THE METHODIC OF MODELING AND CALCULATIONS OF THE OXYGEN REGIME AT THE PURIFICATION OF THE WASTE WATERS IN AEROTANKS WITH SUSPENDED AND FIXED BIOCENOSIS

Abstract. The methodic of mathematical modeling and calculations of oxygen regime at biological treatment of waste waters from organic contaminants in aerotanks with suspended and fixed biocenosis is given. The peculiarities of the simulation of oxygen supply during purification in aerotanks-mixers and aerotanks-displacers are considered at this.

Keywords: model; purification; oxygen; organic pollution; aerotank-mixer; aerotank-displacer; biofilm; active sludge.

Introduction

In biological waste waters treatment reactors in particular in aerotanks the removal of organic contaminants (OC) occurs in aerobic conditions that is when oxygen is consumed for biooxidation of OC and self-oxidation of cell material and also used in other processes that may occur at this time. Therefore the modeling and development of the aeration system is to provide such an oxygen regime in the reactor in which the rate of the biological treatment process should not be limited by the amount of oxygen contained in the reactor. In such reactors the processes of dissolution and consumption of oxygen develop simultaneously and are interconnected. In well-known bioreactors – aerotanks the removing of OC occurs under normal conditions only owing to suspended biocenosis (active sludge) and these processes are sufficiently thoroughly considered in the special literature.
In this paper the peculiarities that occur at the modeling of the oxygen regime in the aerobic biological treatment of waste waters in aerotanks-mixers and aerotanks-displacers with suspended and fixed biocenosis are considered for conditions when the process of biochemical oxidation is provided with oxygen in sufficient quantities and the oxygen supply will not limit the kinetics of biooxidation (removal) of OC in aerotanks with suspended and fixed biocenosis [1].

**The main features of the proposed methodic**

It is known that depending on the hydrodynamic conditions of the flow of the waste waters in bioreactors its are divided on the aerotanks-mixers and aerotanks-displacers [1–4]. If we take into account that oxygen supply takes place using the most commonly used in practice pneumatic (bubble) oxygen delivery technology in the volume of aerotanks due to the use of air then the indicated features of using oxygen with suspended and fixed biocenosis in particular are as follows. If suspended biocenosis (particles of active sludge) is directly used for oxidation of oxygen dissolved in waste waters from oxygen bubbles then in the case of fixed biocenosis (in the form of a biofilm loaded on the surface of the material) it is necessary to determine the flow of dissolved oxygen that enters to the biofilm surface through the boundary layer of the liquid and carry out a quantitative assessment of the consumption of oxygen by microorganisms in the thickness of the biofilm. The solution of these questions allows us to estimate the amount of oxygen needed for biooxidation by suspended and a fixed biocenosis and moreover allows solving such an important question which of the substrates (oxygen or OC) will limit the oxidation process in the biofilm. It has been established by research that at considerable (saturated) arrangement in the aerotank (reactor) of the elements of loading the oxygen can enter in the biofilm not only from the volume of liquid (dissolved oxygen) but also as a result of so-called inter-surface transfer (IST) directly from the bubbles adhering to the surface of the biofilm. The account of IST allows in some cases to increase the concentration of oxygen entering to the biofilm up to 20% [2].

In both cases of the removing of organic contaminants by suspended and fixed biocenosis in aerotanks for growth and livelihoods of microorganisms it is necessary to provide the uninterrupted supply of oxygen and to control its consumption in the amount necessary to maintain the kinetics of reactions with a high rate of utilization of OC in these conditions of the aerobic process. In this work in order to evaluate and analyze the oxygen regime in aerotanks-mixers and aerotanks-displacers under the indicated conditions a general mathematical model was constructed which reduces to the realization of the corresponding equations of the material balance recorded relative to the concentration of oxygen C.

So for aerotank-mixer we have

\[ W_p \frac{\partial C_a}{\partial t} = Q_a \left( C_0 - C_a \right) + W_p \alpha K_c a (\beta C_p - C_a) - F_{d_t} N_c - R_{d_t} W_p, \]  

(1)

and for the aerotank-displacer we have

\[ \varepsilon \frac{\partial C_a}{\partial t} = D_c \frac{\partial^2 C_a}{\partial x^2} - v \frac{\partial C_a}{\partial x} + \varepsilon \alpha K_c a (\beta C_p - C_a) - \frac{F_{d_t}}{W_p} N_c - R_{d_t}, \]  

(2)
In practical calculations it is enough to consider equations (1)–(2) in stationary conditions and to evaluate their members taking into account the known diffusion criterion of Peckle $P_e = \frac{v l}{D_v}$ according to [1]. For further implementation let's bring them to the form:

for aerotank-mixer

$$C_0 - C_a + \alpha K_c a \left( \beta C_p - C_a \right) T_a - R_3 = 0,$$

$$R_3 = \frac{F \delta}{Q_a} N_c + R_{a_v} T_a, \quad T_a = \frac{W_p}{Q_a},$$

for aerotank-displacer

$$-v \frac{dC_a}{dx} + \varepsilon \alpha K_c a \left( \beta C_p - C_a \right) \lambda_c N_c - R_{a_v} = 0, \quad \lambda_c = \frac{F \delta}{F}.$$  

In general case in the above equations the value of the flow of oxygen entering to the biofilm through its surface is determined by the equation:

$$N_c = -D_c \frac{dC}{d\bar{z}} = (1 - \eta) K_C \left( C_a - C|_{\bar{z}=0} \right) + \eta \alpha K_{\bar{C}_n} \left( \beta C_p - C|_{\bar{z}=0} \right),$$

where $\eta$ – the ratio of the surface area of the biofilm in contact with air bubbles to the total surface area of the biofilm.

In other words the equation (5) takes into account the possible additional flow of oxygen into a biofilm both from the volume of liquid in the form of dissolved oxygen and as a result of the so-called inter-surface transfer (IST) directly from the bubbles adhered to the biofilm. The expediency of taking into account IST takes place with sufficiently significant (saturated) of loading of the elements in the aerotank (reactor) which takes place for example in flooded filters with sand-gravel material of loading. In aerotanks with fixed biocenosis (biofilm) it is possible ignoring the IST and some possible positive impact of IST will go into the stock of the calculations. In this case at implementing models it is necessary to take $\eta = 0$ and take into account only the flow of dissolved oxygen from the volume of liquid to the biofilm due to diffusion:

$$N_c = -D_c \frac{dC}{d\bar{z}} = K_C \left( C_a - C|_{\bar{z}=0} \right).$$

Note that the determination of the flow of oxygen through the surface of the biofilm $N_c$ and for the quantitative estimation of the removal of the OC by the biofilm depending on their parameters in particular which of the substrates (pollution or oxygen) limits the purification process in the biofilm is obtained as a result of
solving the following equations which characterize the consumption of oxygen in the removal of OC by a fixed biocenose (biofilm).

In general this equation for a biofilm has the following form:

$$ \frac{\partial C}{\partial t} = D_c \frac{\partial^2 C}{\partial z^2} - R_c $$

(7)

In the case of cylindrical loading elements in which the biofilm is formed the equation for the biofilm will be as follows:

$$ \frac{\partial C}{\partial t} = D_c \left[ \frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right] - R_c $$

(8)

According to the analysis the solution of equations (7)–(8) for practical calculations is sufficient to solve for stationary conditions that occur fairly quickly that is when $$ \frac{\partial C}{\partial t} = 0 $$.

The solution of equation (7) is performed under the following boundary conditions, namely: $N_c$ for $z = 0$, and $\frac{\partial C}{\partial z} = 0$ for $z = \delta$, which allows us to determine the change in the concentration of oxygen in the thickness of the biofilm $l$ and in subsequent calculations to determine the concentration on the surface of the biofilm $C|_{z=0} = C\delta$.

In the general case the reaction rates are described by the following equations:

$$ R_c = \alpha_1 R_L + \alpha_2 b_c \frac{C}{K_{mc}} + X $$

(9)

$$ R_L = \frac{\mu_0 L}{Y} \frac{C}{K_{ml} + L} \frac{C}{K_{mc} + C} X $$

(10)

$$ R_{ca} = \alpha_{1a} R_{aL} + \alpha_{2a} \frac{b_{ac}}{K_{mac} + C_a} \frac{C_a}{K_{mac} + C_a} X_a $$

(11)

$$ R_{aL} = \frac{\mu_{ma} L_a}{Y} \frac{C_a}{K_{ma} + L_a} \frac{C_a}{K_{mac} + C_a} X_a $$

(12)

In the above equations and dependencies we have $C$, $N_\delta$, $C_a$, $C_0$ – respectively the concentration of oxygen in the biofilm, on the surface of the biofilm, in the aerotank and in the waste waters at the entrance to the aerotank; $C_p$ – concentration of saturation (soluble) oxygen in the liquid; $R_c$, $R_{a_c}$ – the rate of reactions of using oxygen in a biofilm and aerotanks, taking into account the oxidation velocity of the isolated substances during the death of microorganisms; $W_a$, $W_p$, $W_\delta$ – respectively the
aerotanks working volume, the volume of the liquid in the aerotank, the volume of the elements of the established loading with the fixed biocenosis \( F_\delta l \), \( F_\delta \) – respectively the total surface area of the biofilm in the aerotank (reactor), the surface area of the biofilm per unit length of the aerotank (reactor); \( K_{ca} \), \( K_{en} \), \( K_C \) – respectively the volumetric mass transfer coefficient, the coefficient between the surface transfer of oxygen in the biofilm, the coefficient of mass transfer of oxygen in the liquid film. The denotation of other variables in the above equations is given in [1, 3].

To assess the impact of these mechanisms of supply and consumption of oxygen in the removal of OC it is advisable to consider the limiting cases of the work of the aerotanks in the system of biological waste water treatment.

1. In the absence of fixed biomass (additional loading) the removal of OC occurs only with the suspended active sludge and for the supply and consumption of oxygen the given equations are solved with \( N_c = 0 \). In this case the calculation of the parameters of the oxygen regime taking into account the specifics of the oxygen supply systems and the work regime of the aerotank was considered in [4].

2. In the case when the removal of OC occurs only on the biomass fixed on the load that is without taking into account the action of suspended active sludge the given equations are solved at \( R_{ac_c} = 0 \).

3. In the case when the removal of OC in aerotanks occurs at the expense of suspended and a fixed biocenosis in determining the optimal parameters of its work the various variants of its location in the volume (in the plan) of the aerotanks and the required area of the surface of the biofilm surface \( F_\delta l \) (loading elements) are possible. At this the loading elements (nozzles, grids, etc.) can be located throughout the aerotank volume or more densely and compactly only in its individual sections. Depending on the technological scheme of the location of the elements in the aerotank for length (in volume) and in connection with the received reactions in the biofilm and aerotank the general equations can be greatly simplified. Let’s consider further the possible following technological schemes:

a) The load elements are not sufficiently close distributed throughout the length of the aerotank. In this case in the above equations we adopt \( \eta = 0 \) that is the inter-surface oxygen transfer may not be taken into account and with sufficient justification the removal of OC in the volume of aerotanks occurs by reaction of zero order and in biofilm by the first order reaction.

Since in equations (9) and (11) \( K_{mc} \ll C \) and \( K_{maC} \ll C_a \) then for oxygen in practical calculations the oxidation occurs by the reaction of zero order in a biofilm and in aerotank. So for reactions we have:

\[
R_c = \alpha_l R_L + \alpha_2 b_c X
\]

\[
R_L = k_L L = \frac{\mu_m X}{Y_{mL}} L
\]

\[
R_{ac} = \alpha_{a_1d} R_a + \alpha_{a_2} b_c X_a
\]

\[
R_a = \frac{\mu_{maC} X_a}{Y_a}.
\]

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Determination of the concentration of OC in a biofilm \( L(z) \) and in particular on its surface \( L_\delta \) is given in [5]. Determination of the concentration of oxygen C in the biofilm and in particular on its surface \( C_\delta \) occurs as a result of the solution of equations (7), (8) depending on the construction of the loading elements on which the biofilm is formed for example or in the form of flat plates with holes or a net of separate cylindrical rods. At the same time with some approximation we can take for the determination of the reaction \( R_{cL} \) the next dependence:

\[
R_{cL} = \alpha_t k_t L_\delta + \alpha_c b_c X,
\]

where \( L_\delta \) is an averaged concentration of OC in a biofilm [5].

b) The loading elements are located at the beginning of the aerotank in its first part – the reactor 1 in which the removal of the OZ occurs due to the fixed biomass and in the second part of it – in the reactor 2 where the removal of OC occurs by a suspended biomass (active sludge) that is a reactor 2 works like a regular aerotank (Fig. 1a).

c) The elements of the load are located at the end of the aerotank in its second part in the reactor 2 in which the removal of the OC occurs due to the fixed biomass and in the first part – the reactor 1 the removal of OC occurs due to the suspended biomass (active sludge) that is the reactor 1 works as a regular aerotank (Fig. 1b).

![Diagram](image)

Fig. 1 – Scheme of biological purification in aerotanks: a – fixed biomass in reactor 1; b – fixed biomass in the reactor 2

Depending on the adopted hydrodynamic regime of the liquid flow the reactors 1 and 2 can work as bioreactors-mixers and bioreactors-displacers. The supply of oxygen for removal of OC in reactors takes place in accordance with the given general mathematical model that takes into account the accepted reactions of OC utilization and oxidation.
The theoretical substantiation and the methods of calculations of the oxygen regime in aerotanks-mixers and aerotanks-displacers for the above described different technological schemes are considered respectively in [6, 7].

To implement the proposed models and calculations we consider some of the features and prerequisites that have been adopted in the formation of the oxygen regime in aerotanks with an fixed biomasses.

Thus in the above models when we remove OC by the suspended and the fixed biocenosis the linear kinetics of the reactions of the first and the zero orders are accepted and the limits of use of which are limited in particular the values of the concentrations of waste waters which enter to the purification. Therefore in the general case with a sufficient justification in the special literature at the removing of the OC it is proposed to use in the models mainly the kinetics of reactions which is described by the known nonlinear Mono equation [5]. Based on the use of the obtained solutions for the reactions of the first and the zero orders the approximate methods for calculating the required parameters are proposed in accordance with the Mono equation [5]. As a result of the aforementioned in [8] and on the base of the implementation of the above mathematical models a methodic of calculations of the removal of the OC in aerotanks with suspended (active sludge) and with fixed biocenosis (biofilm) in which the kinetics of reactions is described by the nonlinear Mono equation is developed, namely:

$$R_L = \frac{p_m L}{K_m + L}, \quad \rho_m = \frac{\mu_m L_a}{Y_a}$$  \hspace{1cm} (18)

$$R_a = \frac{p_{ma} L_a}{K_{ma} + L_a}, \quad \rho_m = \frac{\mu_{ma} L_a}{Y_a}$$  \hspace{1cm} (19)

At the removal of OC by fixed biomass in the reaction of an oxygen regime of zero order instead of a variable concentration $L$ with sufficient justification its average value $L\delta_p$ is taken according to the following dependence:

$$L\delta_p = 0,5(L\delta_{r=0} + L\delta_{z=\delta})$$  \hspace{1cm} (20)

where $L\delta_{r=0}$ is the concentration of OC on the outer surface of the biofilms ($z = 0$), $L\delta_{z=\delta}$ is the concentration of OC on the inner surface of the biofilm ($z = 0$).

In order to determine the concentrations $L\delta_{z=0}$ and $L\delta_{z=\delta}$ the solutions of problems for determining the concentration changes in biofilms at different kinetics of reactions are given in the works [5, 6, 9]. Thus the following equation was obtained in [9] which connects the concentrations $L\delta_{z=0}$ and $L\delta_{z=\delta}$ to the conditions of the nonlinear Mono equation:

$$L\delta_{z=0} = \bar{L}\delta_{z=\delta} - K m_L \ln \left| \frac{L\delta_{z=0} + \bar{K} m_L}{L\delta_{z=\delta} + \bar{K} m_L} \right| + \frac{\beta L^2}{2\alpha L} (L\delta_{z=0} - 1)$$  \hspace{1cm} (21)
\[ N_L = K_L \left( L_a - L_0 \right) = \lambda_L \beta_L \left( 1 - L_0 \right) \]  

(22)

where \( \bar{L} = \frac{L}{L_a}, K_{ml} = \frac{K_{ml}}{L_a}, \alpha_L = \frac{2 m X \delta^2}{Y D L_a L_a}, \beta_L = \frac{K_L \delta}{D_L}, \lambda_L = \frac{D_L}{\delta} L_a. \)

In the case of the necessity of considering the interfacial transfer (IST) according to equation (5) the solution of the problem in particular the determination of oxygen concentration on the surface of the biofilm \( C \delta \) was obtained in [9].

In an aerotank (reactor) where the removal is due to an active sludge it is usually necessary to recirculate the discharge \( Q \) which will be determined by the following formula:

\[ Q_a = Q \left( 1 + r \right) \]  

(23)

where \( Q \) – estimated wastewater discharge, \( m^3/h \), \( r \) – the degree of recirculation of active sludge which is taken according to the work [10].

An important question when using the proposed models and methods for calculations the oxygen supply of the processes the removal of OC is the definition of unknown mass transfer coefficients \( K_c a \) and \( K_{c_a} \) and related to their determination other parameters. If the technological schemes of supplying oxygen and the peculiarities of its use in aerotanks with active sludge were investigated in to a sufficient extent but in the structures in which the removal of OC occurs by fixed on the loading elements biomasses(biofilm) the study of the oxygen regime was provided insufficient. It was assumed at this that the process of removing of OC is not limited by oxygen that is provided in sufficient quantities of oxygen and is maintained mainly at a concentration close to the concentration of saturation. Among other the processes of oxygen supply of microorganisms in the fixed biofilm and in the form of suspended flakes of active sludge are somewhat different that need to take into account when calculating the consumption of oxygen in the utilization of contaminations by fixed and suspended biomasses.

Taking these features into account when calculating the oxygen regime in reactors with suspended and a fixed biomasses allows more basically to substantiate the determination of the coefficients \( K_c a \) and \( K_{c_a} \) as is shown in [1].

In the future on the base of the proposed models and methods of calculations it is necessary to analyze and evaluate their impact in order to ensure the supply of the required amount of oxygen to the place of reactions and the utilization of OC.

As an example of the calculation (simulation) of the oxygen regime consider the aerotank-mixer in which in the reactor 1 the removal of the OC occurs by suspended biocenosis (active sludge) and in the reactor 2 the removal of the OC occurs due to the fixed biomass (biofilm) on the installed load (Fig. 1). This technological scheme of purification from a practical point of view will be more appropriate and more consistent with the current requirements for providing oxygen treatment because in existing traditional aerotanks to provide the proper more higher quality of the waste waters treatment is too difficult and uneconomical.
Conclusions

Thus the implementation of the proposed models allows with known geometric and other characteristics to evaluate the influence of oxygen regime on the processes of purification in aerotanks at the different conditions of their operation and to substantiate an economical and efficient technological supply system with oxygen taking into account the features of removing of OC in aerotanks with suspended and a fixed biocenosis. In this case it is possible to substantiate the criteria in which the biochemical oxidation process will be adequately supplied with oxygen that is it will be not limit the kinetics of biooxidation both suspended and fixed biocenosis.

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