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MATHEMATICAL MODELING OF BIOCHEMICAL WASTEWATER TREATMENT PROCESSES

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Abstract: This paper examines mathematical models of biochemical processes at wastewater treatment plants.

Introduction

In order to predict changes in quantitative indicators of water environment, particularly in natural water reservoirs (receivers of treated wastewater) at various stages of design and decision-making [1], it is necessary to build mathematical models of processes, which occur in main and auxiliary equipment of industrial wastewater treatment plants taking an account of hydrodynamic characteristics of flows, kinetic laws of processes and probabilistic nature of their occurrence. The most important systems that implement the main biochemical treatment processes are: "aeration tank – secondary tank", "denitrifier – secondary tank".

In order to develop mathematical models, the authors have used an approach [2], which enables to generate models in a dialogue mode with the application of PC and user's knowledge about the objects' features.

Mathematical model of an aeration tank

The majority of currently operating biochemical wastewater treatment plants have aeration tanks of corridor type.

In order to create mathematical models of wastewater treatment processes, it is necessary to know the structure of hydrodynamic flows at each facility. In industrial corridor type aeration tanks with dispersed water supply along the corridor hydrodynamics of a suspension flow is at the intermediate position between ideal displacements and complete mixing. Hydrodynamic flows structure is frequently considered as a set of cells with complete mixing with by-passing and recirculation flows. The specific form of hydrodynamic flow structure is determined during tracer experiments [3].

The next stage of bio-chemical processes modeling is the development of analytical biochemical transformation process models that occur in aeration tanks. Work [3] shows that aerobic oxidation processes of carbon and nitrogen containing substances occur in aeration tanks. Oxidation of organic carbon occurs as a result of metabolism of heterotrophic microorganisms (**HMO**) in biological sludge. Oxidation of nitrogen compounds is produced by two types of nitrifying microorganisms (**NMO**): Nitrosomonos bacteria, which oxidizes ammonified nitrogenous compounds to nitrites and Nitrobacter bacteria, which oxidizes nitrites to nitrates.

Nitrification in aeration tanks is necessary for reduction of non-oxidized forms of nitrogen, which flows into water reservoirs (receivers of wastewater) and cause a significant decrease in oxygen content in water. When we include nitrification into treatment scheme, we must perform denitrification at the next stage, which cause reduction of nitrates to nitrogen. The model first described in work [4] is the best analytical model of such biochemical processes. Here we propose the following model for simulation studies to solve the problem of biochemical wastewater treatment facilities design:

$$G\left(Y_{1,j}\right)-\frac{k_1\left(\frac{Y_{1,j}}{Y_{3,j}}\right)^{k_7} Y_{3,j}}{k_2+\left(\frac{Y_{1,j}}{Y_{3,j}}\right)^{k_7}}\frac{Y_{2,j}}{k_3+Y_{2,j}}=0; \tag{1}$$

$$G\left(Y_{2,j}\right)-k_6\left(Y_2^e-Y_{2,j}\right)-1.42(1/k_5-1)\frac{k_1\left(\frac{Y_{1,j}}{Y_{3,j}}\right)^{k_7} Y_{3,j}}{k_2+\left(\frac{Y_{1,j}}{Y_{3,j}}\right)^{k_7}}\frac{Y_{2,j}}{k_3+Y_{2,j}}=0; \tag{2}$$

$$G\left(Y_{3,j}\right)-k_4Y_{3,j}+k_5\frac{k_1\left(\frac{Y_{1,j}}{Y_{3,j}}\right)^{k_7} Y_{3,j}}{k_2+\left(\frac{Y_{1,j}}{Y_{3,j}}\right)^{k_7}}\frac{Y_{2,j}}{k_3+Y_{2,j}}=0; \tag{3}$$

$$G\left(Y_{i,j}\right)=\left(\frac{1}{V_i}\right)\left[R_j^0Y_{i,0}+R_{j-1}Y_{i,j-1}+R_{j-(2+n_\beta)}Y_{i,j-(2+n_\beta)}\beta_{j-(2+n_\beta)}+\right.$$
$$\left.+R_{j+n_\alpha}Y_{i,j+(1+n_\alpha)}\alpha_{j+(1+n_\alpha)}-\left(R_{j-1}\alpha_j+R_{j-1}\beta_j-R_j\right)Y_{i,j}\right], \tag{4}$$

$$i=\overline{1,6},\quad j=\overline{1,m},\quad m=\sum_{k=1}^{K}m_k;$$

$$\beta_j=\tilde{\beta}_1,\quad j=\overline{1,m_1-2};\quad \alpha_j=\tilde{\alpha}_1,\quad j=\overline{2,m_1}; \tag{5}$$

$$\beta_j=\tilde{\beta}_2,\quad j=\overline{m_1+1,m_1+m_2-2};\quad \alpha_j=\tilde{\alpha}_2,\quad j=\overline{m_1+2,m_1+m_2}; \tag{6}$$

. . . .

$$\beta_j=\tilde{\beta}_K,\quad j=\overline{\sum_{k=1}^{K-1}m_k+1,\ m-2};\quad \alpha_j=\tilde{\alpha}_K,\quad j=\overline{\sum_{k=1}^{K-1}m_k+2,m}; \tag{7}$$

$$k_1 = k_{1,20} \cdot 1.047^{T_1 - 20}; \quad (8)$$

$$k_8 = k_{8,20}\{\exp(0.098(T_1 - 15))\}(1 - 0.833(7.2 - \text{pH})); \quad (9)$$

$$Y_2^e = 14.652 - 0.41022T_1 + 0.00791T_1^2 - 0.00007774T_1^3, \quad (10)$$

here $Y_{1,j}$, $Y_{2,j}$, $Y_{3,j}$ – concentration of HMO substrate, oxygen and HMO biomass in cell j, mg/l; k_1 – constant of HMO growth rate, mg/l; k_2, k_3 – constant of HMO substrate and oxygen semi-enrichment, mg/l; k_4 – HMO die-away coefficient, units/day; k_5 – HMO efficiency coefficient, mg/mg; k_6 – volume oxygen transfer ratio, units/day; k_7 – exponent; k_8 – constant of NMO growth rate, units/day; $G(Y_{i,j})$ – hydro-dynamic component of concentration change in a cell j, mg/(units $\cdot$ days); R_j – volume flow from a cell j into a cell $j+1$, units/day; V_j – volume of a cell j, l; m_k – number of cells at a corridor k; m – number of cell in an aeration tank; K – number of corridors in an aeration tank; T_1 – temperature, °C; Y_2^e – oxygen concentration at enrichment level, mg/l; $k_{1,20}, k_{8,20}$ – values of k_1 and k_8 at $T_1 = 20$ °C; $\tilde{\alpha}_1$, $\tilde{\alpha}_2$, $\tilde{\alpha}_3$,..., $\tilde{\alpha}_K$; $\tilde{\beta}_1$, $\tilde{\beta}_2$, $\tilde{\beta}_3$, ..., $\tilde{\beta}_K$ – coefficients of inter-cell recirculation and by-passing in aeration tank's corridors; n_α, n_β – number of cell with inter-cell recirculation and by-passing; R_j^0 – volume inflow of wastewater to a cell j through the system of regulated gates.

In order to obtain kinetic constants of technological processes in a certain aeration tank for model (1) – (10), we have used an approach described in work [2].

Mathematical model of a denitrifier

Significant concentrations of nitrogen compounds in discharged wastewater enhance algae growth, but can be toxic to humans and have harmful effect on water environment. Nitrites and nitrates transformation can be most effectively done by denitrification of wastewater with biological sludge. Denitrifying bacteria are found among Pseudomonas sp., Acrobacterium sp., Micrococcus sp. and others. When they get into oxygen-free conditions, they use oxygen contained in nitrites and nitrates for breathing instead of dissolved oxygen. Denitrifiers are heterotrophs and represent a group of facultative anaerobes. They are present in wastewater in large quantities and can use contaminated substances as a carbon nutrition, which greatly facilitates operation of treatment plants as well as eliminates the need for cultivation of a special adapted microflora.

Transformation of nitrites into nitrogen is a multi-step process: $NO_3 \to NO_2 \to \to NO \to N_2O \to N_2$.

Depending on pH of the environment, we can obtain either NO or N_2O or N_2. Thus, when $\text{pH} < 7.3$, the most probable output is N_2O. When $\text{pH} = [7.5...8.0]$ denitrification output is N_2. Besides pH denitrification is influenced by: source of organic carbon and its concentration, nitrites concentration, oxygen concentration, water temperature, presence of toxic substances, etc.

For practical purposes it is usually recommended to apply a zero order reaction with respect to nitrate concentration. At very low concentrations of nitrate denitrification process is described by Mono's kinetics equation. However, Mono's equation is theoretically derived and best approximates experimental data, if activated sludge biomass is homogeneous and the substrate is represented by one pure organic substance. Multi-component composition of wastewater and sludge heterogeneity in most cases appear in the model in the form correction exponents added to kinetic dependences. Let's consider the following analytical model of denitrification process of a biochemical wastewater treatment plant:

$$\frac{dY_1^d}{dt} = \frac{\widetilde{R}^a}{V^d}\widetilde{Y}_{1,0}^a + \frac{R^a}{V^d}Y_{1,0}^a - k_1^d \frac{\left(\frac{Y_1^d}{Y_3^d}\right)^{k_7^d} Y_3^d}{k_2^d + \left(\frac{Y_1^d}{Y_3^d}\right)^{k_7^d}} - \frac{R^d}{V^d}Y_1^d; \tag{11}$$

$$\frac{dY_2^d}{dt} = \frac{R^a}{V^d}Y_{2,0}^a - \frac{R^d}{V^d}Y_2^d - k_6^d k_1^d \frac{\left(\frac{Y_1^d}{Y_3^d}\right)^{k_7^d} Y_3^d}{k_2^d + \left(\frac{Y_1^d}{Y_3^d}\right)^{k_7^d}} - k_3^d Y_3^d; \tag{12}$$

$$\frac{dY_3^d}{dt} = \frac{R^{dp}}{V^d}Y_3^{dp} - k_5^d k_1^d \frac{\left(\frac{Y_1^d}{Y_3^d}\right)^{k_7^d} Y_3^d}{k_2^d + \left(\frac{Y_1^d}{Y_3^d}\right)^{k_7^d}} - k_4^d Y_3^d - \frac{R^d}{V^d}Y_3^d - k_4^d Y_3^d, \tag{13}$$

here R^a, $Y_{1,0}^a$ – volume flow and chemical oxygen demand (**COD**) of wastewater flowing out of "aeration tank – secondary tank" system, units/day and mg/l; $\widetilde{R}^a$, $\widetilde{Y}_{1,0}^a$ – volume flow and COD of wastewater flowing into denitrificator not through an "aeration tank – secondary tank" system, units/day and mg/l; R^{dp}, Y_3^{dp} – volume flow and COD of denitrificators in the recycle, units/day and mg/l; $Y_{2,0}^a$ – concentration of nitrites in wastewater flowing into denitrificator out of an "aeration tank – secondary tank" system, mg/l; R^d – inflow of wastewater, units/day; V^d – vessel volume, l; Y_1^d – output concentration of COD, mg/l; Y_2^d – output concentration of nitrites, mg/l; Y_3^d – concentration of denitrificators, mg/l; k_1^d – constant of COD elimination rate, units/day; k_2^d – constant of enrichment for eliminated COD; k_3^d – constant of oxygen absorption rate in endogenous respiration, units/day; k_4^d – constant of sludge die-away, units/day; k_5^d – sludge output coefficient in anoxemic conditions; k_6^d – amount of oxygen required for each organic substance, mg of oxygen/mg COD; k_7^d – exponent.

Conclusion

The proposed mathematic models (1) – (10) and (11) – (13) were used for prognosis of output water quality for the reconstructed bio-chemical wastewater treatment plant of Tambov.

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Математическое моделирование биохимических процессов очистки сточных вод

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Ключевые слова и фразы: аэротенк; денитрификатор; математическое моделирование биохимических процессов; очистные сооружения.

Аннотация: Рассмотрены математические модели биохимических процессов, протекающих в основных сооружениях станции очистки сточных вод.

Mathematische Modellierung der biochemischen Prozesse der Reinigung der Abwässer

Zusammenfassung: Es sind die mathematischen Modelle der biochemischen Prozesse, die in den Hauptanlagen der Station der Reinigung der Abwässer betrachtet.

Modélage mathématique des processus biochimiques de l'épuration des eaux des égouts

Résumé: Sont examinés les modèles mathématiques des processus biochimiques se produisant dans les constructions essentielles des stations de l'épuration des eaux des égouts.

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