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MODELING OF BIOLOGICAL WASTEWATER TREATMENT ON THE BASIS OF QUICK-COMPUTING NUMERICAL MODEL

Purpose. The scientific paper involves the development of quick computing numerical model for prediction of output parameters of aeration tank. The numerical model may be used in predicting the effectiveness of aeration tank under different regimes of work. **Methodology.** To simulate the process of biological wastewater treatment in aeration tank numerical models were developed. The flow field in the aeration tank is simulated on the basis of potential flow model. 2-D transport equations are used to simulate substrate and sludge dispersion in the aeration tank. To simulate the process of biological treatment simplified model. For the numerical integration of transport equations implicit difference scheme was used. The difference scheme is built for splitting transport equations. Splitting of transport equation into two equations is carried out at differential level. The first equation of splitting takes into account the sludge or substrate movement along trajectories. The second splitting equation takes into account the diffusive process of substrate or sludge. To solve the splitting equations implicit difference scheme was used. For the numerical integration of potential flow equation the implicit scheme of conditional approximation was used. On the basis of constructed numerical model computer experiment was performed to investigate the process of biological treatment in aeration tank. **Findings.** Quick computing numerical model to simulate the process of biological treatment in the aeration tank was developed. The model can be used to obtain aeration tank parameters under different regimes of work. The developed model takes into account the geometrical form of the aeration tank. **Originality.** The numerical model which takes into account the geometrical form of aeration tank and fluid dynamics process was developed; the model takes into account substrate and sludge transport in aeration tank and process of biological treatment. **Practical value.** Efficient numerical model, so called «diagnostic models» was proposed for quick calculation of biological treatment process in aeration tank.

Keywords: biological treatment; numerical simulation; aeration tank

Introduction

Aeration tanks (AT) are widely used in practice for biological wastewater treatment at treatment plants. AT are used for industrial or municipal wastewaters treatment and may work under different regimes. There are different types of AT but in practice so called «*vitesnitel»* AT (AT of displacement type) is often used: In this AT influent (waste waters) and sludge, which is used for biological treatment, are supplied at one side of the AT (inlet boundary) and are discharged at the opposite side (outlet boundary) (Fig.1).

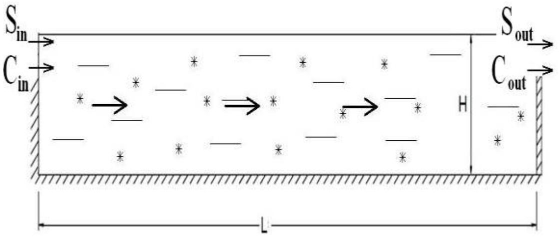

Fig. 1. Aeration tank «*vitesnitel»*
(AT of displacement type)

Literature review

Mathematical models which are used for aeration tank calculation can be separated in some classes. First of all we have to mention empirical models which were built on the basis of physical experiments [5, 7]. These models have the form of

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simple algebraic formulae with some empirical coefficients. These models are widely used in Ukraine but for calculation of typical AT and for the typical regimes of work for which the empirical constants were obtained. We can't use these models for scientific research, for example, to predict the output parameters after treatment in the case which is out of the normal work of aeration tank.

The second class of the models includes mass balance models. These models can be named «zero-dimentional» models. The balance models are very popular [3, 4, 8, 17] and take into account some important parameters of aeration tank work. These models are based on the ordinary differential equations which represent mass balance of sludge, admixture or oxygen in aeration tank. These differential equations can be solved analytically or numerically (for example using Runge – Kutte method). Some commercial codes can be used to perform calculations on the basis of these models. These models are very convenient for prediction of aeration tank output parameters but the models do not take into account the fluid dynamics process in AT.

The models of the third class are based on «one–dimentional» equations of mass transport to simulate, for example, substrate dispersion in AT [6, 9]. The modeling equations are solved analytically. Fluid dynamics is taken into account in these models but for the case of constant velocity in AT.

CFD models are the most «powerful» models at present time to solve the problems of wastewater treatment [1, 2, 10, 12-15]. These models can reproduce the flow field in the AT and admixture transfer for different regimes of work with account of AT geometrical form. As a rule the CFD experiments are performed using commercial codes (for example, ANSYS, Fluent) [11, 12, 16, 17]. CFD experiments comprise of two steps. The first step is computation of flow field. Very often this flow field is computed using of Navier – Stokes equations. The second step is simulation of admixture transfer on the basis of computed flow field. Application of Navier-Stokes equations needs much computing time (to solve some problems it may take from 90h to some weeks to perform CFD experiment). It is not convenient in case of many calculations during AT design or at stage of AT reengineering.

Purpose

The purpose of this work is the development of quick-computing numerical model to simulate the process of biological wastewater treatment in «*vitesnitel»* aeration tank (aeration tank of displacement type).

Mathematical model

To simulate the process of biological treatment in AT, at each time step of mathematical simulation, we separate the process in two stages. At first stage we consider the process of substrate and sludge movement in the aeration tank. It is so called «mass transfer» process. To simulate this process we use the following 2-D transport equations (plan model) [7, 12]:

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial \nu C}{\partial y}=div\left(\mu gradC\right), \tag{1}$$

$$\frac{\partial S}{\partial t}+\frac{\partial uS}{\partial x}+\frac{\partial \nu S}{\partial y}=div\left(\mu\, grad\, S\right), \tag{2}$$

where $C\left(x,y\right)=\frac{1}{H}\int_{0}^{H}C\left(x,y,z\right)dz$ – is the averaged concentration of substrate; H – is the depth of the aeration tank (Fig.1); $S\left(x,y\right)=\frac{1}{H}\int_{0}^{H}S\left(x,y,z\right)dz$ – is the averaged concentration of sludge for biological treatment; u,v – are the flow velocity components in *x, y* direction respectively; $\mu=\left(\mu_x,\mu_y\right)$ – are the coefficients of turbulent diffusion in x, y direction respectively; t – is time.

The boundary conditions for these equations are as following:

1. at the inlet opening the boundary condition is

$$C=C_{in}, S=S_{in}, \tag{3}$$

where C_{in}, S_{in} are known concentrations of substrate and sludge respectively.

2. at the outlet opening the boundary condition in the numerical model (Fig.2) is written as follows

$$\begin{gathered} C\left(i+1,j\right)=C\left(i,j\right), \\ S\left(i+1,j\right)=S\left(i,j\right), \end{gathered} \tag{4}$$

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where $C(i+1,j), S(i+1,j)$ are concentrations at the last computational cell; $C(i,j), S(i,j)$ are concentrations at the previous computational cell.

Boundary condition (4) means that we neglect the diffusion process at the outlet boundary.

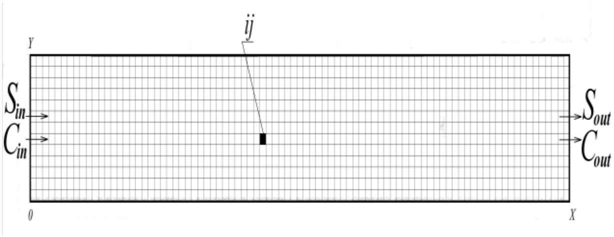

Fig. 2. Sketch of computational domain

3. at the solid walls the boundary condition is

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

where n is normal vector to the boundary.

The initial condition, for $t = 0$, is

$$C = C_0, S = S_0,$$

where C_0, S_0 are known concentrations of substrate and sludge respectively in computational domain.

At the second stage of mathematical simulation we consider the biological process in the aeration tank. To simulate this process in each computational cell inside the aeration tank we use the following simplified model

$$\frac{dC(t)}{dt} = -\frac{\mu(t)}{Y} S(t), \tag{5}$$

$$\frac{dS(t)}{dt} = \mu(t) S(t), \tag{6}$$

where μ is biomass growth rate; Y is biomass yield factor.

To calculate biomass growth rate Monod law is used.

As the initial condition for each equation (5), (6), at each time step, we use the meaning of C, S obtained after computing Eq. 1, 2.

To solve Eq.1, 2 it is necessary to know the flow field in aeration tank. To simulate this flow field we use model of potential flow. In this case the governing equation is

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} = 0, \tag{7}$$

where P is the potential of velocity.

The velocity components are calculated as follows:

$$u = \frac{\partial P}{\partial x}, \ v = \frac{\partial P}{\partial y}. \tag{8}$$

Boundary conditions for equation (7) are [5]:

1. At the inlet boundary $\frac{\partial P}{\partial n} = V$, where V is known velocity.
2. At the outlet boundary P=const.
3. At the solid boundaries $\frac{\partial P}{\partial n} = 0$.

Numerical model

To perform numerical integration of governing equations rectangular grid was used. Concentration of substrate, sludge and P were determined in the centers of computational cells. Velocity components *u, v* were determined at the sides of computational cells.

To solve equation (7) we used the difference scheme of «conditional approximation». To use this scheme we wrote Eq. 5 in «unsteady» form

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2}, \tag{9}$$

where t is «fictitious» time.

It's known that for t solution of Eq.9 tends to the solution of Eq. 7.

We split the process of Eq. 9 in two steps and difference equations at each step are as follows [4]:

$$\frac{P_{i,j}^{n+\frac{1}{2}} - P_{i,j}^{n}}{\Delta t} = \left[\frac{-P_{i,j}^{n+\frac{1}{2}} + P_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2}\right] + \left[\frac{-P_{i,j}^{n+\frac{1}{2}} + P_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2}\right], \tag{10}$$

$$\frac{P_{i,j}^{n+1} - P_{i,j}^{n+\frac{1}{2}}}{\Delta t} = \left[\frac{P_{i+1,j}^{n+1} - P_{i,j}^{n+1}}{\Delta x^2}\right] + \left[\frac{P_{i,j+1}^{n+1} - P_{i,j}^{n+1}}{\Delta y^2}\right]. \tag{11}$$

The calculation on the basis of these formulas is complete if the following condition is fulfilled:

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

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where ε is a small number; n is iteration number.

Difference scheme of splitting (10), (11) is implicit but unknown value of P is calculated, at each step of splitting, using explicit formula of *«running calculation»*. That is very convenient for programming the difference formulae.

To solve Eq. 9 it is necessary to set initial condition for fictitious time $t = 0$. The initial condition is

$$P = P_0,$$

where P_0 is known value of potential in computational domain.

If we know field of P in computational domain we can compute velocity components at the side of computational cells

$$u_{ij} = \frac{P_{i,j} - P_{i-1,j}}{\Delta x}, \tag{12}$$

$$v_{ij} = \frac{P_{i,j} - P_{i,j-1}}{\Delta y}. \tag{13}$$

Main features of the implicit difference scheme to solve numerically Eq. 1, 2 we consider only for equation of substrate transport because Eq. 1 and 2 are similar from mathematical point of view. Before numerical integration we split transport equation in two equations. The scheme of splitting is as follows

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} = 0, \tag{14}$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(\mu \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu \frac{\partial C}{\partial y}\right). \tag{15}$$

From the physical point of view, equation (14) takes into account substrate movement along trajectories, equation (15) takes into account the process of substrate diffusion in aeration tank. After that splitting the approximation of equation (12) is carried out. Time dependent derivative is approximated as follows:

$$\frac{\partial C}{\partial t} \approx \frac{C_{ij}^{n+1} - C_{ij}^{n}}{\Delta t}.$$

The convective derivatives are represented as:

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

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

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

$$\frac{\partial u^{-}C}{\partial x} \approx \frac{u_{i+1,j}^{-}C_{i+1,j}^{n+1} - u_{i,j}^{-}C_{i,j}^{n+1}}{\Delta x} = L_x^{-}C^{n+1},$$

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

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

At the next step we write the finite difference scheme of splitting:

– at the first step k=1/2:

$$\frac{C_{ij}^{n+k} - C_{ij}^{n}}{\Delta t} + \frac{1}{2}\left(L_x^{+}C^{k} + L_y^{+}C^{k}\right) = 0; \tag{16}$$

– at the second step k=1, c=n+1/2:

$$\frac{C_{ij}^{k} - C_{ij}^{c}}{\Delta t} + \frac{1}{2}\left(L_x^{-}C^{k} + L_y^{-}C^{k}\right) = 0. \tag{17}$$

This difference scheme is implicit and absolutely steady but unknown concentration C is calculated using the explicit formulae at each step («method of running calculation»).

Further, Eq. (15) is numerically integrated using implicit difference scheme (10), (11). To solve Eq. 3, 4 we used Eurler method. On the basis of developed numerical model code «*BIOTreat*» was developed. FORTRAN language was used to code the solution of difference equations.

Description of computational procedure

Numerical solution of the whole problem is as follows:

– **Step 1**: we compute potential P in aeration tank (Eq. 8, 9)

– **Step 2:** we compute velocity components (Eq. 10, 11)

– **Step 3**: we compute biological process in aeration tank (Eq. 3, 4)

– **Step 4:** we compute substrate and sludge

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transport in aeration tank (governing equations 1, 3; numerical equations 14, 15 (for C and S) and Eq. 8, 9 written for C and S)

– **Step 5:** for the next time level *t,* the computational procedure repeats from step 3.

Case Study. Developed code «*BIOTrea*» was used to solve the following model problem. The aeration tank is filled with sludge (concentration S_0=2) and substrate (concentration C_0=100) at time t=0. All parameters of the problem are dimensionless. During time period from t=0 till t=*2* the inlet and outlet openings are closed and no flow in the aeration tank. It means that for this time period only biological treatment takes place and we solve only Eq. 3, 4 of the model. At time t=2 the inlet and outlet openings are open and the transport process starts. At the inlet opening the substrate concentration is equal to C_0=100 and sludge concentration is equal to S_0=2. Also at this time five sources of sludge supply inside the aeration tank starts to work with intensity Q_i. Position of these sources can be seen in Fig. 4 where the influence of these sources results in local 'deformation' of concentration field. This field has practically small concentration gradient in aeration tank everywhere except points where sources of sludge supply are situated.

In Fig. 3 we present sludge and substrate concentration change near the outlet opening of the aeration tank (point A in Fig.4). From Fig. 3 we can see that the process of biological treatment accelerates from t=2 and concentration of sludge at the outlet opening increases with time.

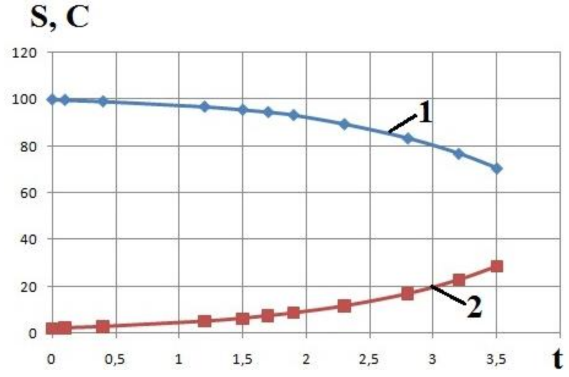

Fig. 3. Sludge and substrate concentration change near the outlet opening:
1 – substrate concentration; *2* – sludge concentration

In Fig. 4 the concentration field of sludge for time step t=4 is shown. It is well seen the zones of sludge sources influences. These zones have form of circles.

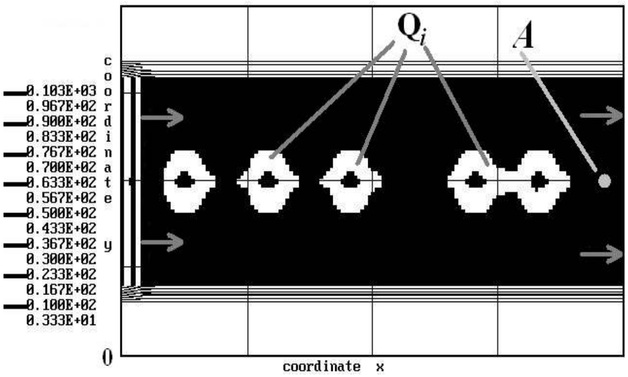

Fig. 4. Field of sludge concentration inside the aeration tank, t=4:
1 – position of sludge supply sources

Findings

Quick computing numerical model was developed to simulate the wastewater treatment in aeration tank. The model does not take much time because the fluid dynamics process is simulated on the basis of potential flow model.

Originality and practical value

A new numerical model to predict the output parameters of aeration tank was developed. The model is based on the 2-D transport equations of substrate and sludge and simplified equations of biological treatment. The developed model takes into account geometrical form of aeration tank. The model can be useful in aeration tanks design.

Conclusions

The article contains results of numerical model development for wastewater treatment in «vitesnitel» aeration tank (aeration tank of displacement type). To simulate the process of biological treatment 2-D transport equations of substrate and sludge are used together with simplified models of biological treatment. The future work in this field will be connected with development of fluid dynamics model which takes into account oxygen transfer in the aeration tank.

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МОДЕЛЮВАННЯ БІОЛОГІЧНОЇ ОЧИСТКИ СТІЧНИХ ВОД НА ОСНОВІ ШВИДКОДІЮЧОЇ ЧИСЕЛЬНОЇ МОДЕЛІ

Мета. Наукова робота передбачає розробку швидкодіючої чисельної моделі для прогнозування вихідних параметрів аеротенка. Чисельну модель можна використовувати для прогнозування ефективності аеротенка при різних режимах роботи. **Методика.** Для моделювання процесу біологічної очистки стічних вод в аеротенках були розроблені чисельні моделі. Поле потоку в аеротенку відтворюється на основі моделі потенційної течії. 2-D рівняння масопереносу використовуються для моделювання розсіювання субстрату і мулу. Для моделювання процесу біологічної обробки застосовується спрощена модель. Для чисельного інтегрування рівнянь переносу вживалася неявна різницева схема. Різницева схема побудована для розщеплення рівнянь переносу. Розщеплення рівняння переносу здійснюється на два рівняння та виконується на диференціальному рівні. Перше рівняння розщеплення враховує рух мулу або субстрату по траєкторіях, а друге – дифузний процес перенесення домішки і мулу. Для вирішення рівнянь розщеплення використовувалася неявна різницева схема. Для чисельного інтегрування рівняння потенційної течії застосовувалася неявна схема умовного наближення. На основі побудованої чисельної моделі був виконаний комп'ютерний експеримент для дослідження процесу біологічної очистки в аеротенку. **Результати.** Розроблена чисельна модель дозволяє швидко моделювати процес біологічної очистки в аеротенку. Модель може використовуватися для оцінки ефективності роботи аеротенків при різних режимах роботи. Розроблена модель враховує геометричну форму аеротенка. **Наукова новизна.** Розроблено чисельну модель, що враховує геометричну форму аеротенка та процес динаміки рідини, а також процес руху субстрату і мулу в аеротенку. **Практична значимість**. Запропоновано ефективну чисельну модель класу «diagnostic models» для швидкого розрахунку процесу біологічної очистки в аеротенку.

Ключові слова: біологічна очистка; чисельне моделювання, аеротенк

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МОДЕЛИРОВАНИЕ БИОЛОГИЧЕСКОЙ ОЧИСТКИ СТОЧНЫХ ВОД НА ОСНОВЕ БЫСТРОДЕЙСТВУЮЩЕЙ ЧИСЛЕННОЙ МОДЕЛИ

Цель. Научная работа предполагает разработку быстродействующей численной модели для прогнозирования выходных параметров аэротенка. Численную модель можно использовать для прогнозирования эффективности аэротенка при различных режимах работы. **Методика.** Для моделирования процесса биологической очистки сточных вод в аэротенке были разработаны численные модели. Поле потока в аэротенке воспроизводится на основе модели потенциального течения. 2-D уравнения массопереноса используются для моделирования рассеивания субстрата и ила. Для моделирования процесса биологической очистки используется упрощенная модель. Для численного интегрирования уравнений переноса применялась неявная разностная схема. Разностная схема построена для расщепления уравнений переноса. Расщепление уравнения переноса осуществляется на два уравнения и выполняется на дифференциальном уровне. Первое уравнение расщепления учитывает движение ила или субстрата по траекториям, а второе – диффузионный про-

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цесс переноса примеси и ила. Для решения уравнений расщепления использовалась неявная разностная схема. Для численного интегрирования уравнения потенциального течения применялась неявная схема условного приближения. На основе построенной численной модели был выполнен компьютерный эксперимент для исследования процесса биологической очистки в аэротенке. **Результаты**. Разработанная быстродействующая численная модель позволяет быстро моделировать процесс биологической очистки в аэротенке. Модель может использоваться для оценки эффективности работы аеротенка при разных режимах работы. Разработанная модель учитывает геометрическую форму аэротенка. **Научная новизна**. Разработана численная модель, учитывающая геометрическую форму аэротенка и процесс динамики жидкости; а также процесс движения субстрата и ила в аэротенке и процесс биологической очистки. **Практическая значимость**. Предложена эффективная численная модель класса «diagnostic models» для быстрого расчета процесса биологической очистки в аэротенке.

Ключевые слова: биологическая очистка; численное моделирование; аэротенк

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