

ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

UDC 504.5:[628.3:519.87]

M. M. BILIAIEV^{1*}, M. V. LEMESH², O. Y. GUNKO³, V. O. ZADOIA⁴,
P. B. MASHYKHINA⁵, Z. M. YAKUBOVSKA⁶

^{1*}Dep. «Hydraulics and Water Supply», Dnipro National University of Railway Transport named after Academician V. Lazaryan, Lazaryana St., 2, Dnipro, Ukraine, 49010, tel. +38 (056) 273 15 09, e-mail water.supply.treatment@gmail.com, ORCID 0000-0002-1531-7882

²Dep. «Hydraulics and Water Supply», Dnipro National University of Railway Transport named after Academician V. Lazaryan, Lazaryana St., 2, Dnipro, Ukraine, 49010, tel. +38 (056) 273 15 09, e-mail water.supply.treatment@gmail.com, ORCID 0000-0002-1230-8040

³Dep. «Hydraulics and Water Supply», Dnipro National University of Railway Transport named after Academician V. Lazaryan, Lazaryana St., 2, Dnipro, Ukraine, 49010, tel. +38 (056) 273 15 09, e-mail water.supply.treatment@gmail.com, ORCID 0000-0001-9257-763X

⁴Dep. «Economics and Management», Dnipro National University of Railway Transport named after Academician V. Lazaryan, Lazaryana St., 2, Dnipro, Ukraine, 49010, tel. +38 (096) 469 60 09, e-mail v.a.zadoia@gmail.com, ORCID 0000-0001-9408-4978

⁵Dep. «Hydraulics and Water Supply», Dnipro National University of Railway Transport named after Academician V. Lazaryan, Lazaryana St., 2, Dnipro, Ukraine, 49010, tel. +38 (056) 273 15 09, e-mail water.supply.treatment@gmail.com, ORCID 0000-0003-3057-9204

⁶Dep. «Power Engineering», Ukrainian State University of Chemical Technology, Haharina Av., 8, Dnipro, Ukraine, 49000, tel. +38 (056) 753 56 38, e-mail zinaidaya25@gmail.com, ORCID 0000-0002-9893-3479

3D MODELING OF BIOLOGICAL WASTEWATER TREATMENT IN AERATION TANK

Purpose. The main purpose of the article is to develop a 3D CFD model for modeling the process of biological wastewater treatment in an aeration tank. **Methodology.** For mathematical modeling of the process of biological wastewater treatment in the reactor, taking into account the flow hydrodynamics, geometric shape of the aeration tank, convective-diffusion transfer of the substrate and activated sludge, a 3D CFD model was built. The model is based on the three-dimensional equation of motion of an ideal liquid and the equation of mass conservation for the substrate, activated sludge. The field of sewage flow rate in the aeration tank is calculated based on the velocity potential equation. The process of biological transformation of the substrate is calculated on the basis of the Monod model. The splitting scheme was used for numerical integration of the equations of convective-diffusion transfer of activated sludge and substrate. The splitting is carried out in such a way to take into account the transfer of substrate (activated sludge) in only one direction at each step of splitting. The calculation of the unknown value of the substrate (activated sludge) concentration is carried out according to an explicit scheme. The Richardson method is used to numerically integrate the three-dimensional equation for the velocity potential, and the unknown value of the velocity potential is calculated by an explicit formula. Euler's method is used for numerical integration of equations describing the process of substrate transformation and change in activated sludge concentration (Monod model). **Findings.** The software implementation of the constructed 3D CFD model is carried out. A description of the structure of the developed software package is provided. The results of a computer experiment to study the process of wastewater treatment in an aeration tank with additional elements are presented. **Originality.** A new multifactor 3D CFD model has been developed, which allows quick assessing the efficiency of biological treatment in an aeration tank. **Practical value.** The constructed 3D CFD model can be used to analyze the efficiency of the aeration tank under different operating conditions at the stage of sketch design of wastewater treatment systems.

Keywords: water treatment; biological water treatment; mathematical modeling; aeration tank; Monod model

Introduction

To determine the efficiency of biological wastewater treatment at the design stage of aeration tanks, it is necessary to use special mathematical models [3, 4, 6]. Nowadays, balance, empirical and analytical models are most often used to solve this problem [1–5, 7–17]. But in some cases, these models cannot provide a reliable result, because they do not take into account primarily the geometric shape of the reactor and the process of hydrodynamics, as well as a number of other parameters. In this regard, the problem of the development of mathematical models that allow theoretical investigation of the process of biological wastewater treatment in aeration tanks, taking into account the most important factors is relevant [1, 2, 6–10].

Purpose

The work is aimed to develop a three-dimensional CFD-model of the process of biological wastewater treatment in aeration tanks. The model must perform real-time calculation. In addition, the model should be acceptable for implementation on low- and medium-power computers.

Methodology

To model the biological wastewater treatment in the aeration tank the following equations are used:

$$\frac{\partial S}{\partial t} + \frac{\partial uS}{\partial x} + \frac{\partial vS}{\partial y} + \frac{\partial wS}{\partial z} = \frac{\partial}{\partial x} \left(\mu_x \frac{\partial S}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_y \frac{\partial S}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu_z \frac{\partial S}{\partial z} \right); \quad (1)$$

$$\frac{\partial X}{\partial t} + \frac{\partial uX}{\partial x} + \frac{\partial vX}{\partial y} + \frac{\partial wX}{\partial z} = \frac{\partial}{\partial x} \left(\mu_x \frac{\partial X}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_y \frac{\partial X}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu_z \frac{\partial X}{\partial z} \right); \quad (2)$$

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

$$\frac{dS}{dt} = -\frac{\mu}{Y} X, \quad (4)$$

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

where K_d – extinction coefficient of activated sludge; t – time; $X(x, y, z, t)$ – concentration of activated sludge in the bioreactor; $S(x, y, z, t)$ – substrate concentration in the bioreactor; $\mu_{x,y,z}(t)$ – empirical parameter; μ_{\max} – parameter in the Mono model; Y – empirical parameter; K_s – parameter in the Mono model; $u(x, y, z)$, $v(x, y, z)$, $w(x, y, z)$ – components of the water flow rate in the bioreactor, in the direction of the axes x, y, z , respectively; μ_x, μ_y, μ_z – diffusion coefficients, respectively, in the direction x, y, z ; t – time.

Let us note that the diffusion coefficients μ_x, μ_y, μ_z are different values, but in the scientific literature there is a significant shortage of data on their values. Therefore, in practice, the calculations are carried out under the condition $\mu_x = \mu_y = \mu_z$. Determining these parameters experimentally is a rather difficult task.

For practical use of equations of model (1) – (4) it is necessary to calculate the non-uniform flow velocity field in the reactor, i.e. to determine the parameters $u(x, y, z)$, $v(x, y, z)$, $w(x, y, z)$, under the action of these parameters there is a convective transfer of substrate and activated sludge in the bioreactor. To calculate the non-uniform flow velocity field in the bioreactor, we use the 3D equation for the velocity potential:

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

$$u = \frac{\partial P}{\partial x}, \quad v = \frac{\partial P}{\partial y}, \quad w = \frac{\partial P}{\partial z}. \quad (6)$$

The boundary conditions for modeling equations are as follows:

– on the surfaces of the building, solid walls,
upper surface: $\frac{\partial P}{\partial n} = 0, \frac{\partial S}{\partial n} = 0, \frac{\partial X}{\partial n} = 0$, where
 n – outward normal to a surface;

ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

– at the entrance boundary:
 $\frac{\partial P}{\partial n} = V_n$, $S = S_{in}$, $X = X_{in}$, where V_n – flow velocity; S_{in} , X_{in} – known concentration;

– at the boundary of outflow of the building:
 $P = P_0 + const$, $\frac{\partial S}{\partial n} = 0$, $\frac{\partial X}{\partial n} = 0$.

CFD model. The method of solving the mass transfer equations from system (1) – (2) will be considered using the example only for the substrate transfer equation. The equation for the transfer of activated sludge has a similar form. The three-dimensional equation for the substrate transfer from the system (1) is split into a system of one-dimensional equations as follows:

$$\begin{aligned} \frac{\partial S}{\partial t} + \frac{\partial uS}{\partial x} &= \frac{\partial}{\partial x} \left(\mu_x \frac{\partial S}{\partial x} \right); \\ \frac{\partial S}{\partial t} + \frac{\partial vS}{\partial y} &= \frac{\partial}{\partial y} \left(\mu_y \frac{\partial S}{\partial y} \right); \\ \frac{\partial S}{\partial t} + \frac{\partial vS}{\partial z} &= \frac{\partial}{\partial z} \left(\mu_z \frac{\partial S}{\partial z} \right). \end{aligned} \quad (7)$$

Equations from system (7) describe the process of substrate transfer in the directions of the x , y , z axes.

The difference equations that make it possible to solve the system of equations (7) are as follows:

– step 1 for the first equation:

$$\begin{aligned} S_{i,j,k}^{n+\frac{1}{2}} &= S_{i,j,k}^n - \Delta t \frac{u_{i+1,j,k}^+ S_{i,j,k}^{n+\frac{1}{2}} - u_{i,j,k}^+ S_{i-1,j,k}^{n+\frac{1}{2}}}{\Delta x} + \\ &+ \Delta t \mu \frac{-S_{i,j,k}^{n+\frac{1}{2}} + S_{i-1,j,k}^{n+\frac{1}{2}}}{\Delta x^2} + \Delta t \mu \frac{-S_{i,j,k}^n + S_{i+1,j,k}^n}{\Delta x^2}; \end{aligned} \quad (8)$$

– step 2 for the first equation:

$$\begin{aligned} S_{i,j,k}^{n+1} &= S_{i,j,k}^{n+\frac{1}{2}} - \Delta t \frac{u_{i+1,j,k}^- S_{i+1,j,k}^{n+1} - u_{i,j,k}^- S_{i,j,k}^{n+1}}{\Delta x} + \\ &+ \Delta t \mu \frac{-S_{i,j,k}^{n+\frac{1}{2}} + S_{i-1,j,k}^{n+\frac{1}{2}}}{\Delta x^2} + \Delta t \mu \frac{-S_{i,j,k}^{n+1} + S_{i+1,j,k}^{n+1}}{\Delta x^2}, \end{aligned} \quad (9)$$

$$\text{where } u^+ = \frac{u + |u|}{2}; \quad u^- = \frac{u - |u|}{2};$$

– step 1 for the second equation:

$$\begin{aligned} S_{i,j,k}^{n+\frac{1}{2}} &= S_{i,j,k}^n - \Delta t \frac{v_{i,j+1,k}^+ S_{i,j,k}^{n+\frac{1}{2}} - v_{i,j,k}^+ S_{i,j-1,k}^{n+\frac{1}{2}}}{\Delta y} + \\ &+ \Delta t \mu \frac{-S_{i,j,k}^{n+\frac{1}{2}} + S_{i-1,j,k}^{n+\frac{1}{2}}}{\Delta y^2} + \Delta t \mu \frac{-S_{i,j,k}^n + S_{i+1,j,k}^n}{\Delta y^2}; \end{aligned} \quad (10)$$

– step 2 for the second equation:

$$\begin{aligned} S_{i,j,k}^{n+1} &= S_{i,j,k}^{n+\frac{1}{2}} - \Delta t \frac{v_{i,j+1,k}^- S_{i,j,k}^{n+1} - v_{i,j,k}^- S_{i,j-1,k}^{n+1}}{\Delta y} + \\ &+ \Delta t \mu \frac{-S_{i,j,k}^{n+\frac{1}{2}} + S_{i-1,j,k}^{n+\frac{1}{2}}}{\Delta y^2} + \Delta t \mu \frac{-S_{i,j,k}^{n+\frac{1}{2}} + S_{i+1,j,k}^{n+\frac{1}{2}}}{\Delta y^2}, \end{aligned} \quad (11)$$

$$\text{where } v^+ = \frac{v + |v|}{2}; \quad v^- = \frac{v - |v|}{2};$$

– step 1 for the third equation:

$$\begin{aligned} S_{i,j,k}^{n+\frac{1}{2}} &= S_{i,j,k}^n - \Delta t \frac{w_{i,j,k+1}^+ S_{i,j,k}^{n+\frac{1}{2}} - w_{i,j,k}^+ S_{i,j,k-1}^{n+\frac{1}{2}}}{\Delta z} + \\ &+ \Delta t \mu \frac{-S_{i,j,k}^{n+\frac{1}{2}} + S_{i,j,k-1}^{n+\frac{1}{2}}}{\Delta z^2} + \Delta t \mu \frac{-S_{i,j,k}^n + S_{i,j,k+1}^n}{\Delta z^2}; \end{aligned} \quad (12)$$

– step 2 the third equation:

$$\begin{aligned} S_{i,j,k}^{n+1} &= S_{i,j,k}^{n+\frac{1}{2}} - \Delta t \frac{w_{i,j,k+1}^- S_{i,j,k+1}^{n+1} - w_{i,j,k}^- S_{i,j,k}^{n+1}}{\Delta z} + \\ &+ \Delta t \mu \frac{-S_{i,j,k}^{n+\frac{1}{2}} + S_{i,j,k-1}^{n+\frac{1}{2}}}{\Delta z^2} + \Delta t \mu \frac{-S_{i,j,k}^{n+1} + S_{i,j,k+1}^{n+1}}{\Delta z^2}, \end{aligned} \quad (13)$$

$$\text{where } w^- = \frac{w - |w|}{2}; \quad w^+ = \frac{w + |w|}{2}.$$

We solve the equation of activated sludge transfer from system (2) according to a similar finite-difference scheme. After solving the transfer equations for X and S , for each difference cell, we solve equations (3) – (4) using the Euler method. That is, we determine new values of the substrate

ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

and activated sludge concentration due to their biological interaction. Difference expressions have the form:

$$S_{i,j,k}^{n+1} = S_{i,j,k}^n - dt \cdot \frac{\mu_{i,j,k}^n}{Y} X_{i,j,k}^n;$$

$$X_{i,j,k}^{n+1} = X_{i,j,k}^n - dt \cdot \mu_{i,j,k}^n X_{i,j,k}^n - K_d X_{i,j,k}^n;$$

$$\mu_{i,j,k}^n = \mu_{\max} \cdot \frac{S_{i,j,k}^n}{S_{i,j,k}^n + K_s}.$$

Next, in a new time step, we repeat the calculation of the change in the concentration of substrate and activated sludge in each difference cell due to their movement, diffusion and biological interaction.

To construct a local one-dimensional scheme for solving equation (5), we perform the following transformations. First, let us present this equation as:

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \frac{\partial^2 P}{\partial z^2}, \quad (14)$$

where t – fictitious time.

Then, we split equation (14) as follows:

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2}; \quad (15)$$

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial y^2}; \quad (16)$$

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial z^2}. \quad (17)$$

The calculated dependencies (Richardson's method) for determining the unknown value P based on equation (15) have the form:

$$P_{i,j,k}^{n+1} = P_{i,j,k}^n + \Delta t \frac{P_{i+1,j,k}^n - P_{i,j,k}^n}{\Delta x^2} + \Delta t \frac{-P_{i,j,k}^n + P_{i-1,j,k}^n}{\Delta x^2}. \quad (18)$$

The calculated dependencies for determining the unknown value P based on equation (16) have the form:

$$P_{i,j,k}^{n+1} = P_{i,j,k}^n + \Delta t \frac{P_{i,j,k+1}^n - P_{i,j,k}^n}{\Delta y^2} + \Delta t \frac{-P_{i,j,k}^n + P_{i,j,k-1}^n}{\Delta y^2}. \quad (19)$$

The calculated dependencies for determining the unknown value of P based on equation (17) have the form:

$$P_{i,j,k}^{n+1} = P_{i,j,k}^n + \Delta t \frac{P_{i,j,k+1}^n - P_{i,j,k}^n}{\Delta z^2} + \Delta t \frac{-P_{i,j,k}^n + P_{i,j,k-1}^n}{\Delta z^2}. \quad (20)$$

The calculation according to these dependencies ends when the condition is met:

$$|P_{i,j,k}^{n+1} - P_{i,j,k}^n| \leq \varepsilon, \quad (21)$$

where ε – small number; n – iteration number.

At the next stage we determine the flow velocities:

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

$$w = \frac{P_{i,j,k+1} - P_{i,j,k}}{\Delta z}.$$

FORTRAN was used to encode the difference equations. The BIO-3K code has been created. To use it, one needs to specify the following input data:

- concentration of the substrate entering the bioreactor and its change over time;
- concentration and consumption of activated sludge entering the bioreactor and its change over time;
- dimensions of the bioreactor, its geometric shape;
- values of Monod model parameters;
- wastewater consumption;
- values of diffusion coefficients.

ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

BIO-3K code includes the following subroutines:

SLE3 – velocity potential calculation in the bioreactor;

SLE3 – velocity field calculation in the bioreactor;

SLM33 – calculation of the substrate concentration field in the bioreactor and its change over time;

SLM33 – calculation of the concentration field of activated sludge in the bioreactor and its change over time;

SLM33 – calculation of changes in the concentration of substrate and activated sludge in the bioreactor according to the dependencies of the Monod model;

SLEM5 – print of the modeling results.

Result of this code is the concentration fields of the substrate and activated sludge in the bioreactor and the change of these fields over time.

Findings

The following are the results of solving the problem of evaluating the efficiency of a biological reactor for wastewater treatment based on the developed three-dimensional CFD model. The calculations are performed on the basis of the following input data:

$S_{in} = 140$ mg/l – the concentration of the substrate ($BOD_{complete}$) entering the structure;

dimensions of the bioreactor 15mx4mx4m;

$Q_s(t) = 1353$ m³ / day – wastewater consumption;

$\mu_x = \mu_y = 2 \cdot 10^{-4}$ m²/day;

$X_{in} = 200$ mg/l – concentration of activated sludge entering the reactor;

$\mu_{max} = 1.04$;

$K_s = 100$ mg/l;

$K_d = 0.055$ 1/day – coefficient that takes into account the death of microorganisms;

$Y = 0.55$.

Initial condition: $S_{in} = 140$ mg/l,

$X_{in} = 200$ mg/l – concentration of substrate and activated sludge in the reactor for the moment of time $t = 0$.

The following scenarios are considered:

– scenario 1: the reactor operates without additional elements inside the building;

– scenario 2: inside the reactor there are two solid plates (calculation area is multiconnected);

– scenario 3: the reactor has three plates, but they have a gap.

Initial condition: $S_{in} = 360$ mg/l, $X_{in} = 200$ mg/l. We study the process of substrate destruction in the reactor over time according to the Monod model and taking into account mass transfer.

It should be noted that the calculation of spatial flow in multiconnected domains is one of the most complex problems of hydrodynamics.

Evaluation of the bioreactor performance is determined by the substrate concentration at the reactor outlet. Fig. 1–6 show the distribution of substrate concentration in the bioreactor for all scenarios, where each number indicates the concentration as a percentage of the maximum concentration in the calculation area (the time shown in the figures is dimensionless). The number 99 corresponds to the maximum value of the concentration in percent. These values are printed in the INTEGER format, i.e. only the integer value of the real number is printed. For example, if at some point in the reactor the concentration is 61.95 %, then the number 61 is printed. Since the three-dimensional problem is being solved, the concentration is shown in different sections of the bioreactor, the time is dimensionless.

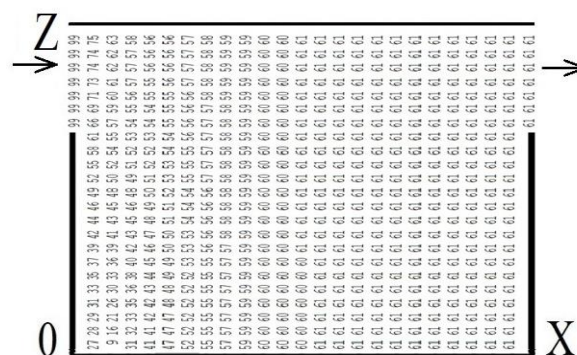


Fig. 1. Distribution of substrate concentration in the bioreactor, cross section $y = 2$ m, $t = 0.24$ (scenario 1)

ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

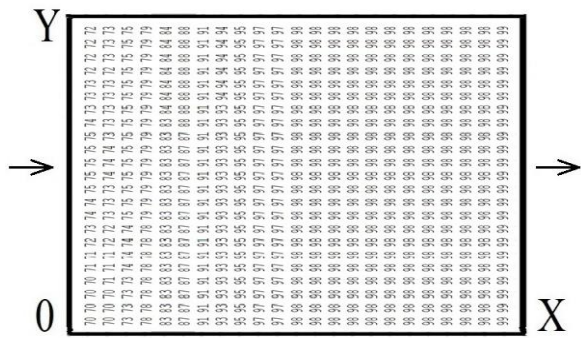


Fig. 2. Distribution of substrate concentration in the bioreactor, cross section $z = 2$ m, $t = 0.24$ (scenario 1)

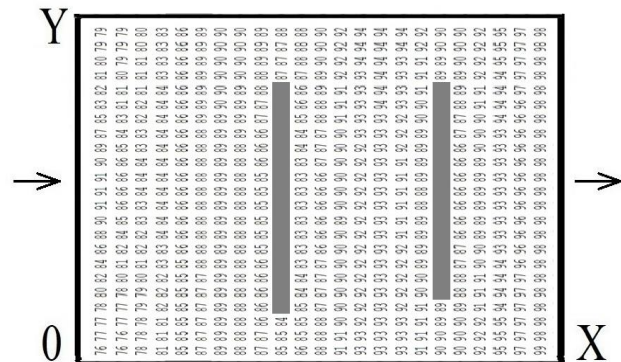


Fig. 5. Distribution of substrate concentration in the bioreactor, cross section $z = 2$ m, $t = 0.40$ (scenario 2)

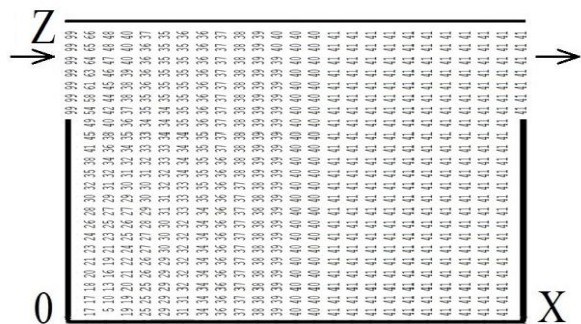


Fig. 3. Distribution of substrate concentration in the bioreactor, cross section $y = 2$ m, $t = 0.40$ (scenario 1)

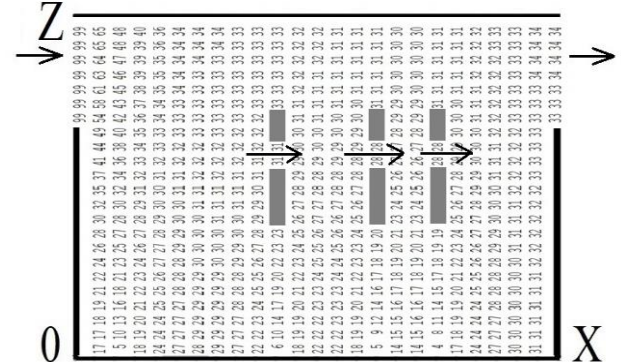


Fig. 6. Distribution of substrate concentration in the bioreactor, cross section $y = 2$ m, $t = 0.40$ (scenario 3)

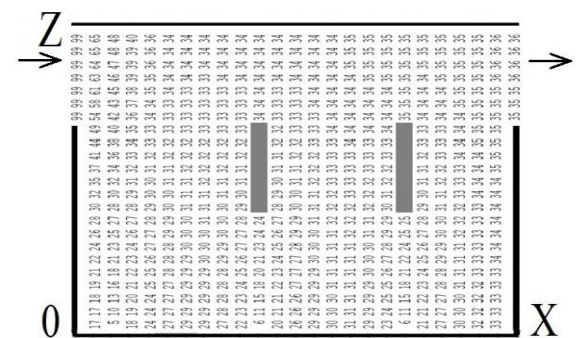


Fig. 4. Distribution of substrate concentration in the bioreactor, cross section $y = 2$ m, $t = 0.40$ (scenario 2)

The figures show that inside the reactor there is a significantly uneven distribution of the substrate concentration, i.e. the process of biological treatment is uneven. The use of plates changes the concentration distribution in the structure, which affects the performance of the reactor.

To analyze the performance of the reactor Table 1 shows the substrate concentration at the outlet for the time $t = 0.40$.

Table 1

Average concentration of substrate at the reactor outlet

Scenario	1	2	3
Concentration	147 mg/l	128 mg/l	118 mg/l

Analysis of data from table 1 shows that the use of plates makes it possible to increase the performance of the biological reactor. That is, we have the opportunity to control the process of wastewater treatment in the bioreactor.

Originality and practical value

A three-dimensional CFD model has been developed to model the process of biological wastewater treatment in an aeration tank. The potential motion model was used to calculate the flow velocity field in the aeration tank. The process of

substrate and activated sludge transfer was determined based on the mass transfer equation. The Monod model was used to calculate the biological treatment process.

The constructed model can be used at the stage of sketch design of structures for wastewater treatment.

Conclusions

The article considers an efficient CFD model that allows you to quickly calculate the process of biological wastewater treatment in the aeration tank, in particular in the presence of additional plates in the middle of the reactor. To solve the problem, the fundamental equations of continuum dynamics are used.

In the future, it is planned to develop a three-dimensional CFD model based on the Navier–Stokes equations.

LIST OF REFERENCE LINKS

1. Беляев Н. Н., Нагорная Е. К. *Математическое моделирование массопереноса в отстойниках систем водоотведения* : монография. Днепропетровск : Новая идеология, 2012. 112 с.
2. Беляев Н. Н., Козачина В. А. *Математическое моделирование массопереноса в горизонтальных отстойниках* : монография. Днепропетровск : Акцент ПП, 2015. 115 с.
3. Василенко О. А., Грабовський П. О., Ларкіна Г. М., Поліщук О. В., Прогульний В. Й. *Реконструкція і інтенсифікація споруд водопостачання та водовідведення* : навч. посіб. Київ : ІВНВКП «Укреліотек», 2010. 272 с.
4. Карелин Я. А., Жуков Д. Д., Журов В. Н., Репин Б. Н. *Очистка производственных сточных вод в аэротенках*. Москва : Стройиздат, 1973. 223 с.
5. Ласков Ю. М., Воронов Ю. В., Калицун В. И. *Примеры расчетов канализационных сооружений*. Москва : Высшая школа, 1981. 237 с.
6. Олійник О. Я., Айрапетян Т. С. Моделювання очисних стічних вод від органічних забруднень в біореакторах-аэротенках зі зваженим (вільно плаваючим) і закріпленим біоценозом. *Доповідь НАН України*. 2015. № 5. С. 55–60. DOI: <https://doi.org/10/15407/dopovidi2015.05.055>
7. Alharbi A. O. M. The biological treatment of wastewater : mathematical models. *Bulletin of the Australian Mathematical Society*. 2016. Vol. 94. Iss. 2. P. 347–348. DOI: <https://doi.org/10.1017/S0004972716000411>
8. Amaral A., Gillot S., Garrido-Baserba M., Filali A., Karpinska A. M., Plósz B. G., ... Rosso D. Modelling gasliquid mass transfer in wastewater treatment : when current knowledge needs to encounter engineering practice and viceversa. *Water Science & Technology*. 2019. Vol. 80. Iss. 4. P. 607–619. DOI: <https://doi.org/10.2166/wst.2019.253>
9. Babaei A., Azadi R., Jaafarzadeh N., Alavi N. Application and Kinetic Evaluation of upflow Anaerobic bio-film Reactor for Nitrogen Removal from Wastewater. *Iranian Journal of Environmental Health Science and Engineering*. 2013. Vol. 10. Iss. 1. P. 1–8. DOI: <https://doi.org/10.1186/1735-2746-10-20>
10. Bomba A., Klymiuk Y., Prysiazhniuk I., Prysiazhniuk O., Safonyk A. Mathematical modeling of wastewater treatment from multicomponent pollution by through microporous filling. *AIP Conference Proceedings*. 2016. Vol. 1773. P. 040003-1–040003-11. DOI: <https://doi.org/10.1063/1.4964966>
11. Dapelo D., Bridgeman G. A CFD strategy to retrofit an anaerobic digester to improve mixing performance in wastewater treatment. *Water Science & Technology*. 2020. Vol. 81. Iss. 8. P. 1646–1657. DOI: <https://doi.org/10.2166/wst.2020.086>
12. Gao H., Stenstrom M. K. Development and applications in CFD modeling for secondary settling tanks over the last three decades : A review. *Water Environment Research*. 2019. Vol. 92. Iss. 6. P. 796–820. DOI: <https://doi.org/10.1002/wer.1279>
13. Gao H., Stenstrom M. K. Influence of Model Parameters and Inlet Turbulence Boundary Specification Methods in Secondary Settling Tanks : Computational Fluid Dynamics Study. *Journal of Environmental Engineering*. 2020. Vol. 146. Iss. 5. P. 04020028-1–04020028-12. DOI: [https://doi.org/10.1061/\(ASCE\)EE.1943-7870.0001689](https://doi.org/10.1061/(ASCE)EE.1943-7870.0001689)

ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

14. Gao H., Stenstrom M. K. Computational Fluid Dynamics Analysis for Improving Secondary Settling Tank Performance. *World Environmental and Water Resources Congress 2020*. 2020. P. 212–224.
DOI: <https://doi.org/10.1061/9780784482988.021>
15. Griborio A. *Secondary Clarifier Modeling : A Multi-Process Approach. Dissertation and Theses*. University of New Orleans : USA, 2004. 440 p.
16. Mocanu C. R., Mihaillescu R. Numerical Simulation Wastewater Treatment Aeration Processes. *U. P. B. Sci. Bull., Series D*. 2012. Vol. 74. Iss. 2. P. 191–198.
17. Pereda M., Zamarrero J. M. Agent – based modeling of an activated sludge process in batch reactor. *19th Mediterranean Conference on Control and Automation Aquis*. 2011. P. 1128–1133.
DOI: <https://doi.org/10.1109/med.2011.5983027>

М. М. БІЛЯЄВ^{1*}, М. В. ЛЕМЕШ², О. Ю. ГУНЬКО³, В. О. ЗАДОЯ⁴, П. Б. МАШИХІНА⁵,
З. М. ЯКУБОВСЬКА⁶

^{1*}Каф. «Гідравліка та водопостачання», Дніпровський національний університет залізничного транспорту імені академіка В. Лазаряна, вул. Лазаряна, 2, Дніпро, Україна, 49010, тел. +38 (056) 273 15 09, ел. пошта water.supply.treatment@gmail.com, ORCID 0000-0002-1531-7882

²Каф. «Гідравліка та водопостачання», Дніпровський національний університет залізничного транспорту імені академіка В. Лазаряна, вул. Лазаряна, 2, Дніпро, Україна, 49010, тел. +38 (056) 273 15 09, ел. пошта water.supply.treatment@gmail.com, ORCID 0000-0002-1230-8040

³Каф. «Гідравліка та водопостачання», Дніпровський національний університет залізничного транспорту імені академіка В. Лазаряна, вул. Лазаряна, 2, Дніпро, Україна, 49010, тел. +38 (056) 273 15 09, ел. пошта water.supply.treatment@gmail.com, ORCID 0000-0001-9257-763X

⁴Каф. «Економіка та менеджмент», Дніпровський національний університет залізничного транспорту імені академіка В. Лазаряна, вул. Лазаряна, 2, Дніпро, Україна, 49010, тел. +38 (096) 469 60 09, ел. пошта v.a.zadoya@gmail.com, ORCID 0000-0001-9408-4978

⁵Каф. «Гідравліка та водопостачання», Дніпровський національний університет залізничного транспорту імені академіка В. Лазаряна, вул. Лазаряна, 2, Дніпро, Україна, 49010, тел. +38 (056) 273 15 09, ел. пошта water.supply.treatment@gmail.com, ORCID 0000-0003-3057-9204

⁶Каф. «Енергетика», Український державний хіміко-технологічний університет, пр. Гагаріна, 8, Дніпро, Україна, 49000, тел. +38 (056) 753 56 38, ел. пошта zinaidaya25@gmail.com, ORCID 0000-0002-9893-3479

3D-МОДЕЛЮВАННЯ БІОЛОГІЧНОГО ОЧИЩЕННЯ СТІЧНИХ ВОД В АЕРОТЕНКУ

Мета. Основною метою статті є розробка тривимірної CFD-моделі для моделювання процесу біологічного очищення стічних вод в аеротенку. **Методика.** Для математичного моделювання процесу біологічного очищення стічних вод у реакторі, з урахуванням гідродинаміки потоку, геометричної форми аеротенка, конвективно-дифузійного переносу субстрату та активного мулу, побудовано тривимірну CFD-модель. В основу моделі покладено тривимірне рівняння руху ідеальної рідини та рівняння збереження маси для субстрату й активного мулу. Поле швидкості потоку стічних вод в аеротенку розраховано на базі рівняння для потенціалу швидкості. Процес біологічного перетворення субстрату розраховано на базі моделі Monod. Для чисельного інтегрування рівнянь конвективно-дифузійного переносу активного мулу та субстрату використано схему розщеплення. Розщеплення здійснено так, щоб на кожному кроці враховувався перенос субстрату (активного мулу) лише в одному напрямку. Розрахунок невідомої величини концентрації субстрату (активного мулу) виконано за явною схемою. Під час чисельного інтегрування тривимірних рівнянь для потенціалу швидкості використано метод Річардсона, розрахунок невідомого значення потенціалу швидкості здійснено за явною формулою. Для чисельного інтегрування рівнянь, що описують процес трансформації субстрату та зміну концентрації активного мулу (модель Monod), використано метод Ейлера. **Результати.** Здійснено програмну реалізацію побудованої тривимірної CFD-моделі. Описано структуру розробленого пакету програм. Подано результати проведеного комп'ютерного експерименту з дослідження процесу очищення стічних вод в аеротенку з додатковими елементами. **Наукова новизна.** Розроблено нову багатofакторну тривимірну CFD-модель, що дозволяє швидко оцінити ефективність біологічного очищення стічних вод в аеротенку. **Практична значимість.** Побудована CFD-модель може бути використана для ана-

ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

лізу ефективності роботи аеротенку за різних умов експлуатації та на етапі ескізного проектування систем очищення стічних вод.

Ключові слова: очищення води; біологічне очищення води; математичне моделювання; аеротенк; модель Monod

Н. Н. БЕЛЯЕВ^{1*}, М. В. ЛЕМЕШ², Е. Ю. ГУНЬКО³, В. А. ЗАДОЯ⁴, П. Б. МАШИХИНА⁵,
З. Н. ЯКУБОВСКАЯ⁶

^{1*}Каф. «Гидравлика и водоснабжение», Днепропетровский национальный университет железнодорожного транспорта имени академика В. Лазаряна, ул. Лазаряна, 2, Днепро, Украина, 49010, тел. +38 (056) 273 15 09, эл. почта water.supply.treatment@gmail.com, ORCID 0000-0002-1531-7882

²Каф. «Гидравлика и водоснабжение», Днепропетровский национальный университет железнодорожного транспорта имени академика В. Лазаряна, ул. Лазаряна, 2, Днепро, Украина, 49010, тел. +38 (056) 273 15 09, эл. почта water.supply.treatment@gmail.com, ORCID 0000-0002-1230-8040

³Каф. «Гидравлика и водоснабжение», Днепропетровский национальный университет железнодорожного транспорта имени академика В. Лазаряна, ул. Лазаряна, 2, Днепро, Украина, 49010, тел. +38 (056) 273 15 09, эл. почта water.supply.treatment@gmail.com, ORCID 0000-0001-9257-763X

⁴Каф. «Экономика и менеджмент», Днепропетровский национальный университет железнодорожного транспорта имени академика В. Лазаряна, ул. Лазаряна, 2, Днепро, Украина, 49010, тел. +38 (096) 469 60 09, эл. почта v.a.zadoya@gmail.com, ORCID 0000-0001-9408-4978

⁵Каф. «Гидравлика и водоснабжение», Днепропетровский национальный университет железнодорожного транспорта имени академика В. Лазаряна, ул. Лазаряна, 2, Днепро, Украина, 49010, тел. +38 (056) 273 15 09, эл. почта water.supply.treatment@gmail.com, ORCID 0000-0003-3057-9204

⁶Каф. «Энергетика», Украинский государственный химико-технологический университет, пр. Гагарина, 8, Днепро, Украина, 49000, тел. +38 (056) 753 56 38, эл. почта zinaidaya25@gmail.com, ORCID 0000-0002-9893-3479

3D-МОДЕЛИРОВАНИЕ БИОЛОГИЧЕСКОЙ ОЧИСТКИ СТОЧНЫХ ВОД В АЭРОТЕНКЕ

Цель. Основной целью статьи является разработка трёхмерной CFD-модели для моделирования процесса биологической очистки сточных вод в аэротенке. **Методика.** Для математического моделирования процесса биологической очистки сточных вод в реакторе, с учетом гидродинамики потока, геометрической формы аэротенка, конвективно-диффузионного переноса субстрата и активного ила, построена трёхмерная CFD-модель. В основу модели положено трехмерное уравнение движения идеальной жидкости и уравнение сохранения массы для субстрата и активного ила. Поле скорости потока сточных вод в аэротенке рассчитано на базе уравнения для потенциала скорости. Процесс биологического превращения субстрата рассчитано на базе модели Monod. Для численного интегрирования уравнений конвективно-диффузионного переноса активного ила и субстрата использована схема расщепления. Расщепление осуществлено так, чтобы на каждом шагу учитывался перенос субстрата (активного ила) только в одном направлении. Расчет неизвестной величины концентрации субстрата (активного ила) осуществлен по явной схеме. Для численного интегрирования трехмерного уравнения для потенциала скорости использован метод Рундсона, расчет неизвестного значения потенциала скорости осуществлен по явной формуле. Для численного интегрирования уравнений, описывающих процесс трансформации субстрата и изменение концентрации активного ила (модель Monod), использован метод Эйлера. **Результаты.** Осуществлена программная реализация построенной трёхмерной CFD -модели. Описана структура разработанного пакета программ. Представлены результаты проведенного компьютерного эксперимента по исследованию процесса очистки сточных вод в аэротенке с дополнительными элементами. **Научная новизна.** Разработана новая многофакторная трёхмерная CFD-модель, позволяющая быстро оценить эффективность биологической очистки сточных вод в аэротенке. **Практическая значимость.** Построенная CFD-модель может быть использована для анализа эффективности работы аэротенка при различных условиях эксплуатации и на этапе эскизного проектирования систем очистки сточных вод.

Ключевые слова: очистка воды; биологическая очистка воды; математическое моделирование; аэротенк; модель Monod

REFERENCES

1. Biliaiev, N. N., & Kozachina, V. A. (2015). *Modelirovaniye massoperenosa v gorizontalnykh otstoynikakh: monografiya*. Dnepropetrovsk: Aktsent PP. (in Russian)
2. Biliaiev, N. N., & Nagornaya, E. K. (2012). *Matematicheskoye modelirovaniye massoperenosa v otstoynikakh sistem vodootvedeniya: monografiya*. Dnepropetrovsk: Novaya ideologiya. (in Russian)
3. Vasilenko, O. A., Grabovskiy, P. O., Larkina, G. M., Polishchuk, O. V., & Progulny, V. Y. (2010). *Rekonstruktsiya i intensyfikatsiya sporud vodopostachannya ta vodovidvedennya: navchalnyy posibnyk*. Kyiv: IVNVKP «Ukrgeiotek». (in Ukrainian)
4. Karelin, Ya. A., Zhukov, D. D., Zhurov, V. N., & Repin, B. N. (1973). *Ochistka proizvodstvennykhstochnykh vod v aerotenkakh*. Moscow: Stroyizdat. (in Russian)
5. Laskov, Yu. M., Voronov, Yu. V., & Kalitsun, V. I. (1981). *Primery raschetov kanalizatsionnykh sooruzheniy*. Moscow: Vysshaya shkola. (in Russian)
6. Oleynik, A. Y., & Airapetyan, T. S. (2015). The modeling of the clearance of waste waters from organic pollutions in bioreactors-aerotanks with suspended (free flow) and fixed biocenoses. *Reports of the National Academy of Sciences of Ukraine*, 5, 55-60. DOI: <https://doi.org/10.15407/dopovidi2015.05.055> (in Ukrainian)
7. Alharbi, A. O. M. (2016). The biological treatment of wastewater: mathematical models. *Bulletin of the Australian Mathematical Society*, 94(2), 347-348. DOI: <https://doi.org/10.1017/S0004972716000411> (in English)
8. Amaral, A., Gillot, S., Garrido-Baserba, M., Filali, A., Karpinska, A. M., Plósz, B. G., ... Rosso, D. (2019). Modelling gas–liquid mass transfer in wastewater treatment: when current knowledge needs to encounter engineering practice and vice versa. *Water Science and Technology*, 80(4), 607-619. DOI: <https://doi.org/10.2166/wst.2019.253> (in English)
9. Babaei, A. A., Azadi, R., Jaafarzadeh, N., & Alavi, N. (2013). Application and kinetic evaluation of upflow anaerobic biofilm reactor for nitrogen removal from wastewater by Anammox process. *Iranian Journal of Environmental Health Science and Engineering*, 10(1), 1-8. DOI: <https://doi.org/10.1186/1735-2746-10-20> (in English)
10. Bomba, A., Klymiuk, Y., Prysiashniuk, I., Prysiashniuk, O., & Safonyk, A. (2016). Mathematical modeling of wastewater treatment from multicomponent pollution by through microporous filling. *AIP Conference Proceedings*, 1773, 040003-1-040003-11. DOI: <https://doi.org/10.1063/1.4964966> (in English)
11. Dapelo, D., & Bridgeman, J. (2020). A CFD strategy to retrofit an anaerobic digester to improve mixing performance in wastewater treatment. *Water Science and Technology*, 81(8), 1646-1657. DOI: <https://doi.org/10.2166/wst.2020.086> (in English)
12. Gao, H., & Stenstrom, M. K. (2019). Development and applications in computational fluid dynamics modeling for secondary settling tanks over the last three decades: A review. *Water Environment Research*, 92(6), 796-820. DOI: <https://doi.org/10.1002/wer.1279> (in English)
13. Gao, H., & Stenstrom, M. K. (2020). Influence of Model Parameters and Inlet Turbulence Boundary Specification Methods in Secondary Settling Tanks: Computational Fluid Dynamics Study. *Journal of Environmental Engineering*, 146(5), 04020028-1-04020028-12. DOI: [https://doi.org/10.1061/\(ASCE\)EE.1943-7870.0001689](https://doi.org/10.1061/(ASCE)EE.1943-7870.0001689) (in English)
14. Gao, H., & Stenstrom, M. K. (2020). Computational Fluid Dynamics Analysis for Improving Secondary Settling Tank Performance. *World Environmental and Water Resources Congress 2020*, 212-224. DOI: <https://doi.org/10.1061/9780784482988.021> (in English)
15. Griborio, A. (2004). *Secondary Clarifier Modeling: A Multi-Process Approach. Dissertation and Theses*. University of New Orleans: USA. (in English)
16. Mocanu, C. R., & Mihaillescu, R. (2012). Numerical Simulation Wastewater Treatment Aeration Processes. *U. P. B. Sci. Bull., Series D*, 74(2), 191-198. (in English)
17. Pereda, M., & Zamarreno, J. M. (2011). Agent–based modeling of an activated sludge process in batch reactor. *19th Mediterrian Conference on Control and Automation Aquis* (pp. 1128-1133). DOI: <https://doi.org/10.1109/med.2011.5983027> (in English)

Received: August 11, 2020

Accepted: December 11, 2020