

ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

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Hierarchy of Mathematical Models for Calculating Aeration Tanks

Purpose. Aeration tanks are widely used in wastewater treatment. Complex processes of mass transfer of impurities, activated sludge, and oxygen occur in an aeration tank. Therefore, it is very important to have specialized mathematical models that allow for a comprehensive consideration of complex multifactorial processes in aeration tanks. The aim of this work is to identify the advantages and disadvantages of mathematical models used to evaluate the efficiency of water treatment in aeration tanks, as well as to develop numerical models for analyzing the operation of aeration tanks. **Methodology.** System analysis methods used in accordance with hydrodynamics and mass transfer models in wastewater treatment tasks in aeration tanks. The solution of the hydrodynamics problem is based on the use of potential flow model. Mass transfer equations that take into account convective and diffusive transport are used to describe the process of impurity movement in an aeration tank. The development of numerical models is based on the use of the method of splitting modeling equations. **Findings.** Numerical models for calculating the efficiency of water purification in an aeration tank have been developed and implemented in software. These models are a modern tool for mathematical modeling of complex, multifactorial mass transfer processes in aeration tanks. **Originality.** Based on a systematic analysis, the advantages and disadvantages of the models used to analyze the efficiency of aeration tanks have been identified. The construction of effective numerical models for calculating hydrodynamics and mass transfer in aeration tanks has been considered. **Practical value.** The proposed numerical models of hydrodynamics and mass transfer in aeration tanks can be useful for rapid assessment of the efficiency of wastewater treatment in aeration tanks.

Keywords: aeration tank; water treatment; numerical modeling; hydrodynamics; mass transfer; treatment facilities

Introduction

Determining the efficiency of wastewater treatment in aeration tanks plays a particularly important role in assessing the efficiency of water treatment throughout the entire technological line at aeration stations [2–5]. The complexity of the wastewater treatment process in aeration tanks (the impact on the treatment process of oxygen concentration in different parts of the facility, activated sludge concentration, wastewater flow velocity, etc.) significantly complicates the process of constructing mathematical models for calculating aeration tanks. Therefore, in practice, mathematical models with varying degrees of simplification are used [6–10].

An analysis of sources devoted to the development of mathematical models of aeration tank operation shows that the most effective approach for theoretical analysis of aeration tank operation is the use of numerical models [1, 7–10].

Purpose

To identify the advantages and disadvantages of mathematical models used to evaluate the efficiency of water purification in aeration tanks: to develop numerical models for analyzing the operation of aeration tank.

Methodology

In this work, system analysis methods and numerical modeling were used to evaluate the efficiency of aeration tanks.

In practice, empirical models are widely used to solve various engineering problems related to evaluating the efficiency of different treatment facilities. With regard to problems related to evaluating the efficiency of aeration tanks, an example of such a model is the following empirical model, which determines the duration of aeration [4]:

$$t = \frac{L_a - L_t}{a \cdot (1 - S_l) \rho},$$

where L_a is BOC_t – wastewater entering the facility; L_t is BOC_t – wastewater leaving the facility S_l – ash content of activated sludge; ρ – oxidation rate; a – activated sludge dose.

Another approach is to use first-order differential equations to describe (with varying degrees of detail) the reactions in the aeration tank (Bertoks):

1) first-order reaction:

$$\frac{dS}{dt} = k_0 XS;$$

2) zero-order reaction:

$$\frac{dS}{dt} = k_1 X;$$

3) mixed-order reaction:

$$\frac{dS}{dt} = kXS,$$

where X – concentration of microorganisms; k , k_0 , k_1 – empirical parameters; S – substrate concentration.

Regarding the models considered, the following should be noted: the models make it possible to perform estimates without the aid of a computer, require a small amount of «input» information, and do not require highly qualified specialists for their application. However, these models do not take into account the hydrodynamics of the flow in the aeration tank and the distribution of active sludge, oxygen, and impurities in the structure.

Balance models are more effective. To describe the wastewater treatment process in an aeration tank, they look like this [10]:

$$\begin{aligned} W \cdot dX &= dt \cdot Q_x(t) \cdot X_{in}(t) - \\ &- dt \cdot Q_x(t) \cdot X + dt \cdot \mu \cdot W \cdot X - \\ &- dt \cdot K_d \cdot W \cdot X ; (1) \end{aligned}$$

$$\begin{aligned} W \cdot dS &= dt \cdot Q_s(t) \cdot S_{in} - \\ &- dt \cdot Q_s(t) \cdot S(t) - dt \cdot \frac{\mu}{Y} \cdot W \cdot X ; (2) \end{aligned}$$

$$\mu = \mu_{\max} \cdot \frac{S}{S + K_s}, \quad (3)$$

where K_s is the *Monod* coefficient; μ_{\max} is the coefficient; $X_{in}(t)$ is the concentration of activated sludge entering the aeration tank; $S_{in}(t)$ is the concentration of substrate entering the facility; W is the reactor volume; $Q_s(t)$ is the substrate flow rate; $Q_x(t)$ is active sludge flow rate; K_d – active sludge decay coefficient; t – time; X – concentration of active sludge in the reactor; S – substrate concentration in the structure; μ – coefficient; Y – parameter.

Balance models (1)–(3) have the following advantages:

1. They take into account a significant number of factors that influence the wastewater treatment process in an aeration tank.

2. Under certain assumptions, they allow for an analytical solution, i.e., an exact solution to the problem.

3. The models can be used to quickly calculate the efficiency of water treatment in an aeration tank.

4. The models can be used to «tune» more powerful, numerical models.

However, these models also have certain disadvantages:

1. The practical application of models requires their solution on a computer.

2. The application of models requires information about certain constants, which is difficult to obtain.

For rapid assessment of oxygen concentration in an aeration tank, 2D models of hydrodynamics and mass transfer can be used [1]:

$$\begin{aligned} \frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} &= \\ &= \frac{\partial}{\partial x} \left(\mu_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_y \frac{\partial C}{\partial y} \right) + \\ &+ \sum Q_i \delta(x - x_i) \delta(y - y_i); (4) \end{aligned}$$

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} = 0; \quad (5) \quad \frac{\partial S}{\partial t} + \frac{\partial uS}{\partial x} + \frac{\partial vS}{\partial y} + \frac{\partial wS}{\partial z} =$$

$$u = \frac{\partial P}{\partial x}, v = \frac{\partial P}{\partial y}; \quad = \frac{\partial}{\partial x} \left(\mu_x \frac{\partial S}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_y \frac{\partial S}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu_z \frac{\partial S}{\partial z} \right);$$

$$\frac{dC}{dt} = K_{La}(C_s - C) - r, \quad (6) \quad \frac{\partial X}{\partial t} + \frac{\partial uX}{\partial x} + \frac{\partial vX}{\partial y} + \frac{\partial wX}{\partial z} =$$

$$= \frac{\partial}{\partial x} \left(\mu_x \frac{\partial X}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_y \frac{\partial X}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu_z \frac{\partial X}{\partial z} \right);$$

where C – oxygen concentration in wastewater; K_{La} – mass transfer coefficient [11, 12]; C_s – maximum value of dissolved oxygen concentration in wastewater; r is the oxygen consumption rate by activated sludge [3]; P – velocity potential; u, v – components of the wastewater flow velocity in the aeration tank; t – time; μ_x, μ_y – diffusion coefficients.

Let us consider the boundary conditions for the modeling equations:

1. At the inlet to the facility: $C = C_{in}$,

where C_{in} is the oxygen concentration in the wastewater stream at the inlet to the aeration tank.

2. At the outlet of the facility: $C(i, j) = C(i+1, j)$, where $C(i+1, j)$ is the oxygen concentration value in the last cell; $C(i, j)$ is the oxygen concentration in the previous cell.

3. On solid surfaces:

$$\frac{\partial C}{\partial n} = 0,$$

where n is the unit normal to the surface.

Initial conditions: at $t = 0$: $C = C_0$, where C_0 is the known oxygen concentration.

For the hydrodynamics equation (5), the boundary conditions are given in [1].

This two-dimensional model has the following advantages:

1. It takes into account the hydrodynamics of flow in the structure.

2. It allows determining the oxygen concentration in different parts of the aeration tank.

3. It can be used for rapid assessment of the oxygen regime in the aeration tank.

However, the model has the following disadvantages:

1. It allows determining the hydrodynamics of the flow only in a two-dimensional representation.

2. It allows determining the oxygen concentration only in a two-dimensional representation.

More powerful are 3D models of hydrodynamics and mass transfer in the aeration tank:

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \frac{\partial^2 P}{\partial z^2} = 0;$$

$$u = \frac{\partial P}{\partial x}, v = \frac{\partial P}{\partial y}, w = \frac{\partial P}{\partial z};$$

$$\frac{dX}{dt} = \mu X - K_d X;$$

$$\frac{dS}{dt} = -\frac{\mu}{Y} X;$$

$$\mu = \mu_{\max} \cdot \frac{S}{S + K_s}.$$

where K_d – active sludge decay coefficient; t – time; $X(x, y, z, t)$ – concentration of active sludge in the bioreactor; $S(x, y, z, t)$ – concentration of substrate in the bioreactor; $\mu_{x,y,z}(t), \mu_{\max}, Y, K_s$ – parameters; $u(x, y, z), v(x, y, z), w(x, y, z)$ – components of the water flow velocity in the bioreactor in the direction of the x, y, z axes, respectively; μ_x, μ_y, μ_z – diffusion coefficients in the direction of the x, y, z axes, respectively.

The boundary conditions for these equations are similar to the boundary conditions for two-dimensional equations.

The three-dimensional model of hydrodynamics and mass transfer has the following advantages:

1. It allows determining the velocity field in the structure and the concentration in three dimensions.

2. The concentrations of activated sludge and impurities are taken into account for the analysis of treatment efficiency.

3. The disadvantages of the model are that the hydrodynamics model does not take into account the viscosity of the wastewater flow in the aeration tank.

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Two-dimensional and three-dimensional equations only allow for numerical solutions. Thus, to integrate a two-dimensional mass transfer equation, the following splitting is performed:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} = 0;$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(\mu_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_y \frac{\partial C}{\partial y} \right);$$

$$\frac{\partial C}{\partial t} = \sum Q_i \delta(x - x_i) \delta(y - y_i).$$

Next, finite difference equations are constructed in the following form:

– step №1 ($k = n+1/2$):

$$\frac{C_{i,j}^k - C_{i,j}^n}{\Delta t} + L_x^+ C^k + L_y^+ C^k = 0;$$

– step №2 ($k = n+1/2$):

$$\frac{C_{i,j}^{n+1} - C_{i,j}^k}{\Delta t} + L_x^- C^{n+1} + L_y^- C^{n+1} = 0.$$

The form of the operators $L_x^+, L_x^-, L_y^+, L_y^-$ is discussed in [1].

The second splitting equation is integrated as follows («conditional approximation scheme»):

$$\frac{C_{i,j}^{n+\frac{1}{2}} - C_{i,j}^n}{\Delta t} = \left[\mu_x \frac{-C_{i,j}^{n+\frac{1}{2}} + C_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} \right] +$$

$$+ \left[\mu_y \frac{-C_{i,j}^{n+\frac{1}{2}} + C_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2} \right],$$

$$\frac{C_{pi,j}^{n+1} - C_{i,j}^{n+\frac{1}{2}}}{\Delta t} = \left[\mu_x \frac{C_{i+1,j}^{n+1} - C_{i,j}^{n+1}}{\Delta x^2} \right] +$$

$$+ \left[\mu_y \frac{C_{i,j+1}^{n+1} - C_{i,j}^{n+1}}{\Delta y^2} \right].$$

Numerical integration for the velocity potential is performed using the «conditional approximation scheme».

The values of the components of the water flow velocity vector in the aerotank are determined as follows:

$$u = \frac{P_{i+1,j} - P_{i,j}}{\Delta x}, v = \frac{P_{i,j+1} - P_{i,j}}{\Delta y}.$$

The three-dimensional equation for the velocity potential is written as follows:

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \frac{\partial^2 P}{\partial z^2}$$

where t is the fictitious time.

Next, Samarsky's method is used for numerical integration of the equation. The two-step splitting scheme has the following form:

$$\frac{P_{i,j,k}^{n+1/2} - P_{i,j,k}^n}{0,5\Delta t} = \frac{P_{i+1,j,k}^n - P_{i,j,k}^n}{\Delta x^2} + \frac{-P_{i,j,k}^{n+1/2} + P_{i-1,j,k}^{n+1/2}}{\Delta x^2} +$$

$$+ \frac{P_{i,j+1,k}^n - P_{i,j,k}^n}{\Delta y^2} + \frac{-P_{i,j,k}^{n+1/2} + P_{i,j-1,k}^{n+1/2}}{\Delta y^2} +$$

$$+ \frac{P_{i,j,k+1}^n - P_{i,j,k}^n}{\Delta z^2} + \frac{-P_{i,j,k}^{n+1/2} + P_{i,j,k-1}^{n+1/2}}{\Delta z^2},$$

$$\frac{P_{i,j,k}^{n+1} - P_{i,j,k}^{n+1/2}}{0,5\Delta t} = \frac{P_{i+1,j,k}^{n+1} - P_{i,j,k}^{n+1}}{\Delta x^2} + \frac{-P_{i,j,k}^{n+1/2} + P_{i-1,j,k}^{n+1/2}}{\Delta x^2} +$$

$$+ \frac{P_{i,j+1,k}^{n+1} - P_{i,j,k}^{n+1}}{\Delta y^2} + \frac{-P_{i,j,k}^{n+1/2} + P_{i,j-1,k}^{n+1/2}}{\Delta y^2} +$$

$$+ \frac{P_{i,j,k+1}^{n+1} - P_{i,j,k}^{n+1}}{\Delta z^2} + \frac{-P_{i,j,k}^{n+1/2} + P_{i,j,k-1}^{n+1/2}}{\Delta z^2}.$$

The calculation based on the difference equations ends when the following condition is met:

$$|P_{i,j,k}^{n+1} - P_{i,j,k}^n| \leq \varepsilon,$$

where ε – small number; n – iteration number (number of steps of time).

The boundary condition of no flow on solid walls is implemented by using fictitious difference cells.

For numerical integration of the three-dimensional mass transfer equation, the splitting scheme is used as for the two-dimensional case.

The solution of the initial equation is broken down into a series of steps:

– first step ($k = 1/4$):

$$\frac{C_{ijk}^{n+k} - C_{ijk}^n}{\Delta t} + \frac{1}{2} (L_x^+ C^k + L_y^+ C^k + L_z^+ C^k) + \frac{\sigma}{2} C_{ijk}^n = 0; \quad (7)$$

– second step ($k = n+1/2$; $c = n+1/4$):

$$\frac{C_{ijk}^k - C_{ijk}^c}{\Delta t} + \frac{1}{2} (L_x^- C^k + L_y^- C^k + L_z^- C^k) + \frac{\sigma}{2} C_{ij}^k = 0; \quad (8)$$

– third step ($k = n+3/4$; $c = n+1/2$):

$$\frac{C_{ijk}^k - C_{ijk}^c}{\Delta t} = \frac{1}{2} \begin{pmatrix} M_{xx}^- C^c + M_{xx}^+ C^k + \\ + M_{yy}^- C^c + M_{yy}^+ C^k + \\ + M_{zz}^- C^c + M_{zz}^+ C^k \end{pmatrix}; \quad (9)$$

– fourth step ($k=n+1$; $c=n+3/4$):

$$\frac{C_{ijk}^k - C_{ijk}^c}{\Delta t} = \frac{1}{2} \begin{pmatrix} M_{xx}^- C^k + M_{xx}^+ C^c + \\ + M_{yy}^- C^k + M_{yy}^+ C^c + \\ + M_{zz}^- C^k + M_{zz}^+ C^c \end{pmatrix}. \quad (10)$$

The form of the operators L_x^+ , L_x^- , L_y^+ , L_y^- , M_{xx}^+ , M_{xx}^- , ... is discussed in [1].

A distinctive feature of all developed numerical models is that the calculation of unknown quantities is performed at each step of the decomposition using explicit formulas.

Findings

Numerical models have been developed to simulate the operation of an aeration tank. The models take into account convection and diffusion processes. The basis for the development of numerical models is the splitting method, which allows the solution of the problem to be reduced to a sequential solution of an equation that has a simpler form.

Originality and practical value

Based on a systematic analysis, the advantages and disadvantages of the models used to analyze the efficiency of aeration tanks have been identified. The development of effective numerical models for calculating hydrodynamics and mass transfer in aeration tanks has been considered. The proposed numerical models of hydrodynamics and mass transfer in aeration tanks can be useful for rapid assessment of the efficiency of wastewater treatment in aeration tanks.

Conclusions

The development of 2D and 3D numerical models of aeration tank operation was considered. These models can be used for operational analysis of water purification, taking into account the hydrodynamics of flow in the treatment plant.

In the future, this scientific direction should be developed in the field of 3D CFD model development for analyzing the complex operation of an «aeration tank+ secondary clarifier».

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Ієрархія математичних моделей для розрахунку аеротенків

Мета. Аеротенки мають широке застосування при очистці стічних вод. Процес очищення стічних вод в аеротенку має дуже складний характер з точки зору математичного опису. В аеротенку відбуваються складні процеси масопереносу домішки, активного мулу, кисню. На процес очистки води в аеротенку суттєво впливає гідродинаміка течії стічних вод, місце подачі кисню, розмір повітряних бульбашок, наявність різного роду перешкод в очисній споруді. Тому для практики дуже важливо мати спеціалізовані математичні моделі, що дозволяють комплексно враховувати складні багатофакторні процеси в аеротенках. Метою роботи є визначення переваг та недоліків математичних моделей, що використовуються для оцінювання ефективності очистки води в аеротенках, а також розробка чисельних моделей для аналізу роботи аеротенків. **Методика.** Методи системного аналізу, використані відповідно до моделей гідродинаміки та масопереносу в задачах очистки стічних вод в аеротенках. Рішення задачі гідродинаміки базується на використанні моделі потенціальної течії. Для опису процесу руху домішки в аеротенку використовуються рівняння масопереносу, що враховують конвективний та дифузійний перенос. Побудова чисельних моделей базується на використанні методу розщеплення моделюючих рівнянь. **Результати.** Розроблено та здійснено програмну реалізацію чисельних моделей розрахунку ефективності очистки води в аеротенку, що являють собою сучасний інструмент математичного моделювання складних, багатофакторних процесів масопереносу в аеротенках. **Наукова новизна.** На основі системного аналізу визначені недоліки та переваги моделей, що використовуються для аналізу ефективності роботи аеротенків. Розглянуто побудову ефективних чисельних моделей для розрахунку гідродинаміки та масопереносу у аеротенках. **Практична значимість.** Запропоновані чисельні моделі гідродинаміки та масопереносу в аеротенках можуть бути корисними для експрес оцінювання ефективності очистки стічних вод в аеротенках.

Ключові слова: аеротенк; очистка води; чисельне моделювання; гідродинаміка; масоперенос; очисні споруди

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