

Calculation of organic substrate decomposition in biofilm and bioreactor-filter taking into account its limitation and inhibition

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Abstract — The mathematical problem of the steady-state biofiltration of an organic substrate is formulated at two levels taking into account the limitation and inhibition of the rate of its decomposition. The exact and approximate solutions to the problem of substrate biooxidation in a representative biofilm were obtained and compared using test examples. Based on them an analysis of the technological process in the porous biofilter medium and the output characteristics was carried out.

Keywords — biofiltration; mathematical model; biofilm; inhibition; calculation; organic substrate; limitation.

I. Introduction

Currently, biological methods are widely used for wastewater treatment [1]. In this way, organic contaminants are removed first. These methods are successfully implemented on submerged bioreactor-filters under aerobic [2, 3] and anaerobic [4] conditions. Organic compounds are directly utilized in the biological phase, which is predominantly formed by a set of biofilms firmly attached to the elements of the solid phase (grains) [5]. Such filters are capable of effectively removing dissolved contaminants over a long period of time. In general, the time of stabilization of the biofiltration characteristics and the output of the filter to the operating mode is short in comparison with the filter run. Therefore, when calculating the technological process in biofilters, it is justified to rely on mathematical models of steady-state biofiltration [6, 7]. Due to the significant difference in the scale (micro and macro) of both physical and biological processes occurring in the layer of filtering material, such models are composed of two (or more) interconnected compartments

II. RESULTS AND DISCUSSION

The first compartment describes the action of a representative biofilm. Inside it, a dissolved organic matter is transferred only due to molecular and surface diffusion. It is important that the rate of biodegradation of organic substrate, as a rule, is significantly limited due to insufficient amount. Decomposition products, such as volatile fatty acids, often inhibit this process [8]. Then, taking the biofilm flat and taking into account the resistance of the surrounding liquid film,

the structural compartment can be represented in the following form

$$D_e \frac{d^2 s}{dx^2} = \frac{\mu_m \rho_B}{Y} \frac{K_i s}{s^2 + K_i s + K_s K_i} = \lambda K_i u(s); \quad (1)$$

$$x = 0, \quad \frac{ds}{dx} = 0; \quad x = l_f, \quad D_e \frac{ds}{dx} = k_L (S - s). \quad (2)$$

Here s is the concentration of the substrate, D_e is the effective diffusion coefficient, μ_m is the maximum specific growth rate of microbial biomass, ρ_B is the density of such biomass, Y is the economic coefficient, K_i is the inhibition coefficient, K_s is the half-saturation constant, l_f is the biofilm thickness, k_L is the transfer coefficient of the substrate in the liquid film, S is the concentration of the substrate in the liquid phase outside the liquid film.

Dimensionless variables and coefficients are introduced: $\bar{s} = s/S_0$, $\bar{S} = S/S_0$, $\bar{x} = x/R_g$, $\bar{l}_f = l_f/R_g$, $\bar{K}_{i,s} = K_{i,s}/S_0$, $\bar{k}_L = R_g k_L/D_e$, $\bar{\lambda} = \mu_m \rho_B R_g^2 / (Y D_e S_0)$, S_0 is the concentration of the substrate at the entrance to the filter, R_g is the radius of the grain. Then the exact solution to the problem (1), (2) is first expressed by the inverse function

$$\bar{x}(\bar{s}) = \bar{l}_f - \frac{1}{\sqrt{2 \bar{\lambda} \bar{K}_i}} \int_{\bar{s}}^{\bar{S}} \frac{d\zeta}{\sqrt{U(\zeta, \bar{s}_g)}}. \quad (3)$$

Here

$$U(\zeta, \bar{s}_g) = \frac{1}{2} \ln \frac{\zeta^2 + \bar{K}_i \zeta + \bar{K}_i \bar{K}_s}{\zeta^2 + \bar{K}_i \zeta + \bar{K}_i \bar{K}_s} - \frac{\bar{K}_i}{2 \sqrt{\bar{K}_i^2 - 4 \bar{K}_i \bar{K}_s}} \times \\ \times \ln \left(\frac{2\zeta + \bar{K}_i - \sqrt{\bar{K}_i^2 - 4 \bar{K}_i \bar{K}_s}}{2\zeta + \bar{K}_i + \sqrt{\bar{K}_i^2 - 4 \bar{K}_i \bar{K}_s}} \frac{2\bar{s}_g + \bar{K}_i + \sqrt{\bar{K}_i^2 - 4 \bar{K}_i \bar{K}_s}}{2\bar{s}_g + \bar{K}_i - \sqrt{\bar{K}_i^2 - 4 \bar{K}_i \bar{K}_s}} \right),$$

$\bar{s}_{g,f} = s_{g,f}/S_0$, $s_{g,f}$ are concentrations of the substrate on the inner and outer surfaces of the biofilm. Initially unknown values \bar{s}_g , \bar{s}_f should be determined

$$\text{by selection from the system of the equations} \\ \bar{k}_L^2 (\bar{S} - \bar{s}_f)^2 = 2 \bar{\lambda} \bar{K}_i U(\bar{s}_f, \bar{s}_g), \quad (4)$$

$$\int_{\bar{s}_g}^{\bar{s}_f} \frac{d\zeta}{\sqrt{U(\zeta, \bar{s}_g)}} = \sqrt{2\lambda K_i} \bar{l}_f. \quad (5)$$

However, this form of solving the internal problem is inconvenient for calculating the action of a separate biofilm and unacceptable for the subsequent analysis of the removal of the substrate within the filter medium. Therefore, it is necessary to find a simpler approximate solution, and to estimate its accuracy using equations (3)–(5).

As the biofilm thickness is small, the equality $\bar{s} = \bar{s}_f$ is assumed for the structural function of utilization. In fact, instead of the indicated function, its some constant (effective) value is taken, which makes it possible to simply solve equation (1) under conditions (2). Its double integration allows to obtain

$$\bar{s}(\bar{x}; \bar{l}_f, \bar{S}) = \bar{S} - \lambda \bar{K}_i u(\bar{s}_f) \left(\frac{\bar{l}_f}{k_L} + \frac{\bar{l}_f^2}{2} - \frac{\bar{x}^2}{2} \right). \quad (6)$$

The cubic equation for the desired relative concentration \bar{s}_f follows from (6) at $\bar{x} = \bar{l}_f$

$$\bar{s}_f^3 + (\bar{K}_i - \bar{S})\bar{s}_f^2 + \left(\bar{K}_i \bar{K}_s - \bar{K}_i \bar{S} + \frac{\lambda \bar{K}_i}{k_L} \bar{l}_f \right) \bar{s}_f - \bar{K}_i \bar{K}_s \bar{S} = 0$$

Its physically meaningful root is calculated using the Cardano formula

$$\bar{s}_f = \sqrt[3]{-\frac{\varphi_1}{2} + \sqrt{\frac{\varphi_1^2}{4} + \frac{\varphi_2^3}{27}}} + \sqrt[3]{-\frac{\varphi_1}{2} - \sqrt{\frac{\varphi_1^2}{4} + \frac{\varphi_2^3}{27}}} - \frac{K_i - S}{3},$$

$$\text{where } \varphi_1 = \bar{K}_i \bar{K}_s - K_i S + \frac{\lambda \bar{K}_i}{k_L} \bar{l}_f - \frac{\bar{K}_i - S}{3},$$

$$\varphi_2 = \frac{2}{27} (\bar{K}_i - S)^3 - \frac{1}{3} (\bar{K}_i - S) \left(\bar{K}_i \bar{K}_s - K_i S + \frac{\lambda \bar{K}_i}{k_L} \bar{l}_f \right) - \bar{K}_i \bar{K}_s S.$$

When \bar{s}_f is known, the second boundary (smallest) concentration is easily calculated

$$\bar{s}_g(\bar{l}_f; \bar{S}) = \bar{S} - \frac{\lambda \bar{K}_i}{2k_L} u(\bar{s}_f(\bar{l}_f, \bar{S})) (2 + k_L \bar{l}_f). \quad (7)$$

Thus, according to (2) the relative amount of the substrate entering a separate biofilm per unit of time \bar{i}_f is

$$\bar{i}_f(\bar{l}_f, \bar{S}) = k_L [\bar{S} - \bar{s}_f(\bar{l}_f, \bar{S})]. \quad (8)$$

Based on equation (8), an expression is derived for the generalized function of substrate utilization (in the operation volume) $I(l_f, S)$. If the porosity of the pure filter medium n_0 , then there are N_g grains of the solid phase in the unit volume of the medium

$$N_g = \frac{3(1 - n_0)}{4\pi R_g^3}. \quad (9)$$

Then the function mentioned above has the dimensional form

$$I(l_f, S) = N_g i_f(l_f, S). \quad (10)$$

It is included as a free term in the steady-state biofiltration equation, so that

$$V \frac{dS}{dz} + I(l_f(z), S(z)) = 0, \quad (11)$$

where V is the biofiltration rate. Thus, for applied calculations it is necessary to establish two functions – $\bar{l}_f(\bar{z}), \bar{S}(\bar{z})$. Therefore, the stationary equation of biomass balance is added to equation (11), which describes the (dynamic) balance between its increase and decrease due to detachment, decay, grazing, namely,

$$YI = k_d B, \quad (12)$$

where k_d is the coefficient of the rate of biomass loss, B is the concentration of biomass. Since the biofilm is considered flat due to $R_g \gg l_f$, it is true

$$B = \rho_B \Omega_B l_f, \quad (13)$$

where ρ_B is the biomass density, Ω_B is the specific surface area of the biological phase. Then the equation of mass transfer using macroscales V and L (height of the bed) is reduced to a dimensionless form

$$\frac{d\bar{S}}{d\bar{z}} + \chi_g \bar{k}_d \bar{l}_f = 0, \quad (14)$$

where $\chi_g = 3(1 - n_0)LD_e/(VR_g^2)$, $\bar{k}_d = k_d \rho_B R_g^2/(YD_e S_0)$. Similarly, the balance equation (12) will be

$$\bar{k}_L [\bar{S} - \bar{s}_f(\bar{l}_f, \bar{S})] = \bar{k}_d \bar{l}_f. \quad (15)$$

The system of equations (14), (15) is supplemented by the boundary condition

$$\bar{z} = 0, \quad \bar{S} = 1. \quad (16)$$

In the general case, the problem (14) - (16) has to be solved numerically using suitable software packages for mathematical analysis (Mathcad, Matlab). However, **when** a high initial concentration of the dissolved organic matter (wastewater) at the inlet section of the bed, the maximum possible amount of biomass is often contained within it above a certain time, characterized by the limiting value of the biofilm thickness l_{fm} . Then the linear distribution of the substrate concentration over the height follows from equation (14) under condition (15)

$$\bar{S}(\bar{z}) = 1 - \chi_g \bar{k}_d l_{fm} \bar{z}. \quad (17)$$

And if the entire bed is maximally saturated with biomass, then the output concentration \bar{S}_e is immediately calculated by formula (17) at $\bar{z} = 1$. At the same time, it is real that the ratio $l_f < l_{fm}$ takes place in the remote part of the bed. Then the concentration of the substrate S_m at the inner boundary ($z = z_m$) is determined by the selection from the equation

$$\bar{k}_d \bar{l}_{fm} + \bar{k}_L \bar{s}_f(\bar{l}_{fm}, \bar{S}_m) = \bar{k}_L \bar{S}_m, \quad (18)$$

and the position of this boundary is calculated by the formula

$$\bar{z}_m = \frac{1 - \bar{S}_m}{\chi_g \bar{k}_d}. \quad (19)$$

Subsequent calculations of \bar{S} , \bar{S}_e on the area $[\bar{z}_m, 1]$ should also be carried out by numerical methods, provided

$$\bar{z} = \bar{z}_m, \quad \bar{S} = \bar{S}_m. \quad (20)$$

III. RESULTS AND DISCUSSION

When conducting a quantitative analysis, a particular importance was attached to the substantiation of the approximate solution obtained above, since on its basis the technological process is modeled on the scale of the bed and, as a result, the content of organic contamination in the filtrate is predicted. The accuracy of this solution can be clearly assessed by comparing it on test examples with the exact solution. The results of exact and approximate calculations are presented in Figs. 1, 2. The relative boundary concentrations of the substrate \bar{S}_g , \bar{S}_f , as well as its inflow per unit time \bar{i}_f to the biofilm located at the entrance to the biofilter ($\bar{S} = 1$) were their subject. The values of the coefficients \bar{K}_s (0.5), \bar{k}_L (25) were also set. Attention was focused on the effect of the inhibition of substrate biodegradation which is less studied. Therefore, concentration \bar{S}_g and flux \bar{i}_f were found as functions of the relative coefficient \bar{K}_i , which varied by three orders of magnitude. The set of the curves in the figures are obtained by varying the coefficient $\bar{\lambda}$. Its large values correspond to aerobic biofiltration, while lower value (25) corresponds to anaerobic biofiltration. It is natural that the unevenness of the microbial mass distribution within the biofilm increases due to an increase in the consumption of the substrate. As a result, the errors in the calculation of microcharacteristics and, first of all, the key microcharacteristic for the subsequent analysis of biofiltration \bar{i}_f (Fig. 2), regardless of the method of averaging the structural function of substrate utilization $u(\bar{S})$, increase. In fact, one of the worst options for simplifying the specified function is implemented above. And nevertheless, even in this case, as follows from both figures, the accuracy of the new approximate solution turned out to be high, and the possible inaccuracies in this case are less than due to the imperfection of experimental methods and the unreliability of the initial information. It should also be noted that with a slow growth of microorganisms, which is characteristic of anaerobes, the calculated errors when using (6) - (8) will be minimal. Therefore, these formulas can serve as a reliable basis for subsequent calculations of biofiltration, taking into consideration its limitation and inhibition, and then for the theoretical substantiation of operating and design parameters.

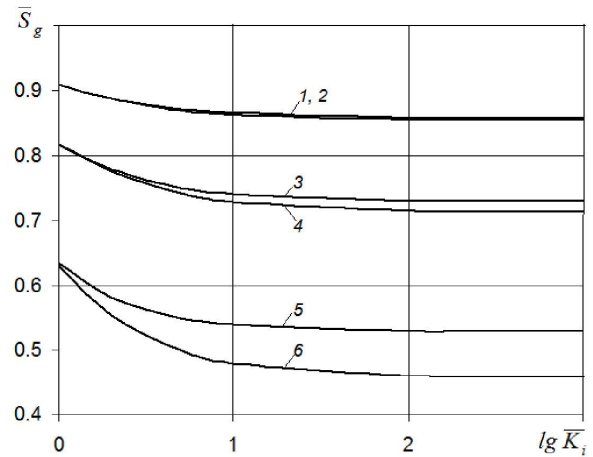


Figure. 1. Relationship $\bar{S}_g(\lg \bar{K}_i)$:

1, 3, 5 – exact calculation; 2, 4, 6 – approximation

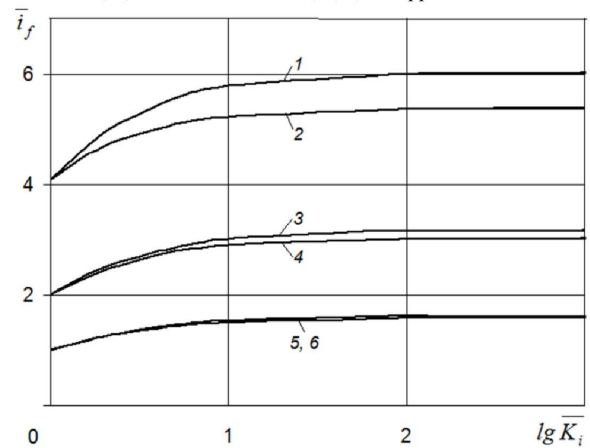


Figure. 2. Relationship $\bar{i}_f(\lg \bar{K}_i)$:

1, 3, 5 – approximation calculation; 2, 4, 6 – exact;
1, 2 – $\bar{\lambda} = 100$; 3, 4 – $\bar{\lambda} = 50$; 5, 6 – $\bar{\lambda} = 25$

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