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Modeling the action of anaerobic biofilm

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A mathematical problem of the action of a representative biofilm in the absence of oxygen is formulated. The anaerobic process of decomposition of a dissolved organic matter is considered as a two-stage process, proceeding due to the vital activity of two groups of microorganisms. An approximate analytic solution allowing one to calculate the concentration and consumption of primary and secondary organic substrates with minimal errors has been obtained. On test examples, their rates of transfer through the biofilm surface are determined, and the possibility of the movement of volatile fatty acids in both directions is discussed.

Keywords*: anaerobic biofilm, organic substrate, decomposition, volatile fatty acids, analytic solution, concentration, consumption.*

Biofiltration of water with a high content of dissolved organic substances has a number of significant advantages and disadvantages in comparison with other methods of biological treatment. A characteristic feature of the aerobic biofiltration is a consistently large amount of the active biomass fixed on the elements of the solid phase, which ensures the rapid removal of organic pollution with the formation of a significant amount of by-products and secondary pollutants of the treated water. At the same time, the free space is seriously reduced, and the hydraulic resistance becomes more significant. It is possible to avoid the noted negative consequences of the intense biooxidation due to the treatment of polluted waters in the absence of oxygen [1, 2]. It is an important feature of the anaerobic wastewater treatment that, as a rule, an increase in the biomass and the release of exudates are considerably reduced, the permeability of the partially clogged filter medium increases, and, finally, the energy is consumed more economically [3—5].

Dissolved organic matter is directly utilized in the biological phase of a biofilter which is formed by numerous biofilms. The rate of degradation of the matter and the composition of its products are closely related to the oxygen content. In its absence, the slow metabolism is a characteristic of vital activities of anaerobic microorganisms [6—8]. As a result, the corresponding biological phase economically consumes the energy for the biosynthesis and respiration and thus

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allows performing a primary wastewater treatment. Therefore, it is natural that the anaerobic biofiltration as a technological process and the action of a representative biofilm under such conditions as its basis are of a great practical interest. The decomposition of organic matter within an anaerobic biofilm is considered below by analytic methods.

Modern ideas of the anaerobic process and its formal description [9] are interpreted with insignificant simplifications. First of all, it is considered as a two-stage process [10]. In the first stage, the organic substrate is transformed into volatile fatty acids and carbon dioxide. In the second stage, the volatile fatty acids eventually decompose to carbon dioxide and methane. Thus, no intermediate oxidation step is distinguished.

Therefore, we will analyze the behavior of the substrate and its by-products (volatile fatty acids, CO_2 CH_4) within an arbitrary flat biofilm l_f in thickness. The mathematical problem is formulated with respect to the corresponding mass concentrations s_i $(i = 1, 2, 3, 4)$ assuming only the diffusion (surface and molecular) transfer, significant limitation of the rates of biodegradation of the substrate and acids, functioning and coexistence within a single biofilm of two groups of microorganisms (acidogenetic and methanogenetic). The model includes, first of all, the following system of equations:

$$D_{e1}\frac{d^2 s_1}{dx^2} = \frac{1}{Y_1}\frac{\mu_{m1}\rho_{B1}s_1}{K_{s1}+s_1}, \tag{1}$$

$$D_{e2}\frac{d^2 s_2}{dx^2} = \frac{1}{Y_2}\frac{\mu_{m2}\rho_{B2}s_2}{K_{s2}+s_2} - \frac{\mu_{m1}\rho_{B1}Y_{s_2/B_1}s_1}{K_{s1}+s_1}, \tag{2}$$

$$D_{e3}\frac{d^2 s_3}{dx^2} = \frac{\mu_{m1}\rho_{B1}Y_{s_3/B_1}s_1}{K_{s1}+s_1} + \frac{\mu_{m2}\rho_{B2}Y_{s_3/B_2}s_2}{K_{s2}+s_2}, \tag{3}$$

$$D_{e4}\frac{d^2 s_4}{dx^2} = \frac{\mu_{m2}\rho_{B2}Y_{s_4/B_2}s_2}{K_{s2}+s_2}. \tag{4}$$

Here, D_{ei} is the effective diffusion coefficients of the i-th substrate, $Y_{1,2}$ are the effective economic coefficients characterizing the decomposition of the initial substrate and volatile fatty acids by the corresponding groups of microorganisms

$$Y_1 = \frac{1}{Y_{s_1/B_1}+Y_{s_2/B_1}+Y_{s_3/B_1}}, \qquad Y_2 = \frac{1}{Y_{s_2/B_2}+Y_{s_3/B_2}+Y_{s_4/B_2}}; \tag{5}$$

Y_{s_i/B_j} are the conversion factors (equal to the mass of the i-th substrate used per unit of the j-th variety of a biomass; and μ_{mj} and ρ_{Bj} are the specific growth rate and density of the j-th biomass. This system is complemented by the usual boundary conditions for a biofilm on a solid element in the liquid medium:

$$x = 0, \quad \frac{ds_i}{dx} = 0; \qquad x = l_f, \quad D_{ei}\frac{ds_i}{dx} = k_{Li}(S_i - s_i), \tag{6}$$

where k_{Li} is the coefficient of transfer of the i-th substrate through the liquid film, S_i is the concentration of the i-th substrate outside both films

Dimensionless variables and parameters are introduced using, as scales, S_0 (reference value for the concentration of the primary substrate, for example, the input value for a fixed-bed reactor), R (a characteristic microsize; for example, radius of a grain or a thread), and D_{e1} as follows:

$$\bar{S}_i = \frac{S_i}{S_0}, \quad \bar{s}_i = \frac{s_i}{S_0}, \quad \bar{x} = \frac{x}{R}, \quad \bar{\lambda}_j = \frac{\mu_{mj}\rho_{Bj}R^2}{Y_j D_{ej} S_0}, \quad \bar{D} = \frac{D_{e2}}{D_{e1}}, \quad \bar{K}_{si} = \frac{K_{si}}{S_0}, \quad \bar{k}_{Li} = \frac{Rk_{Li}}{D_{ei}}, \quad \bar{l}_f = \frac{l_f}{R}.$$

If a theoretical analysis of the anaerobic biofiltration is carried out solely for the purpose of monitoring the quality of the biological purification of water, and if the associated combustible gas is not of practical interest, then it is sufficient to restrict ourselves to a truncated system of equations for $\bar{s}_1$, $\bar{s}_2$, namely:

$$\frac{d^2\bar{s}_1}{d\bar{x}^2} = \frac{\bar{\lambda}_1\bar{s}_1}{\bar{K}_{s1} + \bar{s}_1}, \tag{7}$$

$$\frac{d^2\bar{s}_2}{d\bar{x}^2} = \frac{\bar{\lambda}_2\bar{s}_2}{\bar{K}_{s2} + \bar{s}_2} - \frac{\mathrm{Y}_1\mathrm{Y}_{s_2/B_1}}{\bar{D}} \frac{\bar{\lambda}_1\bar{s}_1}{\bar{K}_{s1} + \bar{s}_1} \tag{8}$$

with the boundary conditions

$$\bar{x} = 0, \qquad \frac{d\bar{s}_{1,2}}{d\bar{x}} = 0; \tag{9}$$

$$\bar{x} = \bar{l}_f, \qquad \frac{d\bar{s}_{1,2}}{d\bar{x}} = \bar{k}_{L1,L2}(\bar{S}_{1,2} - \bar{s}_{1,2}). \tag{10}$$

The solution of problem (7) — (10) can be significantly simplified due to the usually large initial content of an organic substrate in wastewater. In such situations, it is reasonable to believe that the primary substrate decomposes at the maximum rate. It should be noted that this assumption cannot be applied to volatile fatty acids, whose decomposition is limited due to their low content, and, at the same time, an inhibitory effect is possible [11—13]. Therefore, the indicated maximum rate will be $\bar{\lambda}_1$, and Eq. (8) takes the form

$$\frac{d^2\bar{s}_2}{d\bar{x}^2} = \frac{\bar{\lambda}_2\bar{s}_2}{\bar{K}_{s2} + \bar{s}_2} - \tilde{\lambda}_1, \tag{11}$$

where $\tilde{\lambda}_1 = Y_1\mathrm{Y}_{s_2/B_1}\bar{\lambda}_1/\bar{D}$. Then the distribution of the primary substrate across the biofilm is represented by the expression

$$\bar{s}_1(\bar{x}; \bar{l}_f, \bar{S}_1) = \bar{S}_1 - \frac{\tilde{\lambda}_1\bar{l}_f}{\bar{k}_{L1}} + \frac{\tilde{\lambda}_1}{2}(\bar{x}^2 - \bar{l}_f^2). \tag{12}$$

The approximate problem (9) — (11) is solved by averaging the right-hand side of Eq, (11). Previously, this technique was used in the absence of the internal source of a degradable substrate [14]. Then, following the previous procedure, the equation was derived for the mean value u_{av} on the interval $[0, X]$

$$u_{av}(X) = \frac{1}{X}\int_0^X \frac{\overline{s}_2(\overline{x})\,d\overline{x}}{\overline{K}_{s2} + \overline{s}_2(\overline{x})}, \tag{13}$$

which has the form

$$u_{av} + \frac{2\overline{K}_{s2}}{(\overline{\lambda}_s u_{av} - \overline{\lambda}_1)\cdot \Psi_f(u_{av})\overline{x}} \operatorname{arctg} \frac{\overline{x}}{\Psi_f(u_{av})} = 1. \tag{14}$$

Here, $\Psi_f^2 = \dfrac{2(\overline{K}_{s2} + \overline{S}_2)}{\overline{\lambda}_2 u_{av} - \mathrm{X}_1} - \dfrac{2\overline{D}\,\overline{l}_f}{\overline{k}_{L2}} - \overline{l}_f^2$. Now, the function $\operatorname{arctg}\dfrac{\overline{x}}{\Psi_f}$ is expanded in a series in the argument, and only its first term is used. As a result, the quadratic equation for u_{av} was obtained:

$$\overline{\lambda}_2\varphi_f(\overline{l}_f)u_{av}^2 + [\overline{\lambda}_2\varphi_f(\overline{l}_f) + \overline{\lambda}_2\overline{K}_{s2} + \overline{\lambda}_2\overline{S}_2 + \overline{\lambda}_1\varphi_f(\overline{l}_f)]u_{av} + \overline{\lambda}_1\varphi_f(\overline{l}_f) + \overline{\lambda}_2\overline{S}_2 = 0, \tag{15}$$

where $\varphi_f(\overline{l}_f) = \overline{\lambda}_2(\overline{k}_{L2}\overline{l}_f^2 + 2\overline{D}\overline{l}_f)/2\overline{k}_{L2}$. Only one root has the physical meaning, namely,

$$u_{av}(\overline{l}_f, \overline{S}_2) = \frac{1}{2}\left\{\frac{\overline{K}_{s2} + \overline{S}_2}{\varphi_f(\overline{l}_f)} + \frac{\tilde{\lambda}_1}{\overline{\lambda}_2} + 1 - \sqrt{\left(\frac{\overline{K}_{s2} + \overline{S}_2}{\varphi_f(\overline{l}_f)} + \frac{\tilde{\lambda}_1}{\overline{\lambda}_2} + 1\right)^2 - 4\left(\frac{\overline{S}_2}{\varphi_f(\overline{l}_f)} + \frac{\tilde{\lambda}_1}{\overline{\lambda}_2}\right)}\right\}. \tag{16}$$

By simplifying Eq. (11) with regard for (13) and integrating it twice, we get the following expression for the concentration $\overline{s}_2$:

$$\overline{s}_2(\overline{x}; \overline{l}_f, \overline{S}_2) = \overline{S}_2 - [\overline{\lambda}_2 u_{av}(\overline{l}_f, \overline{S}_2) - \tilde{\lambda}_1]\left(\frac{\overline{l}_f}{\overline{k}_{L2}} + \frac{\overline{l}_f^2}{2} - \frac{\overline{x}^2}{2}\right). \tag{17}$$

Thus, the relative value of $\overline{s}_2$ at the biofilm surface is

$$\overline{s}_{2f}(\overline{l}_f, \overline{S}_2) = \overline{S}_2 - [\overline{\lambda}_2 u_{av}(\overline{l}_f, \overline{S}_2) - \tilde{\lambda}_1]\frac{\overline{l}_f}{\overline{k}_{L2}} = \overline{S}_2 - \frac{1}{\overline{k}_{L2}\overline{l}_f + 2\overline{D}}\left\{\overline{K}_{s2} + \overline{S}_2 + \right.$$

$$\left. + \left(1 - \frac{\tilde{\lambda}_1}{\overline{\lambda}_2}\right)\varphi_f(\overline{l}_f) - \sqrt{\left[\overline{K}_{s2} + S_2 + \left(1 - \frac{\tilde{\lambda}_1}{\overline{\lambda}_2}\right)_f \varphi_f(\overline{l}_f)\right]^2 - 4\frac{\varphi_f(\overline{l}_f)}{\overline{\lambda}_2}\left[\overline{\lambda}_2\overline{S}_2 + \tilde{\lambda}_1\varphi_f(\overline{l}_f)\right]}\right\}. \tag{18}$$

Using the representations for $\overline{s}_1$ (12) and $\overline{s}_2$ (17) and doubly integration Eqs. (3) and (4) under the appropriate conditions (6), it is easy to find also the concentrations $\overline{s}_3$ and $\overline{s}_4$ of the final decomposition products $(\mathrm{CO}_2, \mathrm{CH}_4)$.

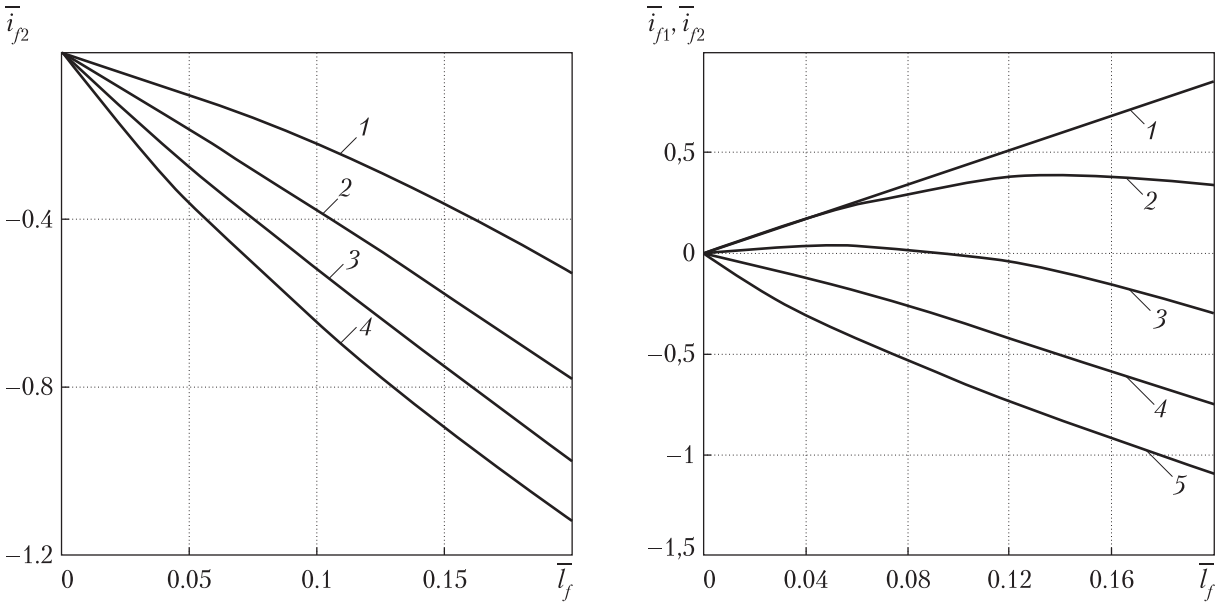

Fig. 1. Dependence $\bar{i}_{f2}(\bar{l}_f)$: *1* — $\bar{S}_{20} = 0$; *2* — $\bar{S}_{20} = 0.1$; *3* — $\bar{S}_{20} = 0.25$; *4* — $\bar{S}_{20} = 0.5$.

Fig. 2. Dependences $\bar{i}_{f1}(\bar{l}_f)$, $\bar{i}_{f2}(\bar{l}_f)$: *1* — $\bar{i}_{f1}$, *2–5* — $\bar{i}_{f2}$; *2* — $\bar{S}_{20} = 0.5$; *3* — $\bar{S}_{20} = 0.25$; *4* — $\bar{S}_{20} = 0.1$; *5* — $\bar{S}_{20} = 0$.

The actual efficiency of a biofilm in relation to both components of the organic pollution can be assessed by calculating their relative flow rates $\bar{i}_{f1}$, $\bar{i}_{f2}$ across the border between both films:

$$\bar{i}_{f1}(\bar{l}_f) = \tilde{\lambda}_1 \bar{l}_f, \tag{19}$$

$$\bar{i}_{f2}(\bar{l}_f) = \bar{l}_f [\bar{\lambda}_2 u_{av}(\bar{l}_f, \bar{S}_2) - \tilde{\lambda}_1]. \tag{20}$$

The approximate solution to the problem of the steady-state action of an anaerobic biofilm obtained above is illustrated by test examples. The possible inaccuracies in calculating the microcharacteristics $(\bar{s}_i, \bar{i}_{fi})$ due to the use of an adaptive averaging of the local organic substrate utilization function (applied before to an aerobic biofilm) were discussed in [14]. It was found that they do not exceed a few percent and are less than the errors due to the experimental determination of the model coefficients.

The subject of many calculations was the relative flow rates of both substrates through the surface of the active biofilm under consideration $(\bar{i}_{f1},\ \bar{i}_{f2})$. It is they that determine the efficiency of the elements of the biological phase (biofilms of any form) in relation to the organic pollution and underlie the modeling of the anaerobic biofiltration. Calculations were performed using formulas (19) and (20) with a continuous change in the relative thickness $\bar{l}_f$ from 0 to 0.2. Thus, the range of its real values was covered with a large margin. The initial content of volatile fatty acids was also discretely varied from 0 to 0.5. In the accepted model, the stable presence of volatile fatty acids is allowed already at the inlet to the filter $(S_2 > 0)$. In practice, a similar situation is typical of the successively acting second and subsequent anaerobic filters [15]. The initial information included the following fixed relative values of the coefficients: $\bar{K}_{s2} = 0.25$, $\bar{k}_{L2} = 10$, $\bar{\rho}_B = \bar{D} = 1$, $\chi = 0.4$, $\bar{\lambda}_1 = 10$. Two characteristic values of (10 and 20) were also selected

for $\bar{\lambda}_2$. Graphs presenting the dependence $\bar{i}_{f2}(\bar{l}_f)$ for $\bar{\lambda}_2 = 10$ are shown in Fig. 1 and, for $\bar{\lambda}_2 = 20$, in Fig. 2. There, the single graph due to the constancy of $\bar{\lambda}_1$ is given for $\bar{i}_{f1}(\bar{l}_f)$ as well. When establishing the quantities $\bar{i}_{f1}$, $\bar{i}_{f2}$, their sign is of fundamental importance, since it determines the direction of the transfer of the corresponding substrate. The "+" sign means that the impurity moves into the biofilm, and the "–" sign — in the opposite direction. It is obvious that the primary substrate is only consumed by the biofilm. Therefore, $\bar{i}_{f1}$ is necessarily positive. The directionality of the secondary substrate is dictated by the ratio between its concentrations outside both films S_2 and at their common boundary s_f. Thus, the volatile fatty acids will diffuse from the outside at $s_f < S_2$ (Fig. 1 and curve *2* in Fig. 2), and $\bar{i}_{f2}$ will be negative at $s_f > S_2$ (curves *3—5* in Fig. 2).

Therefore, the theoretical basis has been developed for a further research of the operation of an anaerobic fixed-bed bioreactor by analytic methods, in essence, thanks to the solution of the problem of the action of a representative anaerobic biofilm. The derived dependences can be used to specify the model coefficients at the structural level.

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МОДЕЛЮВАННЯ ДІЇ АНАЕРОБНОЇ БІОПЛІВКИ

Сформульовано математичну задачу дії репрезентативної біоплівки за відсутності кисню. Анаеробний процес розкладу розчиненої органіки розглядається як двостадійний, який протікає завдяки життєдіяльності двох груп мікроорганізмів. Одержано наближений аналітичний розв'язок, що дозволяє з мінімальними похибками розраховувати концентрації і витрати первинного і вторинного органічних субстратів. На тестових прикладах визначено їх витрати через поверхню біоплівки і демонструється реальність руху летючих кислот в обох напрямках.

Ключові слова: анаеробна біоплівка, органічний субстрат, розклад, летючі кислоти, аналітичний розв'язок, концентрація, витрата.