Computer Simulation of Biological Wastewater Treatment Processes in Aerotanks with Plates

**Purpose.** Efficiency determination of the aeration tank at the stage of design or reconstruction of bioreactors in which biological wastewater treatment is carried out requires the use of special mathematical models and calculation methods. The main purpose of the article is to develop CFD models for evaluating the operation efficiency of aeration tanks.

**Methodology.** A numerical model has been developed for the computer calculation of the biological wastewater treatment process in aerotanks, taking into account hydrodynamics. The model is based on two-level mass conservation equations for the substrate and activated sludge and the velocity potential equation. The process of biological transformation of the substrate is calculated based on the Monod model. For the numerical integration of the mass transfer equations of activated sludge and substrate, the alternating-triangular difference splitting scheme is used. In this case, the basic equations are divided into two equations of a more simplified form. For the numerical integration of the equations for the velocity potential, it is split into two one-dimensional equations. Further, each equation is solved according to explicit scheme. For the numerical integration of equations that describe the process of substrate transformation based on the Monod model, the Euler method is used.

**Findings.** The software implementation of the constructed numerical model has been carried out. The results of a computational experiment on the study of the wastewater treatment process in an aeration tank with plates are presented. This leads to the conclusion that the quality control of wastewater treatment in aeration tanks is possible with the help of plates.

**Originality.** A multivariate CFD model has been developed, which makes it possible to quickly assess the efficiency of the aeration tank. A feature of the model is the ability to evaluate the operation of the aeration tank, taking into account its geometric shape and location of additional plates in the construction. **Practical value.** The constructed numerical model can be used during calculations in the case of designing aeration tanks, or in determining the efficiency of wastewater treatment under new operating conditions.

**Keywords:** water purification; numerical modeling; aerotank; model Mono; CFD models; biological cleaning; wastewater; activated sludge; concentration of pollutants
Introduction

Biological treatment is one of the most effective methods of wastewater treatment [3, 4, 6]. Efficiency determination of this treatment at the stage of design or reconstruction of bioreactors, in which this method of wastewater treatment is carried out, requires the use of special mathematical models and calculation methods. Moreover, these theoretical calculation methods are the main toolkit, since a physical experiment in the field of biological treatment always requires a long time and expensive equipment. To date, a significant number of mathematical models have been developed that allow, with different approximation degrees, determining the bioreactor efficiency. But the existing mathematical models (empirical, balance, analytical) [1–5, 7–17] do not take into account a number of important parameters affecting the efficiency of bioreactors (their geometric shapes and design features, movement hydrodynamics activated sludge and substrate in them, the presence of additional elements, various modes of operation), or require significant time when implemented on computers (CFD-models). Therefore, the development of mathematical models for assessing the efficiency of biological reactors, which allow taking into account these important factors and quickly determining the values of the parameters necessary for the designer, is an important scientific task.

Purpose

This work provides for the development of a numerical model to assess the efficiency of wastewater treatment in aerotanks. The task is to create a multifactorial computer model that makes it possible to quickly calculate the process of biological wastewater treatment, taking into account the geometric shape of the bioreactor.

Methodology

When building a model, we will take into account the following factors:

– the geometric shapes of aerotank;
– the process of changing the substrate concentration in aerotanks over time;
– the process of changing the of activated sludge concentration in aerotanks over time;
– the presence of additional elements in aerotanks.

The material balance equations for the substrate and activated sludge in the reactor based on the Monod model has the following form:

\[
\frac{\partial X}{\partial t} + \frac{\partial uX}{\partial x} + \frac{\partial vX}{\partial y} = \frac{\partial}{\partial x} \left( \mu_x \frac{\partial X}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_y \frac{\partial X}{\partial y} \right) = 0; \quad (1)
\]

\[
\frac{\partial S}{\partial t} + \frac{\partial uS}{\partial x} + \frac{\partial vS}{\partial y} = \frac{\partial}{\partial x} \left( \mu_x \frac{\partial S}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_y \frac{\partial S}{\partial y} \right) = 0; \quad (2)
\]

\[
\frac{dX}{dt} = \mu X - K_d X; \quad (3)
\]

\[
\frac{dS}{dt} = -\frac{\mu}{Y} X; \quad (4)
\]

\[
\mu = \mu_{\text{max}} \cdot \frac{S}{S + K_s}; \quad (5)
\]

where \( K_d \) – activated sludge measurement coefficient; \( t \) – time; \( X \) – averaged concentration of activated sludge in the bioreactor; \( S \) – averaged concentration of substrate in the bioreactor; \( \mu \) – diffusion coefficient; \( Y \) – parameter in the Monod model; \( u, v \) – components of the water flow velocity in the bioreactor in the direction of the \( x \), \( y \) axes, respectively; \( \mu = (\mu_x, \mu_y) \) – components of the diffusion coefficients at the considered plane point in the \( x, y \) direction.

The averaged concentration of activated sludge and substrate over the width of the bioreactor is determined as follows:

\[
X(x,z) = \frac{1}{B} \int X(x,y,z)dy ;
\]

\[
S(x,z) = \frac{1}{B} \int S(x,y,z)dy .
\]

Equations (1) and (2) describe the change in the concentration of activated sludge and substrate over time in the aeration tank due to movement.
ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

and diffusion. Equations (3) – (5) describe the process of substrate consumption by activated sludge.

The limiting conditions for modeling equations are as follows:

1) at the inlet, the boundary condition is:

\[ S = S_0, \quad X = X_0, \]

where \( S_0, X_0 \) – known concentrations of substrate and sludge, respectively;

2) boundary conditions at the exit from the bioreactor:

\[ S(i+1,j) = S(i,j); \quad X(i+1,j) = X(i,j), \]

where \( S(i+1,j), X(i+1,j) \) – concentrations in the last computational cell; \( S(i,j), X(i,j) \) – concentrations in the previous computation cell;

3) on rigid surface:

\[ \frac{\partial X}{\partial n} = 0; \quad \frac{\partial S}{\partial n} = 0, \]

where \( n \) – unit normal to the surface.

The initial conditions are as follows: at \( t=0 \)

\( X=X_0, \quad S=S_0. \)

To solve the hydrodynamics problem – determining the components field of the flow velocity vector in the aerotank – a model of potential motion was used [8, 29]:

\[ \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} = 0, \quad (6) \]

where \( P \) – velocity potential.

Knowing the potential field, the values of the components of the flow velocity vector in the bioreactor are determined by the formulas [8, 9, 14]:

\[ u = \frac{\partial P}{\partial x}, \quad v = \frac{\partial P}{\partial y}. \]

Let us consider the difference in dependencies, with the help of which the numerical integration of the modeling equations is carried out. Thus, to calculate the substrate concentration in the bioreactor, an alternating-triangular two-step splitting scheme is used [2]. At the first stage of splitting, the calculated dependence has the form:

\[ S^{n+1}_{ij} = S^n_{ij} - \frac{u_{i+1,j}^+ S^n_{i,j} + u_{i-1,j}^+ S^{n+1}_{i-1,j}}{Vx} + \frac{Vt\mu}{2Vx^2} \left( -S^n_{ij} + S^{n+1}_{i+1,j} \right). \quad (7) \]

At the second step of splitting, the calculated dependence is as follows:

\[ S^{n+1}_{ij} = S^n_{ij} - \frac{u_{i+1,j}^+ S^{n+1}_{i,j} - u_{i,j}^+ S^n_{i,j}}{Vx} + \frac{Vt\mu}{2Vx^2} \left( -S^{n+1}_{ij} + S^n_{i+1,j} \right), \quad (8) \]

where \( u^+ = \frac{u + |\mu|}{2}, \quad u^- = \frac{u - |\mu|}{2}. \)

For the second equation, the difference schemes have the form:

\[ \begin{align*}
S^{n+1}_{ij} &= S^n_{ij} - \frac{v_{i+1,j}^+ S^{n+1}_{i+1,j} - v_{i,j}^+ S^n_{i,j}}{Vy} + \frac{Vt\mu}{2Vy^2} \left( -S^n_{ij} + S^{n+1}_{i,j+1} \right), \quad (9) \\
S^{n+1}_{ij} &= S^n_{ij} - \frac{v_{i+1,j}^+ S^{n+1}_{i,j} - v_{i,j}^+ S^n_{i,j}}{Vy} + \frac{Vt\mu}{2Vy^2} \left( -S^{n+1}_{ij} + S^n_{i+1,j} \right). \quad (10)
\end{align*} \]

where \( v^+ = \frac{v + |\mu|}{2}, \quad v^- = \frac{v - |\mu|}{2}. \)

To construct a local one-dimensional scheme for solving equation (6), we perform the following transformations. First, let us represent this equation in the form:
\[
\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2},
\]
(11)

where \( t \) – fictitious time.

Further, we divide equation (11) as follows:

\[
\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2};
\]
(12)

\[
\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial y^2}.
\]
(13)

Equation (12) describes the change in the value of \( P \) in the direction of the \( X \) axis, and equation (13) describes the change in the \( Y \) direction.

The calculated dependencies (Richardson’s method) for determining the unknown value of \( P \) based on equation (12) have the form:

\[
P_{i,j}^{n+1} = P_{i,j}^n + V_t \frac{P_{i+1,j}^n - P_{i,j}^n}{\Delta x^2} + V_t \frac{-P_{i,j}^n + P_{i-1,j}^n}{\Delta x^2}.
\]
(14)

Accordingly, the calculated dependencies (Richardson’s method) for determining the unknown value of \( P \) based on equation (13):

\[
P_{i,j}^{n+1} = P_{i,j}^n + V_t \frac{P_{i,j+1}^n - P_{i,j}^n}{\Delta y^2} + V_t \frac{-P_{i,j}^n + P_{i,j-1}^n}{\Delta y^2}.
\]
(15)

Since we solve the evolutionary equation, the calculation by dependencies (14)–(15) ends when the following condition is met:

\[|P_{i,j}^{n+1} - P_{i,j}^n| \leq \varepsilon,\]

where \( \varepsilon \) – small number; \( n \) – iteration number.

We calculate the flow velocity as follows:

\[
u = \frac{P_{i+1,j} - P_{i,j}}{\Delta x},
\]
\[
\nu = \frac{P_{i,j+1} - P_{i,j}}{\Delta y}.
\]

For numerical integration of equations (3)–(4), the Euler method is used.

The algorithm for solving this problem includes two main stages.

At the first stage, the following steps are performed:

1) the velocity potential field \( P \) \((x, y)\) in the aerotank is calculated;
2) the flow velocity field \( u \) \((x, y)\), \( v \) in the aerotank is determined.

The second stage (calculation at the time step \( dt \)) contains the following steps:

1) the change in the concentration of activated sludge in the aerotank due to flow movement and diffusion is calculated;
2) the change in the concentration of the substrate in the aerotank due to the flow movement and diffusion is calculated;
3) the change in the concentration of activated sludge and substrate in each difference cell based on the Monod model is calculated;
4) the calculation is repeated at a new time step, starting from item 1.

Based on the constructed numerical model, the BIO-2K computer program was developed. Programming is carried out in the FORTRAN algorithmic language.

**Findings**

Let us present the results of solving the problem of assessing the efficiency of the aeration tank using the developed CFD model. The following scenarios were considered:

- scenario no. 1: the aerotank works without additional elements inside the structure;
- scenario no. 2: aerotank has one plate inside the structure;
- scenario no. 3: aerotank has two plates inside the structure;
- scenario no. 4: aerotank works as a reservoir for the substrate destruction, but there is no entry and exit of the substrate and activated sludge. That is, in this scenario, the aerotank is a tank filled with activated sludge and substrate, and the process of changing their concentration was studied using the Monod model.

Calculations were performed with the following initial data:

\[S_{in} = 360 \text{ mg/l} – \text{the concentration of the substrate (Biological oxygen demand (complete), which enters the structure)};
\]
Bioreactor dimensions 15x5 m;

\[ Q_s(t) = 3,495 \text{ m}^3/\text{day} \] - waste water consumption;

\[ \mu_0 = \mu_1 = 2 \times 10^{-4} \text{ m}^3/\text{day}; \]

\[ X_{in} = 200 \text{ mg/l} \] - concentration of activated sludge that enters the reactor;

\[ \mu_{max} = 1.04 \] - reproducibility index parameter;

\[ K_s = 100 \text{ mg/l} \] - sludge index parameter;

\[ K_d = 0.055 \text{ 1/day} \] - the death coefficient that takes into account the death of microorganisms;

\[ Y = 0.55 \] - parameter in the Monod model.

Initial condition: \( S_{in} = 360 \text{ mg/l}, X_{in} = 200 \text{ mg/l} \), is the concentration of the substrate and activated sludge in the reactor for the time moment \( t = 0 \).

Figures 1–4 show how the substrate concentration at the reactor outlet changes for the scenarios under consideration. The concentration is averaged over the aerotank width for the time moment \( t = 1.5 \) (dimensionless time). Each number in the Figures shows the substrate concentration as a percentage of the maximum concentration (this is the concentration at the entrance to the reactor \( S_{in} = 360 \text{ mg/l} \)).

As can be seen from the above figures, the field of substrate concentration inside the reactor can be divided into two zones. The first zone corresponds to the concentration range from 99 to 10% and occupies approximately the first half of the reactor. The second zone corresponds to the substrate concentration in the range of 10–3% (output from the reactor). The border between the zones looks like a «slanting» line. The second zone even has a «sparse» view. A significant concentration of the substrate in the first zone is caused by its constant ingress into the structure through the inlet.

As can be seen from Table 1, the plates in the structure affect the efficiency of water purification in the bioreactor. The most active process of water purification takes place if there is no movement in the reactor.
the reactor (scenario no. 4), i.e., if there is no new portions of the substrate entering the reactor. Thus, it can be concluded that the quality control of wastewater treatment in biological reactors is possible through the use of additional elements in the structure – plates.

Data analysis of Table 2 shows that approximately from the moment of time $t = 0.96$, the deceleration of the water purification process starts in the reactor, where the movement takes place, (scenario no. 1). By the time moment $t = 1.5$, the substrate concentration at the outlet from the reactor, where there is movement, is significantly different from the concentration for the reactor, where there is no movement.

Note that the time for calculating each scenario was 5 s.

### Originality and practical value

A new numerical 2D model is proposed to assess the operation efficiency of the aerotank. A feature of the model is the ability to assess the operation of the aerotank, taking into account its geometric shape and location of additional plates in the structure. The simulated equations reflect the fundamental law of continuum mechanics – the law of mass conservation.

The developed numerical model makes it possible to determine the concentration field of the substrate and activated sludge in the bioreactor. The model can be useful when performing calculations in the case of designing biological treatment facilities or when reconstructing existing bioreactors.

### Conclusions

In the article, a new numerical model has been developed that allows one to determine the aerotank operation efficiency, taking into account its geometric shape. The results of computational experiments show that the use of additional elements in the aerotank improves the efficiency of water purification.

In the future, this scientific direction should be developed in the field of development of numerical models for evaluating the aerotank operation efficiency based on the Navier-Stokes equation.
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КОМП’ЮТЕРНЕ МОДЕЛЮВАННЯ ПРОЦЕСІВ БІОЛОГІЧНОГО ОЧИЩЕННЯ СТІЧНИХ ВОД В АЕРОТЕНКАХ ІЗ ПЛАСТИНАМИ

Мета. Визначення ефективності роботи аеротенків на етапі проектування або реконструкції біореакторів, у яких здійснюється біологічне очищення стічних вод, вимагає використання спеціальних математичних моделей і методів розрахунку. Основою метою статті є розробка CFD-моделі для оцінки ефективності роботи аеротенків. Методика. Для комп’ютерного розрахунку процесу біологічного очищення стічних вод в аеротенкі, з урахуванням гідродинаміки, розроблена чисельна модель. В основу моделі покладено двовимірні рівняння збереження маси для субстрату та активного мулу та рівняння для потенціалу швидкості. Процес біологічного перетворення субстрату розраховано на базі моделі Monod. Для чисельного інтегрування рівнянь масопереносу активного мулу та субстрату використано поперемінно-треугольну різницеву схему розщеплення. При цьому базові рівняння розщеплено на два рівняння більш спрощеного вигляду. Для чисельного інтегрування рівняння для потенціалу швидкості здійснено його розщеплення на два одновимірні рівняння. Далі кожне рівняння розщеплено на два рівняння більш спрощеного вигляду. Для чисельного інтегрування рівнянь, що описують процес трансформації субстрату на базі моделі Monod, використано метод Ейлера. Результати. Здійснено програмну реалізацію побудованої чисельної моделі. Наведено результати обчислювального експерименту з дослідження процесу очищення стічних вод в аеротенку за рахунок використання додаткових елементів у споруді–пластині. Це дозволяє зробити висновки, що управління якістю очищення стічних вод в аеротенкі можливе за допомогою застосування пластин. Наукова новизна. Розроблено багатофакторну CFD-модель, що дозволяє швидко оцінити ефективність роботи аеротенка. Особливістю моделі є можливість оцінки роботи аеротенка з урахуванням його геометричної форми та розташування в споруді додаткових пластин. Практична значимість. Побудована чисельна модель може бути використана під час проведення розрахунків у випадку проектування споруд аеротенків або під час визначення ефективності очищення стічних вод за нових умов експлуатації.

Ключові слова: очищення води; чисельне моделювання; аеротенк; модель Monod; CFD-модель; біологічне очищення; стічні води; активний мул; концентрація забруднюючих речовин
КОМПЬЮТЕРНОЕ МОДЕЛИРОВАНИЕ ПРОЦЕССОВ БИОЛОГИЧЕСКОЙ ОЧИСТКИ СТОЧНЫХ ВОД В АЭРОТЕНКАХ С ПЛАСТИНАМИ

Цель. Определение эффективности работы аэротенка на этапе проектирования или реконструкции биореакторов, в которых осуществляется биологическая очистка сточных вод, требует использования специальных математических моделей и методов расчета. Основной целью статьи является разработка CFD-модели для оценки эффективности работы аэротенков.

Методика. Для компьютерного расчета процесса биологической очистки сточных вод в аэротенках, с учётом гидродинамики, разработана численная модель. В основу модели заложены двухуровневые уравнения сохранения массы для субстрата и активного ила и уравнение для потенциала скорости. Процесс биологического преобразования субстрата рассчитан на базе модели Monod. Для численного интегрирования уравнений массопереноса активного ила и субстрата использована поперечно-треугольная разностная схема расщепления. При этом базовые уравнения разделены на два уравнения более упрощенного вида. Для численного интегрирования уравнения для потенциала скорости осуществлено его расщепление на два одномерных уравнения. Далее каждое уравнение решено по явной схеме. Для численного интегрирования уравнений, описывающих процесс трансформации субстрата на базе модели Monod, использован метод Эйлера.

Результаты.Осуществлена программная реализация построенной численной модели. Приведены результаты вычислительного эксперимента по исследованию процесса очистки сточных вод в аэротенке за счет использования дополнительных элементов в сооружении – пластин. Это проводит к выводу, что управление качеством очистки сточных вод в аэротенках возможно с помощью применения пластин.

Научная новизна. Разработана многофакторная CFD-модель, позволяющая быстро оценить эффективность работы аэротенка. Особенностью модели является возможность оценки работы аэротенка с учетом его геометрической формы и расположения в сооружении дополнительных пластин.

Практическая значимость. Построенная численная модель может быть использована при проведении расчетов в случае проектирования сооружений аэротенков или при определении эффективности очистки сточных вод в новых условиях эксплуатации.

Ключевые слова: очистка воды; численное моделирование; аэротенк; модель Monod; CFD-модели; биологическая очистка; сточные воды; активный ил; концентрация загрязняющих веществ

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