate, in which the temperature media are different.

Here, two cases are considered.

- 1) In the first digester, there is mesophilic medium, and in the second - thermophilic medium.
- 2) In the first digester, there is thermophilic medium, and in the second - mesophilic one.

See the optimal parameter values in Table 2.

Fig. 3 shows a graph of the biogas production rate.

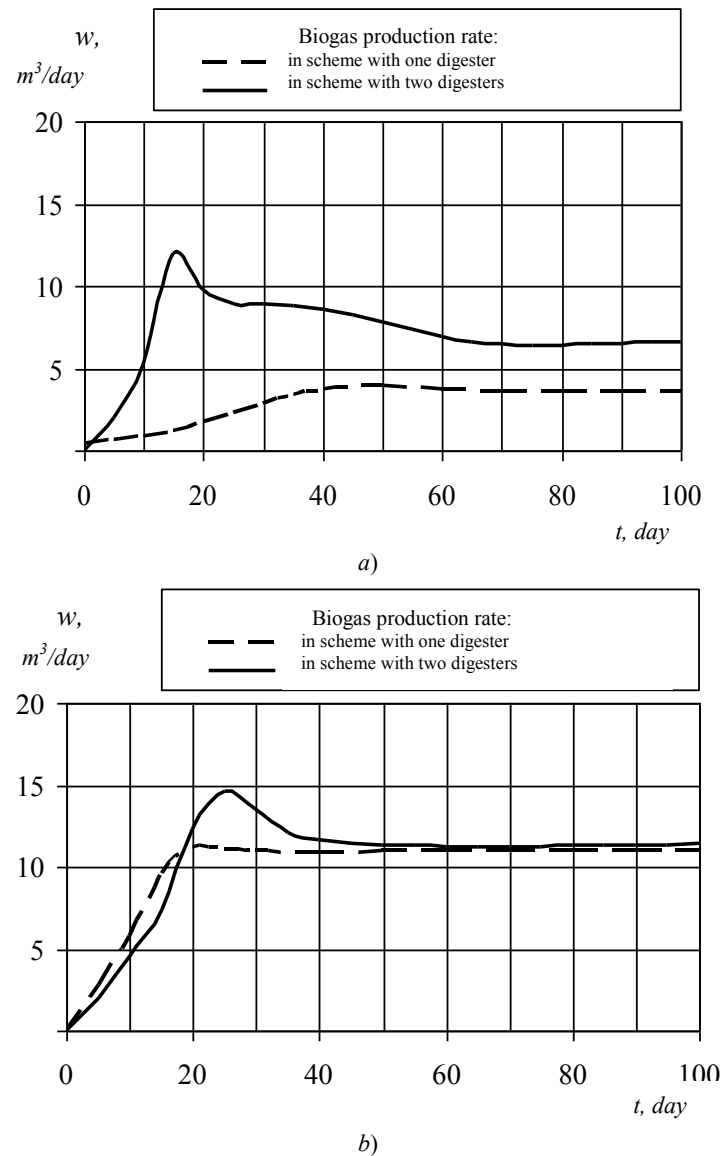


Fig. 3. Biogas production rate when using pig farm waste for two digesters: in the first digester there is mesophilic medium, in the second digester - thermophilic medium (a); in the first digester, there is thermophilic medium, in the second digester – mesophilic medium (b)

The use of a single digester in the continuous mode of fermentation enables to process the substrate nutrients by 40–45% for the mesophilic medium and by 50–55% for the thermophilic one.

When using two digesters with the same temperature media, the share of substrate processing increases by 10% for the mesophilic and by 5% for the thermophilic media. At this, the average daily production of biogas is almost doubled. The biogas production rate for the thermophilic environment is almost twice as high as for the mesophilic one.

Two digesters operating in different temperature media show different results. So, in the first case, the share of substrate processing is about 25% higher than when using a single digester with a mesophilic medium. In the second case, the share of substrate processing is 5–10% higher than when using a single digester with a thermophilic medium. Besides, the organization of the process in the first case provides a nearly twofold increase in the rate of biogas production (when compared to a single digester with a mesophilic medium). In the second case, a significant increase in speed is not observed (if compared to a thermophilic medium). It follows from the above that the second case is not advisable.

The first option loses somewhat in the rate of biogas production in case of using two digesters with a mesophilic medium in each, although it provides a higher (by 10–15%) degree of the substrate processing. This is due to the fact that with the use of two digesters with a mesophilic medium, the optimal values of the relative (and therefore absolute) rates of substrate input are higher, that is, more of the substrate is processed per unit of time. The rate of biogas generation for the second option is twice as low as for the case of using two digesters with a thermophilic medium.

Discussion and Conclusions. Mathematical models are developed that describe the methanogenesis during the downstream substrate processing in two digesters when the temperature media in them coincide and differ. These models correspond to the problem of optimal control of the methanogenesis process on the basis of the Pontryagin maxi-

mum principle. The paper describes an algorithm for its solution. The control parameters are relative rates of the substrate delivery into the digesters.

The numerical study results show that the sequential application of two digesters with the same temperature media allows for an increase in the degree of substrate processing by 5–10%. At the same time, the rate of biogas production is doubled. The degree of processing of the substrate for the mesophilic mode is also 5–10% higher than for the thermophilic one. At the same time, the biogas production rate in a thermophilic medium is almost twice as high as in a mesophilic one. This is due to the higher intensity of the process (higher than the optimal value of the relative rate of the substrate delivery).

The results of the operation of digesters with different temperature media are also shown. In the first case, the substrate is first processed in a mesophilic medium, and then enters the digester with a thermophilic medium. In the second case, on the contrary, the substrate from the digester with a thermophilic medium enters the digester with a mesophilic medium. In the first case, more substrate is processed. When compared to the use of a single digester with a mesophilic medium, the advantage is about 25%. When compared to the use of a single digester with a thermophilic medium, it is 5–10%. In the first case, the rate of biogas production is almost twice as high as in the case of a single digester with a mesophilic medium. In the second case, the rate of biogas production is almost the same as when using a single digester with a thermophilic medium. Thus, the second case is impractical.

In the first case, the biogas formation rate is somewhat lower than in the case of using two digesters with a mesophilic medium in each, but at the same time, the degree of substrate processing is 10–15% higher. In the second case the biogas production rate is twice as low as when using two digesters with a thermophilic medium in each, which again shows the inefficiency of the second case.

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