NUMERICAL SIMULATION OF BIOLOGICAL WASTEWATER TREATMENT IN AERATION TANK

To simulate the process of biological wastewater treatment in aeration tank numerical model was 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 aeration tank. To simulate the process of biological treatment a simplified model is used which takes into account the process of sludge growth and substrate extinction. For the numerical integration of transport equations implicit difference scheme was used.

Keywords: biological treatment; numerical simulation; aeration tank.

Introduction

There are different types of aeration tanks (AT) which are used for biological wastewater treatment but in practice, so called “vitesnitel” AT (AT of displacement type) is very 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

To calculate the efficiency of aeration tank empirical models are often used. These models are built on the basis of physical experiments [5, 8]. These models have the form of simple algebraic formulae with some empirical coefficients. As a rule empiric 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.

Sometimes, in practice, mass balance models are also used. These models can be named ‘zerodimensional’ models. The balance models are very popular [3, 4, 9, 11, 13] and take into account some important parameters of aeration tank work. These models are based on the ordinary differential equa-
tions 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 [11]. 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.

One — dimensional equations of mass transport to simulate, for example, substrate dispersion in AT represent another approach to calculate the aeration tank efficiency [6, 7]. 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, 12, 14, 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) [12, 14]. 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 re-engineering.

**Goal**

The goal of this work is the development of numerical model to simulate the process of biological wastewater treatment in “vitesnitel” aeration tank (aeration tank of displacement type).

**Presenting main material**

**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) [8, 14]:

\[
\frac{\partial C}{\partial t} + \frac{\partial u C}{\partial x} + \frac{\partial v C}{\partial y} = \text{div}(\mu \text{grad} C); \tag{1}
\]

\[
\frac{\partial S}{\partial t} + \frac{\partial u S}{\partial x} + \frac{\partial v S}{\partial y} = \text{div}(\mu \text{grad} S), \tag{2}
\]

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

\[
C = C_{in}, \quad S = S_{in}, \tag{3}
\]

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

\[
C(i+1,j) = C(i,j), \\
S(i+1,j) = S(i,j), \tag{4}
\]
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.

3. at the solid walls the boundary condition is

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

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

\[
\frac{dC(t)}{dt} = -\frac{\mu(t)}{Y} S(t),
\]

(5)

\[
\frac{dS(t)}{dt} = \mu(t) S(t),
\]

(6)

where \( \mu \) is biomass growth rate \([13]\), \( Y \) is biomass yield factor \([13]\).

To calculate biomass growth rate Monod law is used \([13]\).

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

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

(7)

where \( P \) is the potential of velocity.

The velocity components are calculated as follows:

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

(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 \( P = \text{const} \).

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

\[
\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2},
\]

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

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

The calculation on the basis of these formulas is complete if the following condition is fulfilled:
\[ |P_{i,j}^{n+1} - P_{i,j}^n| \leq \varepsilon, \]
where $\varepsilon$ 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
\[ \frac{\partial C}{\partial t} + \frac{\partial u}{\partial x} C + \frac{\partial v}{\partial y} C = 0, \]  \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:
\[ \frac{\partial u}{\partial x} C = \frac{\partial u^+}{\partial x} C + \frac{\partial u^-}{\partial x} C, \]
\[
\frac{\partial v C}{\partial y} = \frac{\partial v^+ C}{\partial y} + \frac{\partial v^- C}{\partial y},
\]
where \( u^+ = \frac{u + |v|}{2}, \ u^- = \frac{u - |v|}{2}, \ v^+ = \frac{v + |v|}{2}, \ v^- = \frac{v - |v|}{2} \).

\[
\frac{\partial u^- C}{\partial x} \simeq \frac{u^-_{i+1,j} C_{i+1,j}^{n+1} - u^-_{i,j} C_{i,j}^{n+1}}{\Delta x} = L^+_x C^{n+1},
\]
\[
\frac{\partial v^+ C}{\partial y} \simeq \frac{v^+_{i,j+1} C_{i,j+1} - v^+_{i,j} C_{i,j}}{\Delta y} = L^+_y C^{n+1},
\]
\[
\frac{\partial v^- C}{\partial y} \simeq \frac{v^-_{i,j+1} C_{i,j+1} - v^-_{i,j} C_{i,j}}{\Delta y} = L^-_y C^{n+1}.
\]

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 \( k = 1, c = n + 1/2 \):
  \[
  \frac{C_{ij}^{c} - C_{ij}^e}{\Delta t} + \frac{1}{2} \left( L^-_x C^k + L^-_y C^k \right) = 0. \tag{17}
  \]

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 Euler method. On the basis of developed numerical model code ‘BIOTreat’ was developed. FORTRAN language was used to code the solution of difference equations.

**Case Study**

Developed code ‘BIOTreat’ was used to solve the following model problem. We consider tree corridor aeration tank. 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. 5, 6 of the model. At time \( t = 2 \) the inlet and outlet openings are open and the transport process starts. Direction of flow is shown in Fig.3 by arrows. 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 nine sources of sludge supply inside the aeration tank starts to work with intensity \( Q_i \). Position of these sources can be seen in Fig.3 where the influence of these sources results in local ‘deformation’ of substrate concentration field which have “circular” form. This field has practically small concentration gradient in aeration tank everywhere except points where sources of sludge supply are situated.

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

In Fig.3 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. 2. Sludge and substrate concentration change near the outlet opening of aeration tank: 1 — sludge concentration; 2 — substrate concentration

Fig. 3. Field of sludge concentration inside the aeration tank, \( t = 4 \)

Conclusions

New numerical model was developed to compute 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.

List of reference links

4. Козачек А.В. Исследование математической модели процесса аэробной очистки сточных вод как стадия оценки качества окружающей водной среды / А.В. Козачек, И.М. Авдасин,
7. Олейник О.Я. Моделирование очистки сточных вод в биореакторах-аэротенках с зваженным (вильно плавающим) и закрепленным биоценозом / О.Я. Олейник, Т.С. Айрапетян // Доповіді НАН України. – 2015. – № 5. – С. 55–60.