# Mathematical modelling of heat and mass transfer processes in wastewater biological treatment systems

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In this paper, a mathematical model is presented for wastewater biological treatment of multicomponent pollutants. The proposed model includes a simulation of the wastewater clarification in the clarifier; simulation of the wastewater aerobic treatment in the porous medium; numerical-asymptotic approximation for solutions of spatial model problems of the wastewater aerobic treatment; simulation of singularly perturbed processes of convective diffusion, taking into account mass transfer and temperature regime; computer modeling of the wastewater biological treatment process in the aerotank regenerator.

The idea of perturbation theory is used for constructing a mathematical model of an appropriate nonlinear problem (this theory is based on the consideration of new factors and effects, by perturbing the output, well-known backgrounds, but not by solving new appropriate intricate modeling problems). The relevant processes, such as "filtration-convection-diffusion-heat and mass transfer", are considered in the media (one connected areas, bounded by equipotential lines and flow lines), which can be deformed depending on the certain process characteristics. This, by turn, predetermine the process nature, i.e. there is a mutual influence of the medium characteristics and the process. Filtration flow is regarded as a certain background for the convective transport of soluble substances (pollutants), taking into account small diffusion effects.

Based on the above, a mathematical model of the wastewater aerobic treatment, taking into account the interaction of bacteria, organic and biologically non-oxidizing substances in conditions of diffuse and mass-transfer disturbances and the influence of temperature regimes, has been constructed.

Keywords: mathematical model, temperature regime, wastewater aerobic treatment

#### INTRODUCTION

Domestic wastewater contains pollutants of mineral and organic origin, while industrial one differs both in composition and concentration, depending on the region. Regardless of the type, the wastewater needs to be cleaned, because it contains pollutants that significantly exceed the permissible concentration levels. To prevent the harmful effects of impurities on the environment, the filter systems that provide acceptable contamination levels are used.

An effective tool for studying the operating modes of such systems and optimizing their parameters is mathematical modeling. In this regard, there is a problem of the creation and implementation of an adequate mathematical model that reflects the physics of phenomena occurring in the systems of biological wastewater treatment. The aim is to develop a mathematical model of the process of biological wastewater treatment, enabling to predict the manufacturing process wastewater treatment in more detail taking into account the temperature regimes, that further enables the implementation of automated control over the process of effective deposition of impurities in biological filters depending on the output data of the aquatic environment, the improvement of these systems in accordance with the accepted conditions and criteria, as well as the possibility of finding an effective combination of wastewater biological treatment schemes with the systems of energy recovery from wastewater treatment (e.g. heat pump installations).

#### LITERATURE REVIEW

In recent years, a large number of scientific researches on the issues of modeling and automation of biochemical wastewater treatment have been carried out. These studies have considerably expanded the concept of water purification, heat and mass transfer, influence of variable parameters necessary for automatic control over output information, and also defined certain principles for the construction of schemes and automation tools.

In some models, wastewater treatment is considered as a technological process with the features of mechanical structures without taking into account the dynamics of time changes of the filter effective operation, in others – interconnections of active sludge and impurities without taking into account the system of interacting parameters, or a set of equations that does not take into account the interconnection between parameters, which are

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clearly expressed in experiments and play an important role.

However, most of these works do not take into account the influence of the environmental temperature, which is one of the main factors affecting the occurring of reactions.

The combination of the above shows the relevance of this work, which is to develop a mathematical model of the process of wastewater treatment from pollutants, which takes into account the interaction of bacteria, active sludge and impurities, as well as temperature regime. The next step is to study the model using computer simulation to calculate the optimal parameters of the technological process [1-9].

## FORMULATION OF THE PROBLEM

It is necessary to consider the process of treating liquids of organic impurities. According to the literary sources, the following stages of wastewater treatment of pollutants are distinguished:

- decomposition of organic contamination by bacteria;

- growth and death of bacteria;

- production of "young" bacteria by active sludge;

- the transfer of impurities to a biologically nonoxidizing substance.

To describe the dynamics of changes in the concentration of pollution, taking into account the influence of activated sludge on the absorption of impurities, there is used the equation of the type [10]:

$$\frac{\partial C_i}{\partial \tau} = v_C \frac{\partial C_i}{\partial x} - \beta_i C_i BT + D_C \frac{\partial^2 C_i}{\partial x^2}, \quad (1)$$

where  $\beta_i$  is the coefficient, which takes into account the design features of the aerotank, the flow rate of the liquid and the absorption of the substrate in accordance with the bacteria activity;

 $C_i$  is the concentration of i-th contamination in water;

T is the temperature of the aerotank;

 $v_c$  is the velocity of the substrate movement;

 $D_c$  is the diffusion coefficient.

Given that the bacteria move along with the contaminated substance in the porous medium, and also settle down in the lower part of the aerotank in the form of active sludge, the following equation for the growth, death and transfer of bacteria taking into account the biological need of oxygen is arrived at:

$$\frac{\partial B}{\partial \tau} = v_B \frac{\partial B}{\partial x} + \beta B K T K_B + w_B + D_B \frac{\partial^2 B}{\partial x^2}, \quad (2)$$

where B is the concentration of activated sludge;

 $K_B$  is the coefficient of oxygen and bacteria absorption;

 $w_B$  is the rate of active sludge accumulation according to the adequacy of the model;

 $v_B$  is the velocity of activated sludge movement;

 $D_B$  is the diffusion coefficient.

In order to improve the efficiency of the process and ensure optimal living conditions of bacteria, oxygen is additionally introduced, and the equation describing the dynamics of this process has the following form:

$$\frac{\partial K}{\partial \tau} = v_K \frac{\partial K}{\partial x} + \beta KT +$$

$$K_K \cdot C \cdot (K_0 - K) + w_K + D_K \frac{\partial^2 K}{\partial x^2},$$
(3)

where K is the oxygen concentration, necessary to maintain the best bacterial absorption of contamination;

 $K_{K}$  is the coefficient of mass transfer of oxygen;

 $K_0$  is the concentration of saturation of water with oxygen at given temperature and pressure;

 $W_{\kappa}$  is the rate of absorption of the oxygen substrate;

 $v_{\kappa}$  is the oxygen flow rate;

+

 $D_{\kappa}$  is the diffusion coefficient.

The basis for the thermal calculation of a biofilter is the equation of the thermal balance of its water mass, which takes into account the following components of heat fluxes:

1. The inflow of heat in a biofilter with a circulation loss of heat input incident, with the outflow of heat supplied to the aerators.

2. The inflow of heat due to the absorption of total solar radiation.

3. The outflow of heat with water at the outlet of the biofilter.

4. The loss of heat due to evaporation.

5. The loss of heat due to convective heat exchange between water and air.

6. The loss of heat due to effective radiation of water surface.

Since the processes occurring in the aerotank (Fig. 1) occur with the release and absorption of energy, the law of thermodynamics is used:

$$Q_{in} + Q_{heat} - Q_w + Q_{bot} - Q_{air} - Q_{evap} - Q_{out} = 0,$$
(4)

where  $Q_{in}$  is the amount of heat coming from the input water;

 $Q_{heat}$  is the amount of heat given by the air;

 $Q_w$  is the amount of heat lost through the aerotank walls;

 $Q_{bot}$  is the amount of heat given to the heating of the earth through the bottom of the aerotank;

 $Q_{air}$  is the amount of heat given to the air on the surface of the water in the aerotank;

 $Q_{evap}$  is the energy of heat that will be emitted for evaporation;

 $Q_{out}$  is the residual heat that will be removed with the outflowing water.



Fig. 1. Thermal balance of aerotank

To determine the energy supplied by the temperature of the incoming water, the formula is used (5):

$$Q_{in} = c_w \cdot m \left( T_{in} - T \right), \qquad (5)$$

where T, K is the water temperature in the aerotank;

 $c_w, \frac{J}{kg \cdot K}$  is the specific heat of water;

*m*, *kg* is the mass of water in which heat transfer occurs;

 $\rho, \frac{kg}{m^3}$  is water density;

 $V = l \cdot h \cdot b, m^3$  is the volume of the aerotank;

l, m is the length of the aerotank;

h, m is the height of the aerotank;

b, m is the width of the aerotank;

 $T_{in}$ , K is the temperature of the water incoming into the aerotank.

The amount of heat transferred from the air is described by Fourier's law:

$$Q_{heat} = -\lambda_p \cdot grad \ T_{air} \cdot h \cdot b \,, \qquad (6)$$

where  $\lambda_p$ ,  $\frac{W}{m^2 \cdot K}$  is the coefficient of thermal conductivity of air;

 $T_{air}, K$  is the air temperature.

But since heat is supplied only in certain areas of the aerotank, the function that describes the amount of heat provided from the outside will look like (7), where we additionally multiply by 2 the area of interaction, because heat is absorbed by water, located on both sides of the point of heat supply:

$$\begin{cases} Q_{heat} = -\lambda_p \cdot grad \ T_{air} \cdot h \cdot b \cdot 2, \ x = 20 \cdot n; \\ Q_{heat} = 0, \ x \neq 20 \cdot n. \end{cases}$$
(7)

where x, m is the coordinate along the aerotank in which the coolant is supplied;

 $n = 1, 2, 3, \dots, k$  are natural numbers.

The loss of heat through the walls of the aerotank is determined by the equation (8):

$$Q_{w} = \frac{\lambda_{w}}{\sigma} (T_{aver} - T) S_{w}, \qquad (8)$$

where  $\lambda_w$ ,  $\frac{W}{m \cdot K}$  is the coefficient of the wall thermal conductivity;

 $\sigma$ , *m* is the wall thickness;

 $T_{aver}$ , K is the average temperature of the air that surrounds the aerotank;

 $S_w = 2 \cdot l \cdot h, m^2$  is the area of the aerotank's lateral surface through which the heat is lost.

The transfer of heat through the bottom of the aerotank to the soil is similar to the formula (8), given that the temperature of the earth is less than the air temperature.

$$Q_{bot} = \frac{\lambda_w}{\sigma} \cdot \left(T_{earth} - T\right) \cdot S_{bot}, \qquad (9)$$

where  $T_{earth}$ , K is the average temperature of the earth;

 $S_{bot} = l \cdot b, m^2$  is the area of the bottom surface through which the heat is emitted to heat the earth.

The transfer of heat from water to air through the aerotank surface is described by Newton-Richman's law:

$$Q_{air} = \alpha \cdot (T_{aver} - T) \cdot F , \qquad (10)$$

where  $\alpha, \frac{W}{m^2 \cdot K}$  is the heat transfer coefficient of air;

 $F = l \cdot b$ ,  $m^2$  is the surface area of the water through which the heat is emitted to heat the air.

The energy of heat that will be emitted for evaporation can be described with the equation (11) from the work [11]:

$$Q_{evap} = \alpha_e \cdot (e_s - e_2) \cdot S_{bot} + \frac{1}{\rho \cdot c_w} \frac{\partial I}{\partial x}, \quad (11)$$

where  $\alpha_e$ ,  $\frac{W}{m^2 \cdot mbar}$  is the coefficient of heat transfer by evaporation;

 $e_s, m^2 \cdot mbar$  is the maximum water vapor moisture, which corresponds to the average temperature of the water surface;

 $e_2, m^2 \cdot mbar$  is the humidity of water vapor at the height of 2 m above the water surface;

- *I* is the flow of solar energy;
- $\rho$  is water density.

The residual heat that will be removed with the outflowing water is determined by the ratio (12):

$$Q_{out} = c_w m \left( T_{out} - T \right), \qquad (12)$$

where T, K is the temperature of water in the aerotank;

 $T_{out}$ , K – the temperature of the water outflowing from the aerotank.

Also, a part of the energy will be transferred along the length of the aerotank due to the motion of water. To do this, in addition to equation (13), we introduce the convective and diffusive components of the mass transfer, as well as the function of the source, which has the following form:

$$k = \gamma \cdot \left(T_{aver} - T_{in}\right) \cdot x, \qquad (13)$$

where  $\gamma, \frac{1}{m \cdot K}$  is the rate of heat transfer along the

aerotank, depending on the environment.

Taking into account the mentioned components of heat fluxes, as well as the corresponding dependences (4)-(13), after carrying out corresponding generalizations, the following equation for the transfer of heat to the aerotank has been obtained:

$$\frac{\partial T}{\partial t} + v_T \frac{\partial T}{\partial x} = D_T \frac{\partial^2 T}{\partial x^2} + F_T + \frac{1}{\rho \cdot c_w} \frac{\partial I}{\partial x}, \quad (14)$$

where  $v_T$  is the velocity of heat motion;

 $D_T$  is the diffusion coefficient;

 $F_{T}$  is heat transfer function.

The set of differential equations (1), (2), (3) and (14) gives complex description of the change in the concentration of bacteria, pollution, oxygen and temperature in the aerotank. Various interactions between the characteristics of the environment and the process should be taken into account by introducing the coefficients into the corresponding equation, which makes it possible to analyze the processes taking place in the aerotank as a set of interconnected influences. Proceeding from the above, the following model problem can be arrived at:

$$\frac{\partial C_i}{\partial t} = v_C \frac{\partial C_i}{\partial x} - \beta_i C_i BT + D_C \frac{\partial^2 C_i}{\partial x^2},$$

$$\frac{\partial B}{\partial t} = v_B \frac{\partial B}{\partial x} + \beta BKTK_B + w_B + D_B \frac{\partial^2 B}{\partial x^2},$$

$$\frac{\partial K}{\partial t} = v_K \frac{\partial K}{\partial x} + \beta KT + K_K \cdot C \cdot (K_0 - K) + (15)$$

$$+ w_K + D_K \frac{\partial^2 K}{\partial x^2},$$

$$\frac{\partial T}{\partial t} + v_T \frac{\partial T}{\partial x} = D_T \frac{\partial^2 T}{\partial x^2} + F_T + \frac{1}{\rho \cdot c_w} \frac{\partial I}{\partial x};$$

$$C_{i}\Big|_{x=0} = C_{i^{*}}^{*}(t), \ B\Big|_{x=0} = B_{*}^{*}(t),$$

$$K\Big|_{x=0} = K_{*}^{*}(t), \ T\Big|_{x=0} = T_{*}^{*}(t),$$

$$\frac{\partial C_{i}}{\partial x}\Big|_{x=l} = 0, \ \frac{\partial B}{\partial x}\Big|_{x=l} = 0,$$

$$\frac{\partial K}{\partial x}\Big|_{x=l} = 0, \ \frac{\partial T}{\partial x}\Big|_{x=l} = 0;$$

$$C_{i}\Big|_{t=0} = C_{i}^{*}(x), \ B\Big|_{t=0} = B^{*}(x),$$

$$K\Big|_{t=0} = K^{*}(x), \ T\Big|_{t=0} = T^{*}(x),$$
(16)

where l is the aerotank length;

 $C_{i^*}^*(t)$ ,  $B_i^*(t)$ ,  $K_i^*(t)$ ,  $T_i^*(t)$ ,  $C_i^*(x)$ ,  $B^*(x)$ ,  $K^*(x)$ ,  $T^*(x)$  given a sufficient number of times, are the numbers of differential functions, coordinated in the angular points of the area  $G = \{(x,t): 0 < x < l, 0 < t < t_* < \infty\}$ .

The solution of the problem (15)-(17) with accuracy  $O(\varepsilon^{n+1})$  are sought in the form of asymptotic series by the power of a small parameter  $\varepsilon$  [12]:

$$C(x,t) = C_0(x,t) + \sum_{i=1}^{n} \varepsilon^i C_i(x,t) +$$

$$+ \sum_{i=0}^{n+1} \varepsilon^i \tilde{C}_i(\tilde{\xi},t) + R_C(x,t,\varepsilon)$$

$$B(x,t) = B_0(x,t) + \sum_{i=1}^{n} \varepsilon^i B_i(x,t) +$$

$$+ \sum_{i=0}^{n+1} \varepsilon^i \tilde{B}_i(\tilde{\xi},t) + R_B(x,t,\varepsilon)$$

$$(19)$$

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$$K(x,t) = K_0(x,t) + \sum_{i=1}^{n} \varepsilon^i K_i(x,t) +$$

$$+ \sum_{i=0}^{n+1} \varepsilon^i \tilde{K}_i(\tilde{\xi},t) + R_K(x,t,\varepsilon)$$

$$T(x,t) = T_0(x,t) + \sum_{i=1}^{n} \varepsilon^i T_i(x,t) +$$

$$+ \sum_{i=0}^{n+1} \varepsilon^i \tilde{T}_i(\tilde{\xi},t) + R_T(x,t,\varepsilon)$$
(21)

where  $R_B, R_K, R_C, R_T$  – reminders;

 $C_i(x,t)$ ,  $B_i(x,t)$ ,  $K_i(x,t)$ ,  $T_i(x,t)$   $(i = \overline{0, n})$  – regular part of the asymptotics;

$$\tilde{C}_i(\tilde{\xi},t), \quad \tilde{B}_i(\tilde{\xi},t), \quad \tilde{K}_i(\tilde{\xi},t), \quad \tilde{T}_i(\tilde{\xi},t) \quad (i = \overline{0,n+1}) -$$
  
function of the borderline type (correspondingly

amendments at the output of purified substance);  $\tilde{z}$  (U ) -1

 $\tilde{\xi} = (L - x) \cdot \varepsilon^{-1}$  – corresponding transformations.

The solution to the corresponding model problem (15)-(17) has been found in the form of asymptotic series, analogous to [13]. The effectiveness of this approach in works [12-15] has been "worked out", in particular, with the consideration of "diffusion contributions" on strong convection and filtration backgrounds. The corresponding processes, such as "filtration-convection-diffusion-heat-mass-

exchange", are considered in environments (singleconnected domains bounded by equipotential lines and flow lines) that can undergo deformations depending on certain process characteristics, which in turn determines the nature of the process (that is, the interaction of the characteristics of the medium and the process takes place), and the filtration flow is considered as a certain background for the convective transfer of soluble substances (pollution), taking into account small diffusion phenomena.

#### CONCLUSIONS

1. The mathematical model of biological wastewater treatment has been developed, taking into account the interaction of bacteria, organic and biologically non-oxidizing substances under conditions of diffusion and mass exchange disturbances and the influence of temperature regimes.

2. The method and the algorithm for solving the corresponding nonlinearly perturbed problem "convection-diffusion-heat-mass-exchange" are offered.

3. The obtained results allow to forecast and automate technological processes of biological wastewater treatment with systems of energy utilization of these waters (for example, heat pump plants) in a more detailed and complex way.

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# МАТЕМАТИЧНО МОДЕЛИРАНЕ НА ТОПЛО И МАСООБМЕННИ ПРОЦЕСИ В СИСТЕМИ ЗА ТРЕТИРАНЕ НА ОТПАДЪЧНИ ВОДИ

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#### (Резюме)

В настоящата работа е представен математичен модел за биологичното третиране на отпадъчни води, съдържащи многокомпонентни замърсители. Предложеният модел включва симулиране на избистрянето на водите в осветител, аеробното третиране в порьозна среда, асимптотична числена апроксимация за решаване на пространствената задача за аеробното третиране и симулиране на сингулярно смутения процес на конвективна дифузия с отчитане на топлообмена и компютърно моделиране на биологичните процеси в аериран танк с регенерация.

Идеята за теорията на пертурбациите е използвана за съставянето на модел на нелинейна задача (отчитат се нови фактори и ефекти чрез смущения на изхода, но без решаването на нови задачи).

Значимите процеси (като филтруване-конвективна дифузия, топло-и масообмен) са разгледани в непрекъсната среда (едно-свързана област, оградена от екви-потенциални и токови линии), която може да се деформира при някои характеристики на процесите. От своя страна това предопределя природата на процесите, т.е. налице е взаимна връзка на характеристиките на средата и на процеса. Филтруването се разглежда като основа за конвективния пренос на разтворимите вещества (замърсители) при слаби дифузионни ефекти.

На тази основа е съставен математичмия модел за аеробното третиране на отпадъчни води с отчитането на влиянието на бактериите, не-окисляемите органични и биологични компоненти в условията на смущения в дифузията, топло и масообмена и влиянието на температурата.