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Mathematical Model of a Filter for Water Treatment Using Biofilms

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Abstract. The paper considers the principles of constructing a mathematical model of water treatment based on the use of a biologically active layer, the bacteria of which absorb harmful impurities contained in water. A system of equations is presented on the basis of which a model of water purification is constructed in the simplest element, which is a rod covered with a biofilm. The system of equations is a system that includes a parabolic equation in a three-dimensional domain and a hyperbolic equation on a part of the surface of this domain, connected to each other through a boundary condition and a potential in an equation of hyperbolic type. Next, an asymptotic analysis of this system is carried out, which allows us to reduce the model of an individual element to the solution of a simple ordinary differential equation. On this basis, a model of the entire water treatment device is proposed.

1. Introduction

The problem of water purification from undesirable impurities is of great practical importance. It has been reviewed by many authors [1-4]. The aim of paper [5] is to find a model of hybrid biofilm reactor under aerobic and anoxic conditions and to simulate the decontamination of petrochemical wastewater. This problem also raises a number of interesting mathematical problems [6-11]. Comparison of multi-dimensional modelling results with those obtained using one-dimensional approaches is made in [12]. In this paper, the authors conclude that it is necessary to use multidimensional modeling to predict the properties that arise from the spatial structure of a biofilm.

The model for a multispecies biofilm growth is in [13]. As a numerical application, simulations for a heterotrophic-autotrophic competition are developed by the method of characteristics. The mathematical model in the work [14] connects the dynamics of biofilm and bulk liquid compartments through which the substrate flow passes. In [15] the authors present a numerical solution of a mathematical model obtained by combining the reactor mass balance for suspended substrates with one-dimensional model of a Wanner-Guger type biofilm.

In this paper, we propose a model of water purification using biologically active films in which bacteria multiply and die. In a special tank of cylindrical shape with a height of about one meter and a diameter of about 20 cm, parallelepipeds consisting of thin pressed polymer fibers are placed. The



volume of such a parallelepiped is about 15-20 cubic centimeters, individual fibers can be considered as rods of a length of about 1 cm. A thin biofilm covers the surface of each such rod, its thickness is about a tenth of a millimeter. Water enters the upper section of the purification device, then water drops flow down on the said rods, wetting the biofilm. Undesirable impurities in water are the food for bacteria in the biofilm, therefore impurities penetrate through the film. The penetration intensity depends on both concentration of bacteria and concentration of undesirable impurities at the film boundary. The average water velocity, which "oozes" over the surface of the biofilm, also affects the absorption rate. Thus, a rod of length l (about a centimeter) is, as it were, an elementary element of a water treatment device. In total, there are several million such elements in the cylinder. If we could build an adequate model of water treatment (i.e., the process of absorption of impurities) for one such element and computer implementation of such a model would take a short time, then we could simulate the entire process of water treatment by quantifying the drop in the level of water pollution during passage through the cleaning device. Similar models were considered in a number of works, in particular, in [16-20]. First, we describe the basic principles of the mathematical model that we use in this paper.

2. Description of the general principle of the mathematical model

We replace the structure of the cleaning elements with a set of rods of length l covered with a cleaning layer of thickness δ . An infinitely thin layer adjoins this layer, through which air and water with undesirable impurities are transported. An absorbing cleaning layer (biofilm) receives impurities in its volume from a surface adjacent to it at a rate that depends on the concentration of bacteria on the surface of the biofilm and impurities in the liquid being cleaned on the same surface, for example, proportional to the difference in concentration in the cleaning layer and on the surface. Inside the cleaning layer, the equation describing the evolution of the concentration of bacteria over time is a diffusion equation with a nonlinear term that models the absorption of harmful impurities by bacteria. At low concentrations, this law can be considered linear. With increasing concentration, the rate of absorption of impurities tends to a constant, since at a high concentration of bacteria they begin to "interfere" with each other. Sometimes this behavior of bacteria in the literature is called the "Mono law." The influx of unwanted impurities is modeled by the condition of contact with the surface adjacent to the biofilm, along which water with undesirable impurities, mixed with air, is transported along the cleaning layer. The field of transportation speeds is considered to be predefined. Its value is calculated for each cleaning element, based on the total consumption of contaminated liquid and the inclination of the element to a horizontal plane (it is clear that water flows off on a vertical surface as quickly as possible, but does not flow on a horizontal surface). The equation of motion of the mixture: water-air-harmful impurities is a hyperbolic type equation (transfer equation) with a potential that describes the removal of harmful impurities into the cleaning layer (this is the amount of "removal" of harmful impurities from water, which determines the potential in this equation, depends on the concentration on the surface bioactive layer of bacteria and harmful impurities, in the simplest case this dependence is linear, for example, the potential value is proportional to the difference in the concentrations of impurities on the surface and in the cleaning layer). The system describing the absorption of harmful impurities in one element is a combination of the diffusion equation in a three-dimensional cylindrical region and the transport equation on an adjacent cylindrical two-dimensional surface. Such a task has no analytical solution. However, it is quite obvious that it is not difficult to build a calculation program. After calculating the degree of absorption of one cleaning element, depending on the concentration of the incoming impurity, the speed of transportation, the thickness of the cleaning layer, the law of absorption of harmful impurities by bacteria and the dependence of the flow of harmful impurities on the difference in concentration in the cleaning layer and on the transport surface, it will be easy to build a model of the entire filter, consisting of thousand of such elements. This is an arithmetic calculation. The most difficult is to build a model and the corresponding calculation programs for one element.

The entire cylindrical tank is divided into separate layers along the height of the tank, and a computer program is built that allows you to calculate the concentration change on each of the layers, from top to bottom, using the model of an elementary cleaning element.

3. System of equations for a mathematical model

Further, we consider the concentration of bacteria in the biofilm and the concentration of impurities at the boundary of the biofilm depend only on the radial variable r and the variable z along the length of the rod. We neglect the dependence on the angular variable.

We introduce the following notation. Ω_0^ε is one rod inside the cube (one fiber of which the cube consists), ε is the diameter of this rod, Ω_1^ε is the surface δ thick layer (biofilm) on the Ω_0^ε , S_ε is the part of the Ω_1^ε lateral border that is not in contact with Ω_0^ε , Γ_ε is the rest of the Ω_1^ε lateral border. $C_\varepsilon(\vec{x}, t)$ denotes the concentration of impurities in Ω_1^ε , $\vec{x} = (r, z)$, t is the time variable, $M_\varepsilon(\vec{x}, t)$ denotes the concentration of impurities on S_ε (on a two-dimensional surface), $\vec{v}(\vec{x}, t)$ is a velocity vector tangential to the surface S_ε . We also denote by D_1, D_2 the upper and lower "covers" of the cylinder (or rod) under consideration.

Functions $C_\varepsilon(\vec{x}, t)$ and $M_\varepsilon(\vec{x}, t)$ must satisfy the following equations in Ω_1^ε and on $S_\varepsilon, \Gamma_\varepsilon$:

$$\dot{C}_\varepsilon = D \cdot \Delta C_\varepsilon + F(t, C_\varepsilon) \text{ in } \Omega_1^\varepsilon, \quad (1)$$

$$\left. \frac{\partial C_\varepsilon}{\partial n} \right|_{\Gamma_\varepsilon} = 0, \quad \left. \frac{\partial C_\varepsilon}{\partial n} \right|_{S_\varepsilon} + k_0 C_\varepsilon = -k_1 (M_\varepsilon - C_\varepsilon)|_{S_\varepsilon}, \quad C_\varepsilon|_{t=0} = 0. \quad (2)$$

In addition, the homogeneous Neumann condition must also be satisfied on D_1, D_2 .

The equation (1) describes the diffusion of bacteria in a layer with the death of bacteria when their concentration increases. The Laplace operator Δ is the Laplace operator in cylindrical variables, r is the radial variable. A non-linear function $F(t, C_\varepsilon)$ models the above Mono law, D is diffusion coefficient, k_0, k_1 are some constants, $\frac{\partial C_\varepsilon}{\partial n}$ is the derivative in the direction of the external normal n to the surface S_ε .

Functions $C_\varepsilon(\vec{x}, t)$ and $M_\varepsilon(\vec{x}, t)$ must satisfy the following equations in Ω_1^ε and on $S_\varepsilon, \Gamma_\varepsilon$:

$$\begin{aligned} \dot{M}_\varepsilon &= \vec{v} \cdot \nabla M_\varepsilon + \bar{k} M_\varepsilon + k_2 (C_\varepsilon - M_\varepsilon), \\ M_\varepsilon|_{\partial S'_\varepsilon} &= C_0, \quad M_\varepsilon|_{t=0} = C_0 \end{aligned} \quad (3)$$

describes the transport of impurities, the content of which we want to reduce, over the surface S_ε with the transition of impurities into Ω_1^ε . Destructible impurities serve as food for bacteria. As $F(t, C_\varepsilon)$ we have designated a nonlinear, generally speaking, function that describes a decrease in the number of bacteria in a biofilm at their high concentration, $\partial S'_\varepsilon$ is a part of the edge S_ε at the upper end of the rod, where the field $\vec{v}$ "enters" into it. In this particular case $\nabla M_\varepsilon = \frac{dM_\varepsilon}{dz}$, as r is constant on the surface S_ε , $\bar{k}, k_2, C_0$ are some constants.

It is easy to construct a direct difference scheme for the posed boundary value problem. However, it should be noted here that this system does not have a specific type, it consists of two equations, the first of which is parabolic and the second hyperbolic. In addition, these systems are defined in domains of various dimensions, system (1) - (2) in a three-dimensional domain, and system (3) in a two-dimensional one. This system is nonlinear, generally speaking, and its correctness raises questions.

Mathematically, this is a new and rather interesting object. We assume that the steady-state regime that the solution reaches for large values of time does not depend on the initial distribution of the density of bacteria, but depends on the density of impurities falling on the upper part of the water treatment device. This is a fairly natural assumption, but as a mathematical statement, it requires proof.

In the statement of the problem given in this paragraph, the dependence in the boundary conditions on the concentration of bacteria and harmful impurities is linear. In this case, it is possible to exclude the value of the density of impurities from the system by solving the linear equation for the density of impurities M at a given value of the concentration density of bacteria C and substituting the resulting expression in the boundary condition for function C . It is obtained by a nonlocal condition of the aftereffect of the integral type, and the past concentration values at various spatial points will affect the flow through the boundary. This is a statement of a boundary value problem with integral “aftereffect”, which is interesting from a mathematical point of view. Currently, such tasks have not yet been adequately studied.

To circumvent these mathematical difficulties, we simplify our model using the additional assumption that the length of an individual cleaning element is significantly greater (about 100 times) the thickness of the biologically active film. This assumption is actually fulfilled for the method of water treatment considered in this paper. Then we can apply the asymptotic method for analyzing the solutions of boundary value problems in the so-called “thin” domains, see, for example [21, 22]. Using this method, with the passage to the limit in thickness, the dimension of the space of independent variables decreases, and the boundary-value problem considered by us for the stationary distribution mode of impurities reduces to solving an ordinary differential equation. The only independent variable is the directional variable along the bar. Such an equation is solved numerically almost instantly on a modern computer, and therefore, the solution of several millions of such equations modeling individual elementary elements of water purification becomes a simple task. The initial conditions for such equations are modeled depending on the layer in height at which such an element is located. Namely, we divide the water treatment device into layers with a thickness of about one centimeter in height. The initial conditions for the equations corresponding to the elements of water treatment in the upper layer are determined by the mode of flow of water into the water purifier. They are predefined. Water may also flow unevenly over the surface area. The distribution of the intensity of water intake with impurities is the initial condition for the model. On the layers of the next level in height, the initial conditions at the upper point of the element will be determined by the group of lower points of elements adjacent to this upper point from the upper layer. Neighboring - means located at a certain distance not exceeding a given value of d . Each element of the upper layer divides in a certain way, for example, evenly, the fraction of impurities still untreated (and these are the values of the concentration of impurities at its lower end) between the input upper points of neighboring elements of the next (lower) layer height.

The slopes of the water treatment elements with respect to the vertical can be modeled as uniformly distributed, and the speeds of movement of the mixture of water and air over individual elements can be selected depending on the slope of the element to the vertical axis.

Now we describe in more detail the procedure of the limiting transition over the film thickness in the original boundary-value problem given in this section, which simplifies the model by reducing it to a system of ordinary differential equations.

4. Asymptotic limit on the water treatment element thickness

This approach, which greatly simplifies the solution of the problem, consists in constructing for the solution of our system in the stationary case an asymptotic approximation with respect to a small parameter $h = R - r_0$ characterizing the thickness of the rod. It turns out that the first approximation in the parameter $h \rightarrow 0$ is easy to construct, and the diffusion value and potential in equation (1) are not significant for it, and the boundary condition on the surface S plays the main role. The role of diffusion coefficients appears only in the next approximation with respect to the parameter h . Indeed, we

consider the equation of system (4) in the stationary version (when the time derivatives are equal to zero) with the boundary condition on S

$$\left(\frac{\partial C}{\partial r} + (k_0 - k_1)C \right) \Big|_{r=R} = \Phi(x). \quad (4)$$

It can be shown that for $C(r, z)$ if $h \rightarrow 0$ we have the asymptotic approximation

$$C^{(1)}(r, z) = \frac{\Phi(x)}{k_0 - k_1} - \frac{\Phi''(x)}{k_0 - k_1} I(r), \quad L_r I(r) = 1, \quad \frac{\partial I}{\partial r} \Big|_{r=r_0} = 0. \quad (5)$$

Here L_r is the radial component of the Laplace operator in cylindrical variables, $I(r)$ is an auxiliary function satisfying the above conditions.

Note that for $C^{(1)}$ approximation, the boundary condition on S is fulfilled with $O(h)$ accuracy, the condition on Σ is satisfied exactly, the conditions on the D_1, D_2 “covers” are not satisfied, but the order areas D_1, D_2 is $O(h)$, and the flow through these surfaces will not affect the solution by more than a $O(h)$ value, this statement can be proved strictly by mathematical methods. The equation for $C^{(1)}$ holds exactly (we consider here $F \equiv 0$ for simplicity, but it is not difficult to consider the more general case when the function F is not identically equal to zero). The term $\frac{\Phi''(x)}{k_0 - k_1} I(r)$ in the expression for $C^{(1)}$ is of $O(h^2)$ order, therefore with $O(h)$ accuracy we will have

$$C^{(1)}(r, z) \sim \frac{\Phi(x)}{k_0 - k_1}. \quad (6)$$

Thus, if we substitute the indicated approximate value (6) for $C(r, z)$ into differential equation (1), then for the proposed approximation for a small value h of the $M(z)$ solution component, from equation (3) we obtain a simple ordinary differential equation

$$\frac{dM}{dz} = -v^{-1} g \left[M(z), \frac{f(M(z))}{k_0 - k_1} \right] \quad (7)$$

with the initial condition $M(0) = m_0$. Here f, g are explicitly defined functions whose specific form is determined by the initial statement of the problem. If f and g are linear functions, then this equation (7) is solved explicitly, and if f and g are functions of a general form, then it can be solved quickly and with high accuracy on a computer.

5. Conclusion

In this work, we propose a model of the water purification process using biologically active elements that is simply implemented as a program. Such a model can help in calculating the parameters of the water treatment device, so that a certain water treatment performance is achieved, and at the same time, the level of harmful impurities in the water at the outlet of the water treatment device does not exceed a predetermined value. Thus, this model can be used to solve the optimization problem of choosing various parameters of a water treatment device with corresponding restrictions on the productivity and quality of water treatment.

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