MATHEMATICAL SIMULATION OF THE PROCESS OF AEROBIC TREATMENT OF WASTEWATER UNDER CONDITIONS OF DIFFUSION AND MASS TRANSFER PERTURBATIONS

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A mathematical model of the process of aerobic treatment of wastewater has been refined. It takes into account the interaction of bacteria, as well as of organic and biologically nonoxidizing substances under conditions of diffusion and mass transfer perturbations. An algorithm of the solution of the corresponding nonlinear perturbed problem of convection–diffusion–mass transfer type has been constructed, with a computer experiment carried out based on it. The influence of the concentration of oxygen and of activated sludge on the quality of treatment is shown. Within the framework of the model suggested, a possibility of automated control of the process of deposition of impurities in a biological filter depending on the initial parameters of the water medium is suggested.

Keywords: aerobic treatment, wastewater, organic and biologically nonoxidizing substance, diffusion and mass transfer perturbations.

Domestic wastewater contains impurities of mineral and organic origin. Industrial wastewater is more dissimilar in the composition and concentration of the impurities in it depending on the region of their origin. Irrespective of the type of wastewater, however, it necessarily needs purification, since the concentrations of the contaminating substances in it greatly exceed permissible ones [1]. To prevent the harmful effect of the impurities, contained in wastewater, on the surrounding medium, systems of magnetic, mechanical, biological, and of other filters are used for its purification. They provide for permissible concentrations of contaminating substances in wastewater. Such systems are to be designed with account for the variety of wastewater and its origin, with the use of the worldwide experience accumulated in this field [1–5].

In the present work, we consider the process of aerobic treatment of wastewater in which the activity of the bacteria contained in it is stimulated by additional supply of air and by maintaining an optimal temperature of the medium. With treatment of such kind, microorganisms are bred in an activated sludge, absorbing impurities and oxygen. However, the absorbability of bacteria decreases with time, and they are deposited in the form of a solid substrate, which is to be removed. Therefore, to ensure effective wastewater treatment it is necessary to sustain the absorbability of bacteria at a respective level.

In recent years, considerable studies have been conducted with respect to the problems of automatization of biochemical treatment of wastewater in aerotanks (settling basins) [1-3] that extended the knowledge of the dynamics of the processes of heat and mass transfer occurring in them and of their individual parameters needed for constructing the schemes and means of automatization of wastewater treatment and of controlling this process. Thus, wastewater treatment is considered in [1] as a technological process with detailed description of the construction of the mechanisms needed for the purpose. The proposed models allow one to calculate the optimal parameters of the aerotank but without accounting for the dynamics of the change in the time of effective action of a filter depending on the initial concentration of impurity, demands for oxygen, and of the speed of growth of activated sludge. The interaction of the activated sludge with impurity is described by the mathematical model suggested in [3]. This model is rather general, however, since it lacks systematic account of the interacting parameters. The system of equations presented in [4] does not account for the mutual effect of the treatment parameters, which, according to experimental data, plays a significant role in this process.

In this connection, the goal of the present work was to improve the mathematical model of the process of clearing wastewater from impurities with account for the interaction of bacteria, activated sludge, and of impurities in a porous medium, and to calculate the optimal technological parameters of this process by means of its computer simulation.

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Formulation of the Problem. We are considering the process of clearing wastewater from organic pollutions by injecting biological bacteria into it. According to theoretical and experimental data [1, 2], one distinguishes the following stages of clearing wastewater from contaminants: decomposition of an organic pollutant by bacteria, growth and dying out of bacteria, production of new bacteria by an activated sludge, and conversion of the impurity into a biologically nonoxidizing substance.

The dynamics of the change in the concentration of organic substance in water is described by the following equation [5, 6] with account for the effect exerted by the activated sludge exerted on the absorption of impurity:

$$\frac{\partial C}{\partial t} = D_{\rm s} \, \frac{\partial^2 C}{\partial x^2} - v_{\rm s} \, \frac{\partial C}{\partial x} - \beta CB \,. \tag{1}$$

Here $\beta = \frac{Q(1+k_i)}{V}$ is the coefficient accounting for the characteristic features of the filter construction and fluid flow velocity, and $D_s = d_s \varepsilon$, where ε is a small parameter that characterizes the advantages of some components of the process over another components, in particular, of the intercomponent interaction and diffusion. Since bacteria move in a porous medium together with a contaminant and settle down in the lower part of the filter in the form of an activated sludge, we arrive at the equation which describes the growth, dying out, and transfer of the bacteria with account for the biological need in oxygen:

$$\frac{\partial B}{\partial t} = D_{\rm b} \frac{\partial^2 B}{\partial x^2} - v_{\rm b} \frac{\partial B}{\partial x} + K_{\rm b}(B)K , \qquad (2)$$

where $K_b(B) = G(K_b - \varepsilon K_b^0 B)$ is the function characterizing the absorption of oxygen by bacteria, $D_b = d_b \varepsilon$. To raise the efficiency of the process of treatment of wastewater and provide for the optimal conditions of the vital activity of bacteria in it, the latter is oxygenated. The equation that describes the dynamics of this process has the form

$$\frac{\partial K}{\partial t} = D_{\rm O} \frac{\partial^2 K}{\partial x^2} - v_{\rm O} \frac{\partial K}{\partial x} + K_{\rm O}(B)(K_{\rm sat} - K) .$$
(3)

Here *K* is the oxygen concentration needed for sustaining the best absorption of the contaminant by bacteria, $K_{O}(B) = \beta(K_{O} + \varepsilon K_{O}^{0}B)$ is the coefficient of oxygen absorption, K_{sat} is the concentration of water saturation with oxygen at given temperature and pressure, and $D_{O} = d_{O}\varepsilon$, where ε , K_{b} , K_{O}^{0} , K_{O} , K_{O}^{0} , $d_{s}d_{b}$, and d_{O} are the "solid" parameters that characterize the "soft" parameters such as $K_{b}(B)$ and $K_{O}(B)$ determined experimentally.

The system of differential equations (1)–(3) describes the change in the concentration of bacteria, contaminant, and of oxygen in a porous medium. It is advisable to take into account the differently interrelated characteristics of the medium and of the process of clearing by supplementing the corresponding equations with the coefficients allowing one to analyze the processes occurring in the aerotank reactor as a set of interrelated phenomena. In real systems, a change of a controlled parameter in response to perturbation occurs with delay for some reasons. In this case, the transfer of a contaminant requires a certain time. We will assume that any change in the external factors, for example, an increase in the concentration of the contaminant or bacteria takes place only after the termination of a certain delay time $\tau > 0$. Proceeding from the foregoing, we arrive at a model perturbed problem:

$$\frac{\partial C}{\partial t} = D_{\rm s} \frac{\partial^2 C}{\partial x^2} - v_{\rm s} \frac{\partial C}{\partial x} - \beta CB ,$$

$$\frac{\partial B}{\partial t} = D_{\rm b} \frac{\partial^2 B}{\partial x^2} - v_{\rm b} \frac{\partial B}{\partial x} + K_{\rm b}(B)K ,$$

$$\frac{\partial K}{\partial t} = D_{\rm O} \frac{\partial^2 K}{\partial x^2} - v_{\rm O} \frac{\partial K}{\partial x} + K_{\rm O}(B)(K_H - K) ,$$
(4)

$$C\Big|_{x=0} = C_*^*(t) , \quad B\Big|_{x=0} = B_*^*(t) , \quad K\Big|_{x=0} = K_*^*(t) ,$$

$$\frac{\partial C}{\partial x}\Big|_{x=L} = 0 , \quad \frac{\partial B}{\partial x}\Big|_{x=L} = 0 , \quad \frac{\partial K}{\partial x}\Big|_{x=L} = 0 ,$$

$$C\Big|_{t=0} = C^*(x) , \quad B\Big|_{t=0} = B^*(x) , \quad K\Big|_{t=0} = K^*(x) ,$$

(5)

where $C_*^*(t)$, $B_*^*(t)$, $K_*^*(t)$, $C^*(x)$, $B^*(x)$, and $K^*(x)$ are the differentiated functions given a sufficient number of times and coordinated at the corner points of the region $G = \{(x, t): 0 \le x \le L, 0 \le t \le t^* \le \infty\}$ [5].

Solution Algorithm. The solution of problem (4), (5) is sought with accuracy $O(\epsilon^{n+1})$ in the form of asymptotic series in powers of the small parameter ϵ [4–6]:

$$C(x, t) = C_0(x, t) + \sum_{i=1}^{n} \varepsilon^i C_i(x, t) + \sum_{i=0}^{n} \varepsilon^i \tilde{C}_i(\xi, t) + R_s(x, t, \varepsilon) , \qquad (6)$$

$$B(x, t) = B_0(x, t) + \sum_{i=1}^{n} \varepsilon^i B_i(x, t) + \sum_{i=0}^{n} \varepsilon^i \tilde{B}_i(\xi, t) + R_b(x, t, \varepsilon) , \qquad (7)$$

$$K(x, t) = K_0(x, t) + \sum_{i=1}^n \varepsilon^i K_i(x, t) + \sum_{i=0}^n \varepsilon^i \tilde{K}_i(\xi, t) + R_0(x, t, \varepsilon) , \qquad (8)$$

where R_s , R_b , and R_0 are the remaining terms, $C_i(x, t)$, $B_i(x, t)$, and $K_i(x, t)$ $(i = \overline{0, n})$ are the terms of the regular parts of the asymptotics, $\tilde{C}_i(\xi, t)$, $\tilde{B}_i(\xi, t)$, and $\tilde{K}_i(\xi, t)$ $(i = \overline{0, n})$ are the functions of the boundary layer type (correspondingly, corrections at the exit of a filtered substance), $\xi = (L - x)\varepsilon^{-1}$ are the corresponding regularizing transformations. As a result of the substitution of (8) into the system (4), (5) and application of a standard procedure of comparison [5, 6] we will obtain problems for determining the functions $B_i(x, t)$, $U_i(x, t)$, and $C_i(x, t)$ $(i = \overline{0, n})$:

$$\begin{aligned} \frac{\partial C_0}{\partial t} &= -v_s \frac{\partial C_0}{\partial x} - \beta C_0 B_0 , \quad \frac{\partial B_0}{\partial t} = -v_b \frac{\partial B_0}{\partial x} + \beta K_b K_0 , \\ \frac{\partial K_0}{\partial t} &= -v_O \frac{\partial K_0}{\partial x} + \beta K_O (K_{\text{sat}} - K_0) , \\ C_0 \Big|_{x=0} &= C_*^*(t) , \quad B_0 \Big|_{x=0} = B_*^*(t) , \quad K_0 \Big|_{x=0} = K_*^*(t) , \\ \frac{\partial C_0}{\partial x} \Big|_{x=L} &= 0 , \quad \frac{\partial B_0}{\partial x} \Big|_{x=L} = 0 , \quad \frac{\partial K_0}{\partial x} \Big|_{x=L} = 0 , \\ C_0 \Big|_{t=0} &= C^*(t) , \quad B_0 \Big|_{x=0} = B^*(x) , \quad K_0 \Big|_{t=0} = K^*(x) ; \end{aligned}$$

$$\begin{aligned} \frac{\partial C_i}{\partial t} &= d_s \; \frac{\partial^2 C_{i-1}}{\partial x^2} - v_s \; \frac{\partial C_i}{\partial x} - \beta C_i B_i \;, \\ \frac{\partial B_i}{\partial t} &= d_b \; \frac{\partial^2 B_{i-1}}{\partial x^2} - v_b \; \frac{\partial B_i}{\partial x} - K_b^0 B_{i-1} K_i + \beta K_b K_i \;, \\ \frac{\partial K_i}{\partial t} &= d_0 \; \frac{\partial^2 K_{i-1}}{\partial x^2} - v_0 \; \frac{\partial K_i}{\partial x} - K_i \; \left(\beta K_0 + \beta K_0^0 B_{i-1}\right) + \beta K_0 K_{sat} + \beta K_0^0 B_{i-1} K_{sat} \;, \\ C_i \Big|_{x=0} &= 0 \;, \quad B_i \Big|_{x=0} = 0 \;, \quad K_i \Big|_{x=0} = 0 \;, \quad C_i \Big|_{t=0} = 0 \;, \quad B_i \Big|_{t=0} = 0 \;, \quad i = \overline{1, n} \;. \end{aligned}$$

As a result of the solution of these problems we have

$$K_{0}(x, t) = \begin{bmatrix} \frac{\beta K_{0} K_{\text{sat}}}{v_{0}} e^{\frac{\beta K_{0} x}{v_{0}}} \int_{0}^{x} e^{-\frac{\beta K_{0} \tilde{x}}{v_{0}}} \tilde{x} d\tilde{x} + K_{*}^{*} \left(t - \frac{x}{v_{0}}\right), \quad t > \frac{x}{v_{0}}, \\ \beta K_{0} K_{\text{sat}} e^{\beta K_{0} t} \int_{0}^{t} e^{-\beta K_{0} \tilde{t}} \tilde{t} d\tilde{t} + K^{*} (x - v_{0} t), \quad t \le \frac{x}{v_{0}}, \end{bmatrix}$$

$$\begin{split} C_{0}(x,t) &= \left| \begin{array}{l} C_{*}^{x} \left(t - \frac{x}{v_{s}} \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} \left(\bar{x}, -\frac{t}{v_{s}} (\bar{x} - x + v_{s} t) \right) d\bar{x}} \\ C_{*}^{x} \left(t - \frac{x}{v_{s}} \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} (x - v_{s} (t - \bar{t}), \bar{t}) d\bar{x}} \\ C^{*} \left(x - v_{s} t \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} (x - v_{s} (t - \bar{t}), \bar{t}) d\bar{t}} \\ C^{*} \left(x - v_{s} t \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} \left(x - v_{s} (t - \bar{t}), \bar{t} \right) d\bar{t}} \\ C^{*} \left(x - v_{s} t \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} \left(x - v_{s} (t - \bar{t}), \bar{t} \right) d\bar{t}} \\ C^{*} \left(x - v_{s} t \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} \left(x - v_{s} (t - \bar{t}), \bar{t} \right) d\bar{t}} \\ C^{*} \left(x - v_{s} t \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} \left(x - v_{s} (t - \bar{t}), \bar{t} \right) d\bar{t}} \\ C^{*} \left(x - v_{s} t \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} \left(x - v_{s} (t - \bar{t}), \bar{t} \right) d\bar{t}} \\ C^{*} \left(x - v_{s} t \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} \left(x - v_{s} (t - \bar{t}), \bar{t} \right) d\bar{t}} \\ C^{*} \left(x - v_{s} t \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} \left(x - v_{s} (t - \bar{t}), \bar{t} \right) d\bar{t}} \\ C^{*} \left(x - v_{s} t \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} \left(x - t + v_{s} t \right) d\bar{t}} \\ C^{*} \left(x - v_{s} t \right) e^{-\frac{\beta}{0} \frac{\beta}{0} B_{0} \left(x - v_{s} t - v_{s} t \right) d\bar{t}} \\ C^{*} \left(v_{0} \left(\bar{t} - t \right) + x, \bar{t} \right) d\bar{t} \\ C^{*} \left(v_{0} \left(\bar{t} - t \right) + x, \bar{t} \right) d\bar{t} \\ C^{*} \left(v_{0} \left(\bar{t} - t \right) + x, \bar{t} \right) d\bar{t} \\ C^{*} \left(v_{0} \left(\bar{t} - t \right) + x, \bar{t} \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(t - \bar{t} \right) \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(t - \bar{t} \right) \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(t - \bar{t} \right) \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(t - \bar{t} \right) \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \left(t - \bar{t} \right) \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \left(x - v_{b} \right) \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x - v_{b} \right) d\bar{t} \\ C^{*} \left(x - v_{b} \left(x$$

$$\left[e^{\int_{0}^{-1} C_{i}(v_{s}(t-t)+x,t)dt} \int_{0}^{-1} e^{\int_{0}^{-1} C_{i}(v_{s}(t-t)+x,t)dt} \tilde{C}_{i}(v_{s}(\tilde{t}-t)+x,\tilde{t})d\tilde{t}, \quad t \leq \frac{x}{v_{s}}, \right]$$

where $\tilde{K}_i = \beta K_0 + \beta K_0^0 B_{i-1}$, $\tilde{C}_i = \beta B_i$, $\tilde{C}_i = d_s \frac{\partial^2 C_{i-1}}{\partial x^2}$, $\tilde{K}_i = d_0 \frac{\partial^2 K_{i-1}}{\partial x^2} + \beta K_0 K_{sat} + \beta K_0^0 B_{i-1} K_{sat}$, $\tilde{B}_i = d_b \frac{\partial^2 B_{i-1}}{\partial x^2} - K_b^0 B_{i-1} K_i + \beta K_b K_i$. The functions $\tilde{C} = \sum_{i=0}^n \tilde{C}_i \varepsilon^i$, $\tilde{B} = \sum_{i=0}^n \tilde{B}_i \varepsilon^i$, and $\tilde{K} = \sum_{i=0}^n \tilde{K}_i \varepsilon^i$ are intended for

removing the inconsistencies introduced by the constructed regular parts $C(x, t) = \sum_{i=0}^{n} C_i \varepsilon^i$, $B(x, t) = \tilde{B} = \sum_{i=0}^{n} \tilde{B}_i \varepsilon^i$, and $K(x, t) = \sum_{i=0}^{n} K_i \varepsilon^i$ in the vicinities of the point x = L (exit of filtered flow), i.e., they ensure the fulfillment of the condition

$$\frac{\partial}{\partial x} (C + \tilde{C}) = O(\varepsilon^{n+1}), \frac{\partial}{\partial x} (B + \tilde{B}) = O(\varepsilon^{n+1}), \frac{\partial}{\partial x} (K + \tilde{K}) = O(\varepsilon^{n+1}).$$
 For finding these functions we have the problems which

are analogous to the problems considered in [5, 6]. Estimation of the remaining terms is made analogously to what was done in [5]. As was expected, it is enough to take three or four terms of each of the asymptotic series (8) in the calculations to obtain an approximation of the solution accurate to four meaningful figures in the space of the computational time of the filter cycle.

Results of Numerical Calculations. The results of a numerical experiment at $C|_{t=0} = 1 \text{ mg/L}$, $B|_{t=0} = 35e^{\mu x} \text{ g/L}(\mu=1)$, $K|_{t=0} = 0.1 \text{ g/L}$, $Q = 7.2 \text{ m}^3/\text{h}$, $V = 0.7 \text{ m}^3$, $k_i = 0.5$, $K_b = 0.001 \text{ h}^{-1}$, $K_O = 100 \text{ h}^{-1}$, $K_b^0 = K_O^0 = 1$, $C_0 = 6 \text{ mg/L}$, $v_s = 1.26 \text{ m/h}$, $v_b = 1.92 \text{ m/h}$, $v_O = 1.26 \text{ m/h}$, $d_s = 0.721 \text{ m}^2/\text{h}$, $d_b = d_O = 10^{-3} \text{ m}^2/\text{h}$, L = 1 m, and $\varepsilon = 0.01$ are presented in Figs. 1–3.

As is seen from Fig. 1, the concentration of the activated sludge increases with time along the filter as a result of the formation of favorable conditions for the reproducition of bacteria, namely, a constant arrival of contaminants in the form of admixtures and a regular supply of oxygen (Fig. 2)Figure 3 depicts the change in the concentration of impurity particles with time along the filter length. These particles interact with one another and settle in the lower parts of the filter



Fig. 1. Change in the concentration of activated sludge with time at different points of the filter (a) and along its length at different instants of time (b): (a) 1) x = 0.1 m; 2) 0.3; 3) 0.5; 4) 0.7; 5) 0.9; (b) 1) t = 10 h; 2) 20; 3) 30; 4) 40; 5) 50.



Fig. 2. Change in the concentration of oxygen with time at different points of the filter (a) and along its length at different instants of time (b): (a) 1) x = 0.1 m; 2) 0.3; 3) 0.5; 4) 0.7; 5) 0.9; (b) 1) t = 10 h; 2) 20; 3) 30; 4) 40; 5) 50.



(a) and along its length at different instants of time (b): (a) 1) *x* = 0.1 m; 2) 0.3; 3) 0.5; 4) 0.7; 5) 0.9; (b) 1) *t* = 10 h; 2) 20; 3) 30; 4) 40; 5) 50.

in the form of an activated sludge. A decrease in the concentration of impurity along the length of the filter with time points to the efficiency of its operation. At the early stage of clearing, however, the needed amounts of bacteria and oxygen were not obtained at the exit from the filter, which predetermines the increase in the concentration of the contaminant.

Conclusions. The model of aerobic treatment of wastewater, improved by taking into account the interaction of bacteria, organic substance, and of a biologically nonoxidizable substance in this water under conditions of their diffusion and mass transfer perturbations, makes it possible to more thoroughly predict the technological processes of treatment of this water. The proposed method and the corresponding algorithm allow one to account for different kinds of perturbations, in particular, the small backward effect of the process characteristics on the characteristics of the medium with the use of different kinds of corrections for the main parameters of the process without solving the problem each time from the very beginning, which, in turn, provides a possibility of paralleling out computations. Based on the proposed model, a computer experiment is carried out, as a result of which numerical characteristics of the effect of the concentration of oxygen and of the activated sludge on the quality of the process of treatment have been obtained. With the use of this model it is possible to implement the control of the process of impurity deposition in a biological filter depending on the initial parameters of the water medium. Further improvement of the model is planned which will account for the age of the activated sludge and of such parameters of the medium as oxidity and temperature.

NOTATION

B, concentration of activated sludge; *C*, concentration of a contaminant in water; D_s , D_b , and D_O , diffusion coefficients of the substrate, activated sludge, and of oxygen; k_i , coefficient of activated sludge recirculation; *K*, oxygen concentration; *L*, length of the filter, *V*, volume of the filter; v_s , v_b , and v_O , velocities of motion of substrate, activated sludge, and of oxygen. Indices: b, bacteria; O, oxygen; s, substrate; sat, saturation.

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