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ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

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Mathematical models for water treatment problems

Purpose. Assessing the efficiency of water treatment in different structures is a problem of big importance. To solve this a problem, it is necessary to have mathematical models that allow to quickly obtain data on the cleaning effect in different structures. The aim of the work is to develop numerical models to determine the efficiency of water treatment in an aeration tanks, settlers and mixers. **Methodology**. For mathematical modeling of the process of water treatment in a bioreactor, balance equations were used. These equations allow to determine concentrations of substrate, activated sludge and dissolved oxygen in s structure. The Monod model is used to calculate the substrate oxidation process. To study effectiveness of water treatment process in vertical settler Euler's equation were used with convective-diffusive equation. To simulate reagent mixing in mixer equation of potential and convective-diffusive equation were used. To solve governing equations finite- difference schemes of splitting were used. **Findings.** A tool for theoretical assessment mass transfer processes in aeration tank, vertical settler, mixer was developed. **Originality.** Effective numerical models to simulate water treatment in bioreactor, vertical settler, mixer were developed. Fundamental equations of Fluid Dynamics and Mass Transfer were used to build the models. Proposed models can be used in practice at the stage of «sketch designing». The models take into account the main physical parameters which influence the process of Mass Transfer and are quick computing. **Practical value**. The constructed mathematical model can be useful during the reconstruction and designing structures for water treatment. Computer programs have been developed to carry out numerical experiment. The results of a computer experiment are presented.

Key words: water treatment; aeration tank; settler; mixer; mathematical modelling; water use

Introduction

The problem of water treatment is very important in the field of water use. Water treatment requires the use of various structures operating under different load conditions reagent mixer, air tanks, settlers, etc (Fig. 1–3) [2–3, 5–14]. The use of these structures requires application of efficient mathematical models. In practice for water treatment empirical, analytical models [2, 3, 5, 6] and numerical models [1, 9–11] are used.

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Fig. 1. Biological filter (https://cutt.ly/fe5McbC7)

Fig. 2. Aeration tank (https://cutt.ly/ue5MWnqx)

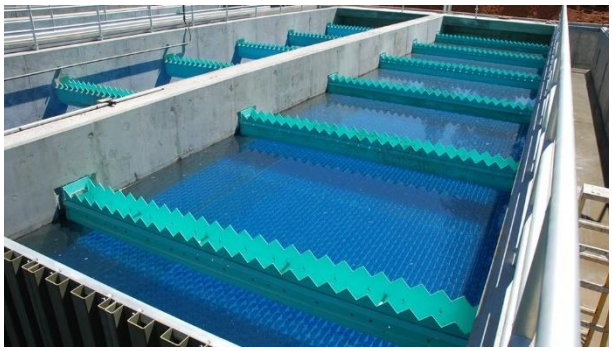

Fig. 3. Settler (https://cutt.ly/Oe5ME8xR)

It should be emphasized that for practice it is important to have quick computing numerical models. It is important that these models must take into account the most important physical factors. Such models are called “screening models” and are an effective tool in designing.

Purpose

The objective of this paper is development of numerical models to simulate mass transfer processes in bioreactors, settlers, mixers.

Methodology

Modeling biological wastewater treatment.

To describe the biological wastewater treatment process in the aeration tank the following equations are used [1, 13]:

$$\frac{dX}{dt} = Q(t)\cdot X_{in}(t) - \cdot Q(t)\cdot X + \mu\cdot X - K_d\cdot X; \quad (1)$$

$$\frac{dDO}{dt} = Q(t)\cdot DO_{in}(t) - Q(t)\cdot DO(t) + $$

$$+ \mathrm{K}_{La}(DO_{\max} - DO) - \frac{K_0\mu X}{Y}; \quad (2)$$

$$\frac{dS}{dt} = Q(t)\cdot S_{in}(t) - Q(t)\cdot S(t) - \frac{\mu X}{Y}; \quad (3)$$

$$\mu = \mu_{\max}\cdot\frac{S}{S+K_s}\cdot\frac{DO}{k_{DO}+DO}, \quad (4)$$

where t – time; $Q(t)$ – wastewater flow; $X_{in}(t)$ – concentration of activated sludge entering the aeration tank; S_{in} – the concentration of the substrate entering the aeration tank; K_d – coefficient that takes into account the rate of biomass extinction; DO – oxygen concentration in wastewater; $DO_{\max}$– the maximum value of oxygen concentration in wastewater; DO_{in} – oxygen concentration in wastewater entering the reactor; K_0, K_S, K_{La}, $\mu_{\max}$, k_{DO}, Y – parameters [13].

Equations (1)–(3) express the law of conservation of mass for substrate, dissolved oxygen and activated sludge in the reactor. Equation (4) shows the relationship between the biomass growth rate in the bioreactor as a function of the dissolved oxygen concentration and the substrate concentration in the bioreactor.

For the system of equations (1)–(3) it is necessary to set the initial conditions at t=0:

$$X = X_0; S = S_0; DO = DO_0.$$

Modeling equations (1)–(3) make it possible to determine how the concentration of the substrate (impurity) in the bioreactor, as well as dissolved oxygen and activated sludge, changes over time.

To solve governing equations Euler’s method was used, so difference equations were as follows:

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$$X^{n+1} = X^n + dt \cdot Q_w(t^n) \cdot X^n{}_{in}(t^n) - $$

$$-dt \cdot Q_w(t^n) \cdot X^n + dt \cdot \mu^n \cdot X^n, \quad (5)$$

$$S^{n+1} = S^n + dt \cdot Q_w(t^n) \cdot S^n{}_{in} -$$

$$-dt \cdot Q_w(t^n) \cdot S^n{}_{in}(t) - dt \cdot \frac{\mu^n}{Y \cdot W} X^{n+1}, \quad (6)$$

$$DO^{n+1} = DO^n + dt \cdot Q_w(t^n) \cdot DO^n{}_{in} -$$

$$-dt \cdot Q_w(t^n) \cdot DO^n\ (t) - dt \cdot \frac{K_o \mu^n}{Y \cdot W} X^{n+1}, \quad (7)$$

where $Q_w = \frac{Q}{W}$.

Coding of numerical model was carried out using FORTRAN.

Modeling water treatment in Settler.

To study effectiveness of wastewater treatment process in vertical settler the following equation was used:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial (v - w_g)C}{\partial y} =$$

$$= \frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right), \quad (8)$$

where C – pollutant concentration in wastewater which is treated in vertical settler; u, v – components of velocity vector; μ_x, μ_y – diffusion coefficients; w_g – Stocks's velocity of fallout.

Boundary conditions are as follows:

1) at inlet boundary:

$$C=C_{in},$$

where C_{in} is known concentration in wastewater;

2) at outlet boundary:

$$C(i+1, j)=C(i, j),$$

where $C(i+1, j)$ – concentration in the last computational cell; $C(i, j)$ is concentration in the previous computational cell;

3) at the solid surfaces: the boundary condition was as follows:

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

The initial condition is $C = C_0$, where C_0 – known concentration.

To construct numerical model of pollutant dispersion, equation (8) is split as follows:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} = \frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right), \quad (9)$$

$$\frac{\partial C}{\partial t} + \frac{\partial \nu C}{\partial y} = \frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right), \quad (10)$$

Further, the following transformation were made:

$$\frac{\partial uC}{\partial x} = \frac{\partial u^+ C}{\partial x} + \frac{\partial u^- C}{\partial x},$$

$$\frac{\partial vC}{\partial y} = \frac{\partial v^+ C}{\partial y} + \frac{\partial v^- C}{\partial y},$$

$$u^+ = \frac{u + |u|}{2}, u^- = \frac{u - |u|}{2}, v^+ = \frac{v + |v|}{2}, v^- = \frac{v - |v|}{2},$$

$$\frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) \approx \mu_x \frac{C^{n+1}_{i+1,j} - C^{n+1}_{i,j}}{\Delta x^2} -$$

$$-\mu_x \frac{C^{n+1}_{i,j} - C^{n+1}_{i-1,j}}{\Delta x^2} = M^-_{xx} C^{n+1} + M^+_{xx} C^{n+1},$$

$$\frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right) \approx \mu_y \frac{C^{n+1}_{i,j+1} - C^{n+1}_{i,j}}{\Delta y^2} -$$

$$-\mu_y \frac{C^{n+1}_{i,j} - C^{n+1}_{i,j-1}}{\Delta y^2} = M^-_{yy} C^{n+1} + M^+_{yy} C^{n+1},$$

$$\frac{\partial u^+ C}{\partial x} \approx \frac{u^+_{i+1,j} C^{n+1}_{i,j} - u^+_{i,j} C^{n+1}_{i-1,j}}{\Delta x} = L^+_x C^{n+1},$$

$$\frac{\partial u^- C}{\partial x} \approx \frac{u^-_{i+1,j} C^{n+1}_{i+1,j} - u^-_{i,j} C^{n+1}_{i,j}}{\Delta x} = L^-_x C^{n+1},$$

$$\frac{\partial \nu^+ C}{\partial y} \approx \frac{\nu^+_{i,j+1} C_{i,j} - \nu^+_{i,j} C_{i,j-1}}{\Delta y} = L^+_y C^{n+1},$$

$$\frac{\partial \nu^- C}{\partial y} \approx \frac{\nu^-_{i,j+1} C_{i,j+1} - \nu^-_{i,j} C_{i,j}}{\Delta y} = L^-_y C^{n+1}.$$

After these transformations, the following finite difference scheme was used to solve equation (6):

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– at the first step:

$$\frac{C^k_{i,j,k} - C^n_{i,j,k}}{\Delta t} + L^+_x C^k = M^+_{xx} C^k + M^-_{xx} C^n;$$

– at the second step:

$$\frac{C^{n+1}_{i,j,k} - C^k_{i,j,k}}{\Delta t} + L^-_x C^{n+1} = M^+_{xx} C^n + M^-_{xx} C^{n+1}.$$

Finite difference scheme to integrate equation (7) has the following view

– at the first step:

$$\frac{C^k_{i,j,k} - C^n_{i,j,k}}{\Delta t} + L^+_y C^k = M^+_{yy} C^k + M^-_{yy} C^n,$$

– at the second step:

$$\frac{C^{n+1}_{i,j,k} - C^k_{i,j,k}}{\Delta t} + L^-_y C^{n+1} = M^+_{yy} C^n + M^-_{yy} C^{n+1}.$$

To integrate equation (5) it is necessary to know the velocity inside settler. To solve this problem the following governing equations were used:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\omega; \qquad (11)$$

$$\frac{\partial \omega}{\partial t} + \frac{\partial u\omega}{\partial x} + \frac{\partial v\omega}{\partial y} = 0 \qquad (12)$$

where $\omega = \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}$ – vorticity; ψ – flow function.

Velocity components are determined as follows:

$$\frac{\partial \psi}{\partial x} = -v; \quad \frac{\partial \psi}{\partial y} = u.$$

Boundary and initial conditions are described in [4].

To solve equation of vorticity transfer two-steps scheme of splitting was used:

– at the first step:

$$\frac{\omega^{n+1/2}_{i,j} + \omega^n_{i,j}}{\Delta t} + \frac{u^+_{i+1,j}\omega^{n+1/2}_{i,j} - u^+_{i+1,j}\omega^{n+1/2}_{i-1,j}}{\Delta x} + \frac{\nu^+_{i,j+1}\omega_{i,j} - \nu^+_{i,j-1}\omega_{i,j-1}}{\Delta y} = 0;$$

– at the second step:

$$\frac{\omega^{n+1}_{ij} - \omega^{n+1}_{ij}}{\Delta t} + \frac{u^-_{i+1,j}\omega^{n+1}_{i+1,j} - u^-_{i,j}\omega^{n+1}_{i,j}}{\Delta x} + \frac{\nu^-_{i,j+1}\omega^{n+1}_{i,j+1} - \nu^-_{i,j-1}\omega^{n+1}_{i,j}}{\Delta y} = 0.$$

To solve equation for flow function, it was written in the following form:

$$\frac{\partial \psi}{\partial \eta} = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \omega,$$

where η – «fictitious» time.

Further, the following scheme of splitting was used:

– at the first step:

$$\frac{\psi^{n+1/4}_{ij} - \psi^n_{ij}}{\Delta t} = \frac{\overline{\psi_{ij}}}{2};$$

– at the second step:

$$\frac{\psi^{n+1/2}_{i,j} - \psi^n_{i,j}}{\Delta t} = -\frac{\psi^{n+1/2}_{i,j} - \psi^{n+1/2}_{i-1,j}}{\Delta x^2} - \frac{\psi^{n+1/2}_{i,j} - \psi^{n+1/2}_{i,j-1}}{\Delta y^2};$$

– at the third step:

$$\frac{\psi^{n+3/4}_{i,j} - \psi^{n+1/2}_{ij}}{\Delta t} = \frac{\psi^{n+3/4}_{i+1,j} - \psi^{n+3/4}_{i,j}}{\Delta x^2} + \frac{\psi^{n+3/4}_{i,j+1} - \psi^{n+3/4}_{i,j}}{\Delta y^2};$$

– at the fourth step:

$$\frac{\psi^{n+1}_{ij} - \psi^{n+3/4}_{ij}}{\Delta t} = \frac{\overline{\omega_{i,j}}}{2},$$

where $\overline{\omega_{i,j}} = \frac{1}{4}\left(\omega_{i,j} + \omega_{i-1,j+1}\omega_{i-1,j-1} + \omega_{i,j-1}\right)$.

Computational procedure is finished when the following condition is fulfilled:

$$\left|\psi^{n+1}_{i,j} - \psi^n_{i,j}\right| \le \varepsilon,$$

where $\varepsilon = 0.001$, n – iteration number.

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To compute vorticity at the corner points special procedure was used [4]. Velocity components were calculated as follows:

$$u_{i,j} = \frac{\psi_{i,j+1} - \psi_{i,j}}{\Delta y}, \quad v_{i,j} = -\frac{\psi_{i+1,j} - \psi_{i,j}}{\Delta x}.$$

Velocity components were used when numerical integration of equation (5) was carried out.

Modeling reagent transfer in mixer.

To simulate the process of reagent dispersion in mixer two governing equations were used:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial (v - w_g)C}{\partial y} = $$

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

$$+ Q\delta(x - x_i)\delta(y - y_i), \quad (13)$$

$$\frac{\partial R}{\partial t} + \frac{\partial uR}{\partial x} + \frac{\partial vR}{\partial y} =$$

$$= kC + \frac{\partial}{\partial x}\left(\mu_x \frac{\partial R}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial R}{\partial y}\right), \quad (14)$$

where C – insoluble reagent concentration in water; R – dissolved reagent concentration in water; k – coefficient of dissolution rate; u, v – components of water velocity vector; w_g – gravity fallout speed; μ_x, μ_y – diffusion coefficients; Q – reagent rate supply into mixer; x_i, y_i – coordinates of reagent supply.

Boundary conditions for equation (13) and equation (14) are similar to the boundary conditions for equation (8).

Flow in the mixer was simulated using model of potential flow. In this case the governing equation was:

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} = 0, \quad (15)$$

where P is velocity potential.

Components of velocity vector are determined as follows:

$$u = \frac{\partial P}{\partial x}, v = \frac{\partial P}{\partial y}.$$

Boundary conditions are:

1. At inlet boundary: $\frac{\partial P}{\partial x} = V_0$, where V_0 – known velocity.

2. At outlet boundary: P=Const.

3. At the solid boundaries: $\frac{\partial P}{\partial n} = 0$, n – normal to the solid surface.

Method of equations numerical integration is considered only for equation (14), because equation (13) and equation (14) are equivalent from mathematical point of view, both are convective-diffusive equations.

Firstly equation (14) was split as follows:

$$\frac{\partial R}{\partial t} + \frac{\partial uR}{\partial x} + \frac{\partial vR}{\partial y} = 0, \quad (15)$$

$$\frac{\partial R}{\partial t} = \frac{\partial}{\partial x}\left(\mu_x \frac{\partial R}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial R}{\partial y}\right), \quad (16)$$

$$\frac{\partial R}{\partial t} = kC. \quad (17)$$

Finite difference scheme for equation (15) is written as follows:

– at the first step:

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

– at the second step:

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

where $L_x^+, L_y^+, L_y^+, L_y^-$ are finite-difference operators which were mentioned above.

To solve equation (16) two steps scheme of conditional approximation was used:

– at the first step:

$$\frac{R_{i,j}^{n+\frac{1}{2}} - R_{i,j}^n}{\Delta t} =$$

$$= \left[\mu_x \frac{-R_{i,j}^{n+\frac{1}{2}} + R_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2}\right] + \left[\mu_y \frac{-R_{i,j}^{n+\frac{1}{2}} + R_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2}\right];$$

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– at the second step:

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

Euler's method was used for equation (17) integration.

FORTRAN was used for coding equations of all described numerical models.

Findings

Below are the results of model problem solution for vertical settler. The aim of simulation was to be ensure that developed models can model mass transfer in regions with comprehensive geometrical form without losing stability.

Four Scenarios were considered for vertical settler:

1. Scenario # 1: vertical settler, no additional elements inside (Fig. 4).
2. Scenario # 2: vertical settler with additional element: short plate (Fig. 5).
3. Scenario # 3: vertical settler with additional element: long plate (Fig. 6).
4. Scenario # 4: vertical settler with two additional elements (Fig. 7).

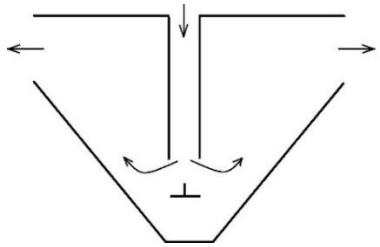

Fig. 4. Sketch of computational region, Scenario #1, no additional elements in settler

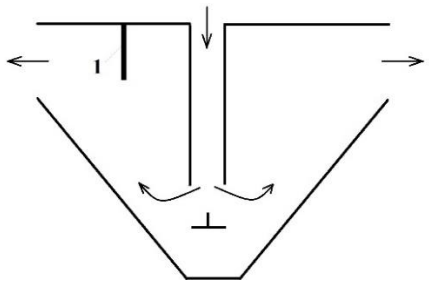

Fig. 5. Sketch of computational region, Scenario #2, short plate

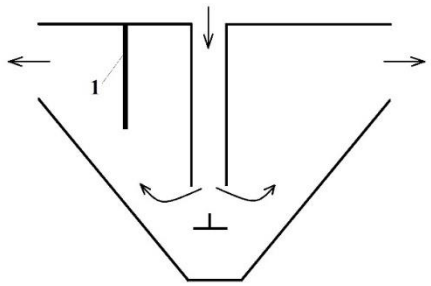

Fig. 6. Sketch of computational region, Scenario #3, long plate

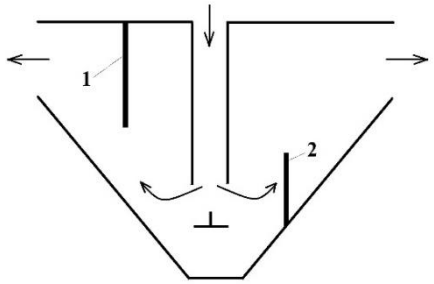

Fig. 7. Sketch of computational region, Scenario #4, two additional plates

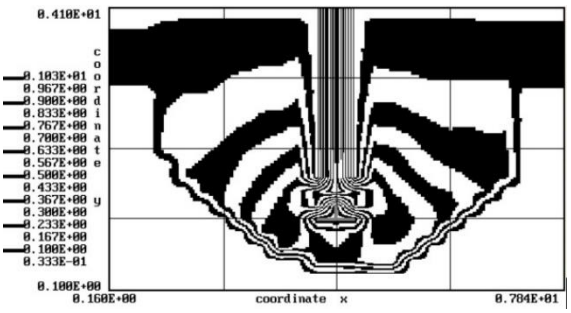

Fig.8 Pollutant concentration inside settler, Scenario #1

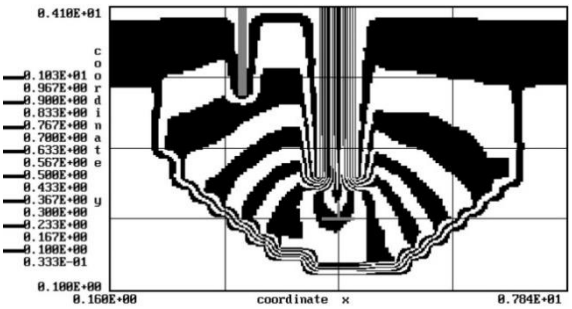

Fig. 9. Pollutant concentration inside settler, Scenario #2

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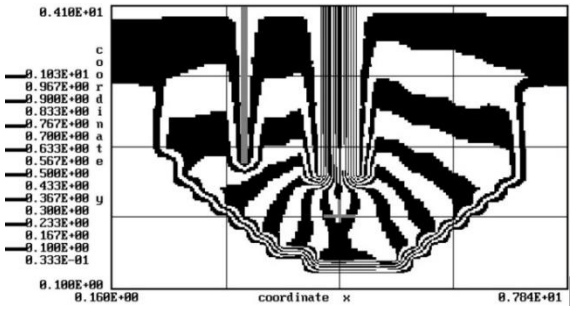

Fig. 10. Pollutant concentration inside settler, Scenario #3

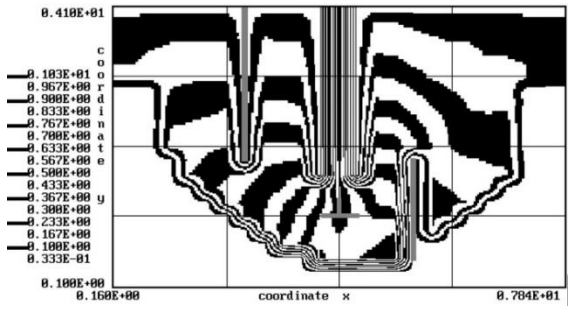

Fig. 11. Pollutant concentration inside settler, Scenario #4

As can be seen from the figures above, additional elements inside the settler causes deformation of pollutant concentration field. Near these elements regions with high gradient concentrations were formed.

Loss of stability was not occurred during the computational experiment. The calculation time was 3 s for each scenario.

Originality and Practical value

The article discusses effective numerical models to simulate water treatment in bioreactor, vertical settler, mixer. Fundamental equations of Fluid Dynamics and Mass Transfer were used to build the models.

The proposed models can be used in practice at the stage of «sketch designing». The models take into account the main physical parameters wch influence the process of Mass Transfer and are quick computing.

Conclusions

1. The article proposes effective numerical models for analyzing the processes of mass transfer in different structures for water treatment.
2. The models will be useful at the stage of «sketch designing».
3. In the future, this scientific direction should be developed in the field of developing three-dimensional numerical models for analyzing the processes of mass transfer.

LIST OF REFERENCE LINKS

1. Біляєв М. М., Козачина В. А., Гунько О. Ю., Лемеш М. В. *Комп'ютерне моделювання процесів біологічної очистки стічних вод*. Дніпро : Журфонд, 2023. 186 с.
2. Василенко О. А., Грабовський П. О., Ларкіна Г. М., Поліщук О. В., Прогульний В. Й. *Реконструкція і інтенсифікація споруд водопостачання та водовідведення*. Київ : Укргеліотех, 2010. 272 с.
3. Гіроль М. М., Гіроль А. М., Гіроль А. М. *Технології водовідведення промислових підприємств*. Рівне : НУВГП, 2013. 625 с.
4. Згуровский М. З., Скопецкий В. В., Хрущ В. К., Беляев Н. Н. *Численное моделирование распространения загрязнения в окружающей среде*. Киев : Наукова думка, 1997. 368 с.
5. Ковальчук В. А. *Очистка стічних вод*. Рівне : ВАТ «Рівненська друкарня», 2002. 622 с.
6. Олійник О. Я., Айрапетян Т. С. Моделювання очистки стічних вод від органічних забруднень в біореакторах-аеротенках зі зваженим (вільноплаваючим) і закріпленим біоценозом. *Доповіді Національної академії наук 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. Babaei A., Azadi R., Jaafarzadeh N., Alavi N. Application and Kinetic Evaluation of upflow Anaerobic biofilm 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
9. 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

doi: https://doi.org/10.15802/stp2025/324157

10. 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
11. Gao H., Stenstrom MK 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
12. Mocanu C. R., Mihaillescu R. Numerical Simulation of Wastewater Treatment Aeration Processes. *UPB Scientific Bulletin, Series D: Mechanical Engineering.* 2012. Vol. 74. Iss. 2. P. 191–198.
13. Pereda M., Zamarreno J. M. Agent – based modeling of an activated sludge process in batch reactor. *2011 19th Mediterranean Conference on Control & Automation (MED)* (Corfu, 20-23 June 2011). Corfu, 2011. P. 1128–1133. DOI: https://doi.org/10.1109/med.2011.5983027
14. Vilanova R., Rojas J. D., Alfaro V. M. Digital Control of a Waste Water Treatment Plant. *International Journal of Computers Communications & Control*. 2011. Vol. 6, No. 2. P. 367–374. DOI: https://doi.org/10.15837/ijccc.2011.2.2184

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Математичні моделі в задачах очищення води

Мета. Оцінка ефективності очищення води в різних спорудах є актуальною проблемою. Для її вирішення необхідно мати математичні моделі, які дозволяють швидко отримувати дані про ефективність очищення в різних спорудах. Основною метою роботи є розробка чисельних моделей для визначення ефективності очищення води в аеротенках, відстійниках та змішувачах. **Методика**. Для математичного моделювання процесу очищення води в біореакторі використано балансові рівняння. Ці рівняння дозволяють визначити концентрації субстрату, активного мулу та розчиненого кисню в його складі. Для розрахунку процесу окислення субстрату використано модель Моно. Під час дослідження ефективності процесу очищення води у вертикальному відстійнику рівняння Ейлера було доповнено конвективно-дифузійним рівнянням. Для моделювання перемішування реагентів у змішувачі використано рівняння потенціалу та конвективно-дифузійне рівняння. Розв'язання моделювальних рівнянь здійснено за допомогою скінченнорізницевих схем розщеплення. **Результати**. Розроблено інструмент для теоретичної оцінки масообмінних процесів в аеротенку, вертикальному відстійнику, змішувачі. **Наукова новизна**. Розроблено ефективні чисельні моделі для визначення процесів очищення води в біореакторі, вертикальному відстійнику, змішувачі. Для побудови моделей взято фундаментальні рівняння гідродинаміки та масообміну. Запропоновані моделі можуть бути використані на практиці на стадії «ескізного проєктування». Моделі враховують основні фізичні параметри, які впливають на процес масообміну, і є швидкими в обчисленні. **Практична значимість**. Побудовані матема-

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тичні моделі можуть бути корисними під час реконструкції та проєктування споруд для водопідготовки та очистки стічних вод. Розроблено комп'ютерні програми для проведення чисельного експерименту. Представлено результати комп’ютерного експерименту.

Ключові слова: водопідготовка; аеротенк; відстійник; змішувач; математичне моделювання; водокористування

REFERENCES

1. Biliaiev, M. M., Kozachyna, V. A., Gunko, O. Yu., & Lemesh, M. V. (2023). *Kompiuterne modeliuvannia protsesiv biolohichnoi ochystky stichnykh vod*. Dnipro: Zhurfond. (in Ukrainian)
2. Vasylenko, O. A., Grabovsky, P. O., Larkina, G. M., Polishchuk, O. V., & Progulny, V. Y. (2010). *Rekonstruktsiia i intensyfikatsiia sporud vodopostachannia ta vodovidvedennia*. Kyiv: IVNVKP «Ukrgeliotek». (in Ukrainian)
3. Hirol, M. M., Hirol, A. M., & Hirol, A. M. (2013). *Tekhnolohii vodovidvedennia promyslovykh pidpryiemstv*. Rivne: NUWEE. (in Ukrainian)
4. Zgurovsky, M. Z., Skopetsky, V. V., Khrushch, V. K., & Biliaiev, M. M. (1997). *Chyslennoe modelyrovanye rasprostranenyia zahriaznenyia v okruzhaiushchei srede*. Kyiv: Naukova dumka. (in Russian)
5. Kovalchuk, V. A. (2002). *Ochystka stichnykh vod*. Rivne: «Rivnenska drukarnia». (in Ukrainian)
6. Oliinyk, O. Ya., & 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. 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)
9. 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)
10. Gao, H., & Stenstrom M. K. (2019). Development and applications in CFD 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)
11. 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 (in English)
12. Mocanu, C. R., & Mihaillescu, R. (2012). Numerical Simulation of Wastewater Treatment Aeration Processes. *UPB Scientific Bulletin, Series D: Mechanical Engineering, 74*(2), 191-198. (in English)
13. Pereda, M., & Zamarreno, J. M. (2011, June). Agent-based modeling of an activated sludge process in a batch reactor. In *2011 19th Mediterranean Conference on Control & Automation (MED)* (pp. 1128-1133). Corfu, Greece. DOI: https://doi.org/10.1109/med.2011.5983027 (in English)
14. Vilanova, R., Rojas, J. D., & Alfaro, V. M. (2011). Digital Control of a Waste Water Treatment Plant. *International Journal of Computers Communications & Control, 6*(2), 367-374. DOI: https://doi.org/10.15837/ijccc.2011.2.2184 (in English)

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