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Original Research

Kinetics of Oxygen Dissolution and Modeling of the Aeration Process in Wastewater Treatment Bioreactors

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Abstract

Aeration is a key and the most energy-intensive process in biological wastewater treatment using activated sludge systems in aeration tanks, accounting for up to 50-90% of the total energy consumption of wastewater treatment plants. The efficiency of biological treatment largely depends on providing activated sludge microorganisms with a sufficient concentration of dissolved oxygen as well as ensuring proper mixing of the sludge mixture within the reactor. Therefore, improving the efficiency of aeration systems is an important task for reducing operational costs and increasing the overall sustainability of wastewater treatment facilities.

This paper examines the theoretical foundations of the aeration process in biological wastewater treatment systems. Particular attention is given to the mechanisms of oxygen mass transfer from the gas phase into the liquid phase and the factors influencing this process. The key parameters characterizing oxygen transfer efficiency are analyzed, including the volumetric oxygen mass transfer coefficient (KLa) and the α-factor, which reflects the influence of wastewater properties on oxygen transfer. Understanding these parameters is essential for the correct design, optimization, and operation of aeration systems in activated sludge reactors. The presented theoretical analysis contributes to improving the energy efficiency and operational performance of modern wastewater treatment plants.

Keywords: aeration, activated sludge, oxygen mass transfer, dissolved oxygen

Introduction

Aeration in biological wastewater treatment systems is a complex multiphase mass transfer process that combines physical, chemical, and biological phenomena. In general, the process involves the transfer of oxygen from the gas phase (air) to the liquid phase (water), its dissolution, and subsequent consumption by microorganisms involved in the biological oxidation of organic pollutants. The efficiency of this process determines the stability of wastewater treatment plant operation, the rate of biochemical reactions, and the overall environmental effect of the treatment process.

The main objective of aeration is to create and maintain a concentration of dissolved oxygen (DO) sufficient to ensure aerobic conditions in the bioreactor.

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An optimal DO level enables activated sludge microorganisms to oxidize organic substances, perform nitrification of ammonium nitrogen, and carry out other important biochemical processes. Excessively low DO concentrations lead to the formation of anaerobic zones, accumulation of toxic intermediate products, and a decrease in treatment efficiency. At the same time, excessive aeration is also undesirable because it leads to unnecessary energy consumption for air supply and may cause excessive foaming in the reactor.

The oxygen mass transfer process includes several sequential stages: formation of air bubbles in the liquid, their rise through the water column, diffusion of oxygen molecules across the gas-liquid interface, dissolution in the aqueous medium, and subsequent distribution due to turbulent mixing. The final stage involves the biological consumption of oxygen by microorganisms, which determines the balance between oxygen supply and demand [1-3].

Aeration efficiency is influenced by numerous factors, including the size and number of air bubbles, the immersion depth of diffusers, temperature and pressure conditions, mixing intensity, as well as the chemical composition of wastewater and the biochemical oxygen demand (BOD). These parameters collectively determine the rate of mass transfer and the concentration of dissolved oxygen in different zones of the bioreactor.

One of the key parameters is the size of air bubbles. Fine-bubble aeration is considered more efficient compared to coarse-bubble aeration because it provides a significantly larger gas–liquid contact surface area and increases the residence time of bubbles in the water column, promoting more complete oxygen dissolution.

Another important factor is the diffuser immersion depth. The longer the path traveled by a bubble in the liquid, the longer the mass transfer process can continue, and consequently, the greater the amount of oxygen that can dissolve in the water (Fig. 1).

Temperature and pressure also have a significant impact. The solubility of oxygen in water increases with decreasing temperature and increasing pressure. Therefore, during colder periods of the year, the oxygen saturation coefficient is naturally higher than in warmer conditions.

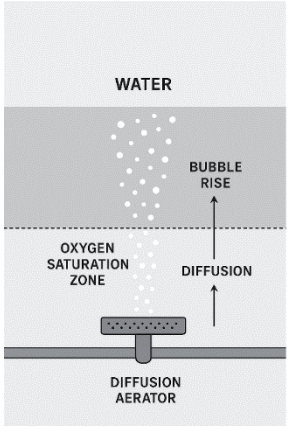

Fig. 1. Bubble formation process in the liquid.

Hydrodynamic conditions within the reactor are also crucial. Mixing of liquid flows improves the uniform distribution of oxygen and prevents the formation of stagnant zones where mass transfer efficiency is significantly reduced.

In addition, the chemical composition of wastewater plays an important role. The presence of organic and inorganic impurities, as well as the level of biochemical oxygen demand (BOD), determines the overall consumption of dissolved oxygen in the system. Some substances, particularly surfactants, may reduce the mass transfer rate by altering the properties of the gas-liquid interface.

Therefore, aeration efficiency depends on a complex set of interacting factors (Table 1), the optimization of which is necessary to ensure stable operation of wastewater treatment plants and to achieve regulatory standards for treated water quality.

Under current conditions of increasing wastewater generation, stricter environmental regulations, and global decarbonization policies, the issue of energy efficiency of wastewater treatment plants (WWTPs) has become particularly relevant. According to international greenhouse gas emission statistics, the water supply and wastewater sector contributes a significant share of indirect emissions associated with electricity consumption.

Biological treatment processes remain the basis of modern technologies for the removal of organic matter as well as nitrogen and phosphorus compounds. However, these processes are accompanied by significant electricity consumption. According to research results, the energy consumption of biological treatment can account for 30-80% of the total energy balance of WWTPs [4-7].

Aeration is the most energy-intensive stage of the treatment process and supplies microorganisms with the required amount of dissolved oxygen necessary for biochemical oxidation processes of pollutants [8, 9].

Aeration in secondary treatment can account for up to 50-80% of the total energy consumption of a treatment plant, making it a key factor in determining operational costs and the carbon footprint of the facility. At the same time, the average specific energy consumption of wastewater treatment plants in different countries ranges from 0.3 to 0.8 kWh/m^3 [10], indicating a significant potential for optimization of technological processes.

Recent technological developments provide new opportunities for reducing energy consumption in the aeration process. These directions include improvements in aerator design, increasing the oxygen mass transfer coefficient (KLa), the application of micro- and nanobubble systems [11], as well as the use of CFD modeling for analyzing hydrodynamics and mass transfer in bioreactors [12, 13]. Modern studies are also focused on improving mathematical models of

Table 1. Factors influencing the aeration process.

Factor	Influence on the aeration process
Bubble size	The smaller the bubble diameter, the larger the gas–liquid contact area and the longer the residence time in water → higher oxygen mass transfer coefficient (K_La).
Diffuser immersion depth	Increases the bubble travel path and the time available for oxygen dissolution.
Water temperature	As temperature increases, oxygen solubility decreases.
Pressure	Higher pressure → greater solubility of gases in the liquid.
Hydrodynamic conditions	Poor mixing promotes the formation of stagnant zones and reduces aeration efficiency.
Wastewater composition	High BOD and COD values increase oxygen demand. The presence of surfactants may reduce mass transfer efficiency.
Aerator design	Determines the uniformity of air distribution and the hydraulic resistance of the system.
Energy consumption	Aeration may account for up to 70% of the total energy consumption of wastewater treatment plants.

oxygen dissolution kinetics, digital twin technologies, AI-based prediction of dissolved oxygen concentration, and optimization of aeration regimes using software platforms such as BioWin and CFD-based simulation tools. Particular attention is paid to the investigation of spatial heterogeneity of oxygen transfer, identification of stagnant zones, and enhancement of oxygen transfer efficiency under varying hydrodynamic conditions [14-17].

In addition, modern algorithms for controlling dissolved oxygen concentration play an important role, ranging from classical PID controllers to adaptive, fuzzy, and neural network-based control systems [18, 19].

Given the significant operational costs associated with aeration, understanding and optimizing its theoretical foundations is of great scientific and practical importance [20, 21].

Despite significant advances in modeling mass transfer processes in bioreactors, conventional approaches typically rely on the assumption of ideal mixing, treating the entire reactor volume as hydrodynamically and spatially homogeneous. However, in real-scale operating packed and pneumatic aeration systems, oxygen dissolution is highly heterogeneous due to the existence of localized high-turbulence mass transfer zones surrounding the diffusers or packing elements. The critical research gap lies in the lack of analytical models that couple this spatial heterogeneity with the cyclic circulation of liquid.

To address this gap, this study provides new knowledge by developing an improved mathematical model that fundamentally differentiates itself from classical formulations. Instead of using a single global mass transfer coefficient, the proposed model explicitly segregates the total reactor volume (V) into a high-intensity working volume of the aerator (Va) and a residual volume where only macro-mixing occurs. This allows for the evaluation of oxygen dissolution kinetics as a function of the number of liquid circulation cycles (n) and the geometric layout of the packing.

Hence, the main objective of this research is to develop, theoretically substantiate, and validate a mathematical model for the kinetics of air oxygen dissolution in a batch reactor that accounts for the spatial heterogeneity of mass transfer zones, thereby providing a tool to optimize aeration systems and reduce energy consumption.

Materials and Methods

Research Concept and Hydrodynamic Assumptions

The aeration process in activated sludge aeration tanks is based on the transfer of oxygen from the gas phase (air) into the liquid phase – the mixed liquor – where it is subsequently utilized by microorganisms during the biochemical oxidation of organic pollutants. Oxygen transfer is a complex multiphase mass transfer phenomenon involving several sequential stages: diffusion of oxygen from the interior of the gas bubble to its surface, transfer across the gas-liquid interface, dissolution and diffusion through the liquid film surrounding the bubble, transport into the bulk liquid, and finally biochemical consumption by microorganisms [22].

The rate of oxygen transfer across the gas–liquid interface is commonly described by the general mass transfer equation:

$$\frac{dC}{dt} = K_L a(C^* - C) \quad (1)$$

where C is the instantaneous dissolved oxygen concentration in water (mg/L); C^* is the equilibrium or saturation concentration of oxygen at a given temperature and pressure; and K_La is the volumetric oxygen mass transfer coefficient, s^{-1}. The driving force of oxygen transfer is the concentration gradient (C^*-C), which determines the intensity of the dissolution process.

The coefficient $K_L a$ is widely used as an integrated indicator of aeration performance. Its magnitude depends on a number of physical and operational parameters, including the physicochemical properties of the liquid, diffuser immersion depth, bubble size distribution, airflow rate, aerator design, and the level of turbulence in the reactor. Reducing bubble diameter increases the gas-liquid interfacial area and thereby enhances oxygen transfer efficiency. However, smaller bubbles may also lead to increased hydraulic resistance and higher energy demand for air supply.

According to the classical film theory of mass transfer, the kinetics of oxygen dissolution are largely controlled by the liquid boundary layer surrounding the gas bubble. This layer represents the main resistance to mass transfer. Its thickness is inversely related to the intensity of turbulent mixing. Therefore, increased mixing intensity reduces the thickness of the liquid film and enhances the overall mass transfer coefficient.

The equilibrium concentration of dissolved oxygen C^* is determined in accordance with Henry's law:

$$C^* = H \cdot p_{O_2} \tag{2}$$

where H is Henry's constant, which is temperature-dependent, and p_{O_2} is the partial pressure of oxygen in the gas phase. As water temperature increases, oxygen solubility decreases due to the reduction in Henry's constant.

Under real wastewater treatment conditions, aeration efficiency is often evaluated using the α-factor, which accounts for the influence of wastewater characteristics, including suspended solids, surfactants, and foam formation, all of which may reduce oxygen transfer efficiency compared with clean water conditions [23]. For activated sludge systems, the α-factor typically ranges from 0.6 to 0.85.

Overall, oxygen transfer in aeration systems results from the interaction of physicochemical and hydrodynamic processes that jointly determine the performance of biological wastewater treatment. A thorough understanding of these mass transfer mechanisms enables engineers to optimize aeration system design and operation by selecting appropriate diffuser types, immersion depths, and air supply rates, thereby achieving improved treatment efficiency while minimizing energy consumption.

Governing Equations of Heterogeneous Mass Transfer

As noted above, the rate of oxygen dissolution represents the limiting step in the biochemical process. Therefore, both theoretical and experimental investigations of this phenomenon are necessary.

To further improve the research methodology, systematize experimental data, and develop engineering approaches for process calculations, an improved mathematical model of the aeration process was developed.

Under laboratory conditions, as well as in most practical cases, the process of oxygen dissolution from air into water occurs in batch mode. As an example, consider the scheme of a reactor equipped with a packed aerator (Fig. 2), containing a liquid volume V, m³.

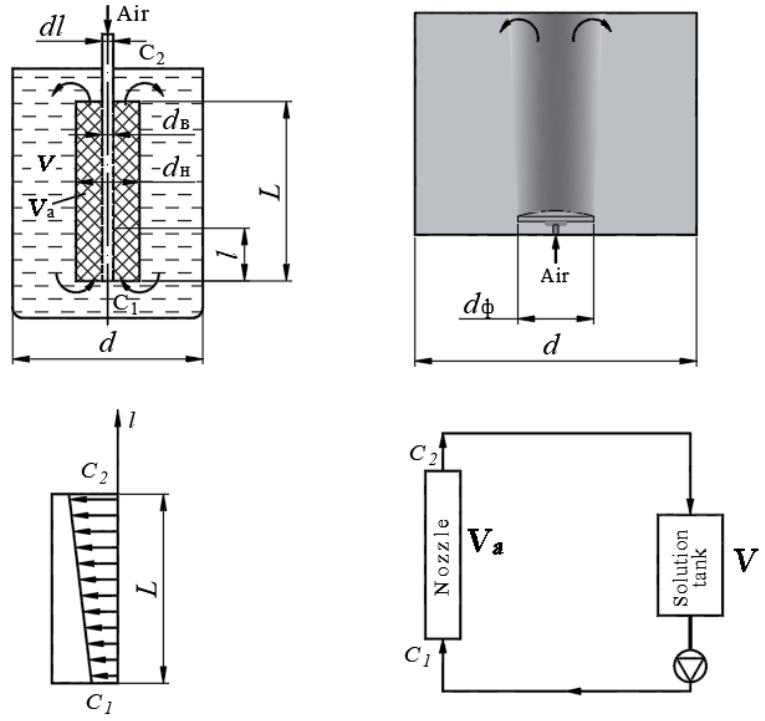

Fig. 2. Schematic diagram of a reactor with a packed aerator.

The initial concentration of dissolved oxygen is denoted as C_p. The main portion of oxygen dissolves within a specific part of the liquid volume referred to as the working volume of the aerator (V_a). In this zone, intensive mass transfer occurs between the gas and liquid phases. After leaving the packing, the oxygen-enriched liquid mixes with the bulk liquid volume, which results in an increase in oxygen concentration from C_1 to C_2 during one circulation cycle. Gradually, as the process is repeated multiple times, the oxygen concentration increases from the initial value C_p to the final concentration C_k.

The process is described by an equation based on a modified form of Fick's law of diffusion [24, 25]:

$$\frac{dC}{dt} = K_v(C_s - C) = K_{\text{П}}\sigma(C_s - C) \quad (3)$$

where $K_v = K_{n\sigma}$ is the volumetric mass transfer coefficient, s^{-1}; $K_{\text{П}}$ is the mass transfer coefficient through the bubble surface, m/s; σ is the specific interfacial area between phases ($m^2/m^3 = m^{-1}$).

The working volume of the aerator is determined by the following expression:

$$V_a = FL = \frac{\pi}{4}(d_{\text{П}}^2 - d_{\text{В}}^2) \quad (4)$$

where d_n and $d_в$ are the outer and inner diameters of the packing, respectively, m, and L is the height of the packing layer, m.

In other cases, for example, in pneumatic aeration, the term ($d_n - d_в$) in Equation (2) may be replaced by the diameter of the bubble plume $d_ф$. When porous diffuser plates are used in aeration tanks, the total surface area of the plates F is used instead.

Unlike classical approaches [24-26], the proposed model accounts for the heterogeneity of mass transfer by dividing the total reactor volume (V) into a working volume (V_a) and a residual volume. This approach corresponds to modern concepts of local turbulence zones and non-uniform mass transfer in gas-liquid systems [27, 28].

Mathematical Modeling Implementation and Software

The computational implementation of the proposed implicit kinetic algorithms was performed in MATLAB (MathWorks, Natick, MA, USA). Numerical analysis of the experimental data, including estimation of the volumetric oxygen mass transfer coefficient (K_v), was conducted using custom-developed computational routines. Model calibration was performed by nonlinear least-squares regression employing the Levenberg–Marquardt optimization algorithm, which iteratively minimizes the objective function defined as the sum of squared deviations between the predicted and experimentally measured dissolved oxygen concentrations.

Results and Discussion

Mathematical Model of the Process of Dissolution of Air Oxygen in Water in a Batch Reactor

The change in concentration C_2 along the packing height at a distance l with a water flow velocity W is described by the system of Equations (5), (6):

$$\frac{dC_2}{dl} = \frac{K_v}{W}(C_s - C_2) \quad (5)$$

$$\frac{dM}{dt} = V_a K_v (C_s - C_2) \quad (6)$$

Boundary conditions:

$$t = 0,\ C_1 = C_n,$$
$$l = 0,\ C_1 = C_2,$$
$$l = l_s,\ C_2 = C_s.$$

Integration of Equation (5) gives:

$$ln = \frac{C_s - C_1}{C_s - C_2} = \frac{K_v}{W} l \quad (7)$$

From Equation (7) it follows that when $C_2 \to C_s$; $l \to l_s$, the left-hand side tends to infinity. This means that in order to achieve saturation at the outlet of the packing, its height must be infinite ($l = L_s = \infty$).

From Equation (7), we determine the oxygen concentration at the outlet of the packing with height L, kg/m^3:

$$C_2 = C_s - (C_s - C_1)exp\left(-\frac{K_v}{W}L\right) \quad (8)$$

The mass balance at any time t:

$$M = M_v + M_a = V(C_1 - C_{\text{П}}) + V_a(C_2 - C_1) \quad (9)$$

where M_v and M_a are the amounts of oxygen dissolved in volumes V and V_a, respectively, kg; $\bar{C}_2$ is the average concentration of dissolved oxygen over the packing height L, kg/m^3.

$$\bar{C}_2 = \frac{1}{L}\int_0^L C_2(l)dl \quad (10)$$

Substituting C_2 (l) from Equation (8) into Equation (10), we obtain:

$$\bar{C}_2 = \frac{1}{L}\int_0^L \left[C_s - (C_s - C_1)\,exp(-\frac{K_v}{W}L)\right]dl$$
$$= C_2 - (C_s - C_1)\frac{W}{K_v L}\left[1 - exp(-\frac{W}{K_v}L)\right] \quad (11)$$

Taking into account Equation (11), the mass of oxygen M_a dissolved in the aerator packing is:

$$M_a = V_a(\overline{C_2} - C_1) = V_a(C_s - C_1)\left\{1 - \frac{W}{K_v L}\left[1 - exp\left(-\frac{K_v}{W}L\right)\right]\right\} \quad (12)$$

$$dM_a = -V_a\left\{1 - \frac{W}{K_v L}\left[1 - exp\left(-\frac{K_v}{W}L\right)\right]\right\}dC \quad (13)$$

Since the turbulence of the liquid is maximal in the working volume of the aerator V_a, it can be assumed that the actual dissolution of oxygen occurs in this volume, whereas in the liquid volume V only mixing of solutions with different oxygen concentrations occurs. Therefore, $C_1 > Cn$ when $t > 0$.

Substituting $dM = dM_a$ from Equation (13) into the left-hand side of Equation (12), and C_2 from Equation (8) into the right-hand side, we obtain:

$$V\frac{dC_1}{dt} = V_a(C_s - C_1)exp\left(-\frac{K_v}{W}L\right) \quad (14)$$

$$\frac{dC_1}{C_s - C_1} = \frac{V_a}{V}exp\left(-\frac{K_v}{W}L\right)dt \quad (15)$$

Integration of Equation (15) gives:

$$\ln\frac{C_s - C_п}{C_s - C_1} = \beta t \quad (16)$$

where $\beta = \frac{V_a}{V}exp\left(\frac{K_v}{W}L\right)$.

Since saturation is achieved at $L_s = \infty$, the curve C_2 (l) can be replaced by a straight line over a small segment L.

Then

$$\overline{C_2} = \frac{C_1 + C_2}{2},\ \overline{C_2} - C_1 = \frac{C_2 - C_1}{2} \quad (17)$$

Substituting $C_2 - C_1$ from this equation into Equation (12), we obtain:

$$M_a = \frac{1}{2}V_a(C_2 - C_1) \quad (18)$$

From Equation (8) we obtain:

$$C_2 - C_1 = (C_s - C_1)\left[1 - exp\left(-\frac{K_v}{W}L\right)\right] \quad (19)$$

Substituting this value of $C_2 - C_1$ into Equation (17), we obtain:

$$M_a = \frac{1}{2}V_a(C_s - C_1)\left[1 - exp\left(-\frac{K_v}{W}L\right)\right] \quad (20)$$

or

$$dM_a = \frac{1}{2}V_a\left[1 - exp\left(-\frac{K_v}{W}L\right)\right]dC_1 \quad (21)$$

Differentiation of the left-hand side of Equation (9), taking into account Equation (21), gives

$$dM = dM_v + dM_a = \left\{V - \frac{1}{2}V_a\left[1 - exp\left(-\frac{K_v}{W}L\right)\right]\right\}dC_1 \quad (22)$$

Substituting this value of dM into Equation (6) and integrating the result, we obtain:

$$\ln\frac{C_s - C_п}{C_s - C_1} = \frac{b}{a}K_v t \quad (23)$$

where

$$a = V - \frac{1}{2}V_a\left[1 - exp\left(-\frac{K_v}{W}L\right)\right],\ b = V_a\,exp\left(-\frac{K_v}{W}L\right)$$

The volumetric mass transfer coefficient K_v enters Equation (23) in an implicit form; therefore, it can be determined from experimental data using a computer.

Let us consider the second approach to solving this problem by tracking the change in the mass M_a and concentration C_1 over n cycles of water circulation with time $t = nl/W$.

The concentration C_1 after the first cycle:

$$C_1' = C_п + \frac{M_1}{V} \quad (24)$$

The mass of dissolved oxygen after n cycles from Equation (20):

$$M_a = m(C_s - C_1) \quad (25)$$

where $m = V_a\left[1 - exp\left(-\frac{K_v}{W}L\right)\right]$.

Table 2 presents the results of summing the mass M_a and concentration C_1 according to Equations (24) and (25) at time t as the number of cycles n increases.

From the table we obtain:

$$M_a = M_1 + M_2 + \cdots + M_n = m(C_s - C_п) + m(C_s - C_п)\left(1 - \frac{m}{V}\right) + + \cdots + m(C_s - C_п)\left(1 - \frac{m}{V}\right)^{n-1} = m(C_s - C_п)\frac{1 - (1-\varepsilon)^n}{\varepsilon} \quad (26)$$

where $\varepsilon = \frac{m}{V} = \frac{1}{2}\frac{V_a}{V}\left[1 - exp\left(-\frac{K_v}{W}L\right)\right]$

$$C_1 = C_п + \frac{M_a}{V} = C_п + (C_s - C_п)[1 - (1 - \varepsilon)^n] \quad (27)$$

In this case, the “net contact time” of oxygen with water is:

$$t_n = \frac{nL}{W} \quad (28)$$

Obviously, the current time required to complete one cycle is

Table 2. Change in the current mass M_a and oxygen concentration C_1 with an increasing number of dissolution cycles n.

n	Time, *t*	Current mass, M_a	Current concentration, C_1
1	$t_1 = \frac{L}{W}$	$M_1 = m(C_s - C_{\text{п}})$	$C_1' = C_{\text{п}} = \frac{M_1}{V}$
2	$t_1 = 2\frac{L}{W}$	$M_1 = m(C_s - C_1') = m(C_s - C_{\text{п}})\left(1 - \frac{m}{V}\right)$	$C_1'' = C_1' + \frac{M_2}{V} = C_{\text{п}} = \frac{M_1 + M_2}{V}$
3	$t_1 = 3\frac{L}{W}$	$M_1 = m(C_s - C_1'') = m(C_s - C_{\text{п}})\left(1 - \frac{m}{V}\right)^2$	$C_1''' = C_1'' + \frac{M_1 + M_2 + M_3}{V}$
n	$t_1 = n\frac{L}{W}$	$M_n = m(C_s - C_{\text{п}} - \frac{M_1 + M_2 + \cdots + M_{n-1}}{V}) = m(C_s - C_{\text{п}})\left(1 - \frac{m}{V}\right)^{n-1}$	$C_1 = C_{\text{п}} + \frac{M_1 + M_2 + \cdots + M_n}{V}$

$$t_a = {}^{L}/_{W_a} \tag{29}$$

where $t_a = {}^{L}/_{W_a}$ – time of water residence in the aerator packing; $t_2 = {}^{L}/_{W}$ – time of water residence in the apparatus before reaching the packing; W_a, W – average velocities of water movement in the aerator packing and after it.

Then the total current time is

$$t = nt_1 = nL\left(\frac{1}{W_a} + \frac{1}{W}\right) \tag{30}$$

From the continuity equation of the flow, it follows that

$$Q = W_a f_a = W(f - f_a)$$

where Q – water circulation capacity, m³/s; f, f_a – cross-sectional areas of the reactor and aerator, respectively:

$$f = \frac{\pi d^2}{4}, \qquad f_a = \frac{\pi d_{\text{н}}^2}{4}$$

from which

$$W = W_a \frac{f_a}{f - f_a} = W_a \frac{d_{\text{н}}^2}{d^2 - d_{\text{н}}^2} \tag{31}$$

Taking into account Equation (29), Expression (30) takes the form

$$t = nL\left\{\frac{1}{W_a} + \frac{1}{W_a}\left[\left(\frac{d}{d_{\text{н}}}\right) - 1\right]\right\} = \frac{nL}{W_a}\left(\frac{d}{d_{\text{н}}}\right)^2 \tag{32}$$

From Equation (32) it follows that

$$n = \frac{W_a}{L}\left(\frac{d_{\text{н}}}{d}\right)^2 t = \psi t \tag{33}$$

Substituting the value of n from Equation (32) into Equation (27), we obtain the final result:

$$C_1 = C_{\text{п}} + (C_s - C_{\text{п}})\left[1 - (1 - \varepsilon)^{\psi t}\right] \tag{34}$$

where $\psi = \frac{W_a}{L}\left(\frac{d_{\text{н}}}{d}\right)^2$

$$\text{Or } \frac{C_1 - C_{\text{п}}}{C_s - C_{\text{п}}} = 1 - (1 - \varepsilon)^{\psi t} \tag{35}$$

This equation, like Equation (23), requires processing of experimental data using a computer to determine K_v, since the function appears in an implicit form.

The third approach to solving the problem is based on the same conclusion that saturation of the solution with oxygen is achieved when $L_s = \infty$. Therefore, it can be assumed that over a small segment L, the concentration C_2 will not differ significantly from C_1. In this case, the driving force $C_s - C_2$, which appears in Equation (6), can, with some approximation, be replaced by $C_s - C_1$:

$$\frac{dM}{dT} = V_a K(C_s - C_1)_{\text{v}} \tag{36}$$

From Equation (9), when $M_v = 0$ due to the practical absence of oxygen dissolution (according to the reasoning after relation (13)), we obtain $dM = VdC_1$.

Substituting this value of dM into the left-hand side of Equation (36) and integrating the res ult, we obtain:

$$\ln\frac{C_s - C_{\text{п}}}{C_s - C_1} = \frac{V_a}{V} K_{\text{v}} t \tag{37}$$

This equation of a straight line makes it possible to easily determine K_v by processing experimental data using the tangent of the slope of the line. In contrast to known relations, dependence Equation (37) takes into account the influence of the ratio V_a/V on the kinetics of oxygen dissolution.

The relations obtained above have physical meaning as long as the air passing through the packing contains oxygen. At an air flow rate G, m³/s, and an initial oxygen concentration Y_n, kg/m³, the oxygen concentration

at the outlet of the packing decreases to Y_2 according to the mass balance:

$$M_a = G(Y_{\text{П}} - Y_2)t \tag{38}$$

Substituting into this equation M_a from Equation (20) and t from Equation (37), we obtain:

$$Y_2 = Y_{\text{П}} - \frac{M_a}{Gt} = Y_{\text{П}} - \frac{\frac{1}{2}K_{\text{V}}V_a^2\left[1-exp\left(-\frac{K_{\text{V}}}{W}L\right)\right]}{GV\ln\frac{C_S-C_{\text{П}}}{C_S-C_1}} \tag{39}$$

Equation (39) makes it possible to estimate the oxygen utilization coefficient of air.

$$\eta = \frac{Y_{\text{П}}-Y_2}{Y_{\text{П}}} = 1 - \frac{Y_2}{Y_{\text{П}}} \tag{40}$$

Model Sensitivity and Physical Discussion

A sensitivity analysis was conducted to evaluate the influence of the ratio V_a/V on the overall performance of the aeration system. The obtained results demonstrate that increasing the active aeration volume V_a or the specific gas-liquid interfacial area σ significantly accelerates oxygen transfer, resulting in an exponential reduction in the time required to reach the saturation concentration C_s. Physically, this behavior is explained by the enlargement of the effective mass-transfer region, which increases the gas–liquid contact area and shortens the characteristic diffusion path. Consequently, the proposed model confirms that both reactor geometry and the extent of the localized active mass-transfer zone are key parameters governing oxygen dissolution kinetics.

Comparison with Prior Studies

The proposed mathematical model (Equation (34)) was compared with conventional oxygen transfer models commonly applied in wastewater treatment research. Unlike classical approaches, such as those proposed by Downing et al. [23, 24], where the volumetric oxygen mass-transfer coefficient K_La is assumed to be spatially uniform throughout the reactor, the present model explicitly incorporates the spatial heterogeneity of the mass-transfer process. In particular, the oxygen dissolution kinetics are directly related to the reactor geometry through the generalized kinetic parameter $\psi = \frac{W_a}{L}\left(\frac{d_{\text{н}}}{d}\right)^2$, which accounts for the circulation characteristics of the liquid and the dimensions of the active aeration zone. This formulation enables the model to describe localized oxygen transfer occurring in the vicinity of packing elements or diffusers rather than assuming ideal mixing throughout the entire reactor volume. Consequently, the proposed approach provides a more physically realistic representation of oxygen dissolution in packed and pneumatic aeration systems.

Validation of the Developed Model

To verify the adequacy of the proposed mathematical formulation (Equation (34)), model predictions were validated against independent experimental data on oxygen dissolution kinetics in packed bubble columns reported by Akita and Yagi [26], as well as Henkel [28]. A comparison between the predicted oxygen concentration profiles $C_l = f(t)$ and the published experimental data demonstrated good agreement over a wide range of operating conditions, indicating that the proposed model adequately reproduces the observed oxygen dissolution kinetics.

The validation results support the underlying assumption that oxygen transfer is predominantly localized within the active aeration volume V_a, while the remaining reactor volume mainly contributes to macroscopic mixing. Furthermore, the predicted oxygen utilization efficiency (η, Equation (40)) is consistent with trends reported in previous studies by Drewnowski et al. [2] and Gu et al. [19], suggesting that minimizing inactive aeration zones may contribute to improved oxygen transfer efficiency and lower energy demand.

Conclusions

The theoretical analysis and mathematical modeling of the aeration process made it possible to determine the main mechanisms governing oxygen transfer from the gas phase into the aqueous medium. The rate of oxygen dissolution was shown to be the limiting step in the biochemical oxidation of organic compounds and is primarily determined by mass transfer characteristics at the gas-liquid interface. Key factors influencing this process include hydrodynamic flow conditions, bubble size distribution, temperature, pressure, and aerator design.

A comparative analysis of different modeling approaches showed that the proposed improved mathematical model accounts for the heterogeneity of the mass transfer process by dividing the total reactor volume into a working volume and a residual volume. This approach provides a more realistic representation of actual aeration conditions. In contrast to classical formulations based on Fick's diffusion law, the proposed model allows consideration of local turbulence zones as well as the temporal and spatial variation of dissolved oxygen concentration along the height of the packing layer.

The derived relationships for determining the volumetric mass transfer coefficient (K_{v}) indicate that increasing the specific interfacial area and enhancing turbulence intensity significantly improves oxygen transfer efficiency. However, excessive aeration intensification may lead to increased energy consumption, which necessitates optimization of air supply regimes.

Thus, the obtained results provide a scientific basis for further optimization of fine-bubble and packed aeration systems in biological reactors. The proposed model can be applied to predict oxygen dissolution kinetics under real wastewater treatment plant conditions and to design energy-efficient aeration systems.

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Conflict of Interest

The authors declare no conflict of interest.

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