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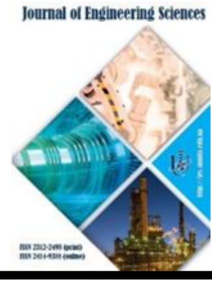

# Formalization of the Task of Creating a Mathematical Model of Combined Wastewater Treatment Processes

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**Abstract.** This paper focuses on the formation approach to formalize the mathematical modeling of wastewater treatment processes for further forming decision support systems for wastewater treatment facilities management on such a theoretical basis. To create an experimental model of formalization of modeling problems, research was conducted on activated sludge from municipal sewage treatment facilities by introducing an oxidant (H2O2) during standard operation of wastewater treatment facilities and introducing a toxicant (sulfur compounds). It was determined that under conditionally standard conditions, the influence of the oxidant is negative: exceeding technological standards of the concentration of dissolved oxygen in water solutions (3.0–13,7 mg/l), low water column transparency (1.4–1.6 cm), higher concentrations of ammonia nitrogen and phosphorus. With the appearance of a toxicant in the form of reduced sulfur compounds (sulfide ions and hydrogen sulfide 1.4–2.8 mg/l), on the contrary, the positive effect of $H_2O_2$ on biological water treatment processes was determined: the concentration of dissolved oxygen increases to 3.4 mg/l and the swelling of activated sludge stops. In this case, using a simplified scheme of expert evaluation as a global quality criterion of the biological stage management process of water treatment for rapid assessment of the vitality of activated sludge is justified. As parameters available for direct automatic measurement, it was proposed to use ORP and pH approximated by the regression equation. Also, a conditional scheme of the decision support system for water treatment management was proposed, which will provide two-level hierarchical control: situational and operational in real-time with a preventive response to emergencies; tactical with daily, at least daily, forecasting of the treatment plants.

**Keywords:** formalization, mathematical model, activated sludge, toxicant, wastewater treatment, biological stage.

## 1 Introduction

Analyzing the composition of technical regulations and peculiarities of functioning of water treatment equipment, we can conclude that the key and most difficult tasks in the implementation of technological regulations directly at the production are [1]:

– control of the parameters of technological processes, characteristics of the equipment of treatment facilities;

– technological analysis of equipment operation according to operational production indices, resource consumption, cleaning efficiency according to regulations and established criteria and indices.

Even more complicated situation with technical devices capable of operating in real-time (RT) in industrial conditions – and they are essential for monitoring compliance with regulatory requirements for water treatment efficiency [2].

Accordingly, justification of approaches to formalizing mathematical modeling of water treatment processes with further creation of an appropriate decision support system (DSS) is a relevant and promising scientific and applied task.

## 2 Literature Review

The combination of physical and mathematical modeling in a single instrumental engineering complex will integrate the approaches' strengths, minimizing the weaknesses. When creating such tools and complexes, it is advisable to take into account as much as possible the possibility of emergencies (ES) - expanding their area of effective practice-oriented use [2]. At the same time, the operation of the activated sludge system at high values of its retention time in the aeration tanks contributes to endogenous respiration of biomass, which increases the amount of chemical oxygen demand (COD) oxidized to $CO_2$ and reduces the total production of sludge biomass [3]. It is essential to control the influx of electron donors to the system for different groups of microorganisms. Thus, limiting the concentration of reduced sulfur compounds in wastewater is associated with their toxic effects on biota and the fact that they are energy donors for aerobic bacteria of the genus Thiobacillus [4]. The ratio of microbial groups affects the qualitative and quantitative yield of greenhouse gases and the efficiency of the oxidation process of organic pollutants in wastewater, which also requires an efficient mathematical apparatus to describe this process in practice. Baresel et al. (2016) calculated nitrous oxide emissions from a conventional biological treatment process using mathematical modeling while monitoring dissolved $N_2O$ in the aqueous phase using a sensor [5], which was necessary for monitoring system automation. Monitoring the structure, size, and morphology of aerobic pellets is increasing in importance and can be used for operation and process control purposes. For example, Leal et al. (2021) verified a sampling technique to estimate pellet and flocculus biomass using quantitative image analysis in the presence of biochemically active compounds [6].

Dychko et al. (2020) presented a methodology for environmental monitoring of natural and engineered wastewater treatment systems, including determining the dichotomous fractal structure of the measuring network, the boundaries of the polygon, and the density of pollution by Peano and Koch curves [7]. Modeling is also essential in assessing the effectiveness of biological treatment processes using activated sludge (AS). Thus, the work of Mir-Tutusaus et al. (2020) evaluated the combination of advanced oxidation processes (AOPs) based on UV/$H_2O_2$ treatment in combination with biological treatment (aerobic activated sludge or fungal enzyme-based treatment). Twenty-two PhACs (a pharmacological drug) were found in wastewater and were effectively removed (93–95 %) by a combination of biological treatments followed by UV/$H_2O_2$ treatment [8]. Spina et al. (2020) studied the enzymatic degradation of micropollutants in real, unmodified municipal wastewater with modeling of process optimization criteria [9].

The study by Breithaupt and Wiesmann (1998) used Haldane kinetics to mathematically model the biodegradation of organics in an anaerobic wastewater treatment system. The model took into account all local parameters (pH value, acetic acid concentration, biomass, and ion activity) and showed the influence of ion activity, which also requires refinement of the dispersion model [10].

Thus, previous studies presented the experimental modeling of treatment plant operation systems according to existing regulations, using the parameters of microbial growth kinetics. However, the systematization of parameters of influence on the efficiency of activated sludge in biological treatment systems with the formation of an adequate mathematical model of the process remains an unsolved problem.

This study aims to substantiate approaches to the formalization of mathematical modeling of wastewater treatment processes using different ways of removing pollutants from municipal wastewater for further formation of decision support systems for the management of wastewater treatment facilities on such a theoretical basis.

## 3 Research Methodology

To create an experimental basis for formalizing the tasks of mathematical modeling, we used active sludge (AS) of biological treatment facilities of Baranovichi city (Belarus) and additionally added oxidant $H_2O_2$ (one of the approaches of AOPs) according to the following sequence:

1) a revolving AS of the functioning sewage treatment plants was taken;

2) a zero sample (initial AS) was settled, and its qualitative indices were assessed: water column transparency, the concentration of dissolved oxygen, phosphorus, ammonia nitrogen, assessment of species composition;

3) different doses of oxidizer $H_2O_2$ (concentration of 3 %) were added to a zero sample (initial AS), the solution was retained, and its qualitative indicators were evaluated: transparency of water column [11]; concentration of dissolved oxygen was determined by an electrochemical method [12]; concentration of total dissolved phosphorus was determined by a photometric method after combustion with persulfate [13]; concentration of ammonium nitrogen by persulfate photometric method with Nessler reagent [14]; the species composition was assessed [11].

Also, the presence of sulfide ions and hydrogen sulfide at the treatment plant's inlet and its effect on the AS was investigated in a passive experiment mode. The results were analyzed to build mathematical models and form a hierarchical structure for solving such a complex problem. The basis of such conclusions justified the "global" criterion of quality of the management process of combined pollutant removal processes.

## 4 Results and Discussion

### 4.1 Experimental study

Three doses of $H_2O_2$ (3 %) were introduced into the activated sludge of the treatment plant: 0.5, 1.0, and 1.5 ml/l. Comparison of dissolved oxygen concentration in the aqueous solution of activated sludge was performed at intervals equal to 2 hours (Figure 1). The influence of various toxicants leads to a disturbance of the flocculation process and the destruction of floccules, which are already formed. This entails an increase in the amount of finely dispersed suspended fraction and, accordingly, a decrease in the transparency of supernatant (Figure 2).

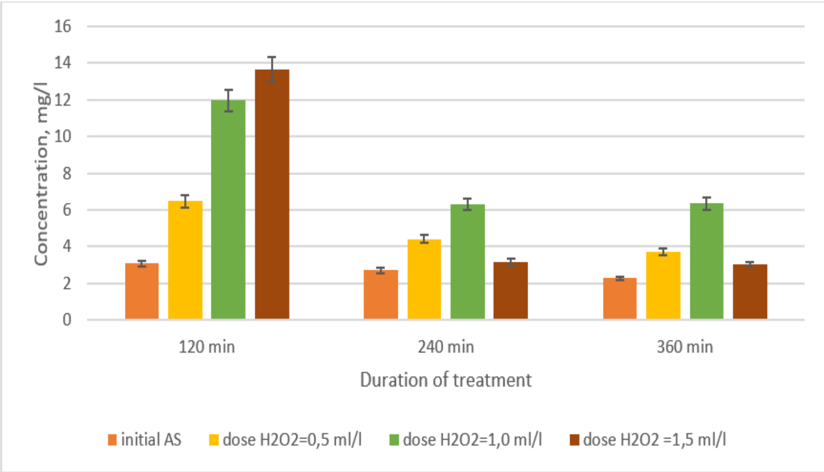


Figure 1 – The concentration of dissolved oxygen in the activated sludge of wastewater treatment plants and after adding different doses of hydrogen peroxide to AS (3 % concentration)

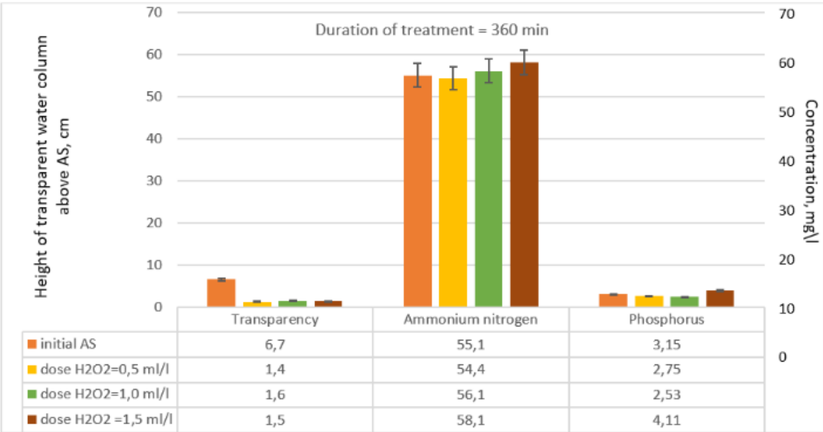


Figure 2 – Wastewater quality control by indicators of water column transparency over AS, the concentration of ammonia nitrogen and phosphorus when treated with different doses of hydrogen peroxide (3 % concentration)

The degree of biological treatment is satisfactory if the water transparency is at least 12 cm. In this case, it was initially (in the initial AS) was 8 cm. When applying different doses of hydrogen peroxide, it decreased. Other indices, in particular the concentration of ammonia nitrogen and phosphorus, did not vary significantly from the initial AS without adding hydrogen peroxide (3% solution), but still higher concentrations of ammonia nitrogen and phosphorus were observed in the series of experiments.

After 6 hours from the start of the experiments, an analysis of the species composition of AS was performed (Table 1).

The results obtained (Figures 1–2, Table 1) allow us to formulate the following conclusions about the conditionally standard modes of operation of biological wastewater treatment systems:

– in general, the initial AS, functioning treatment plants (without adding additional oxidant $H_2O_2$), more consistent with the technological objectives of wastewater treatment in terms of "Concentration of dissolved oxygen", "Transparency", "Concentration of phosphorus", "Concentration of ammonium nitrogen", the species composition;

– additional oxidizer $H_2O_2$ has a negative impact on the AS by the indicators mentioned above.

At the same time to the inlet of sewage treatment plants after a certain period began to arrive sewage with an impermissibly high concentration of reduced sulfur compounds (the total concentration of sulfide ions and hydrogen sulfide 1.4–2.8 mg/l) - as a result, began to swell the AS, reducing the concentration of dissolved oxygen in the water solution, reducing the transparency of the water column above the silt. Following the rules for the reception of industrial wastewater in the sewer system of settlements, the maximum allowable concentration of hydrogen sulfide in the effluent sent for biological treatment should not exceed 1 mg/l. At pH < 10, the content of sulfide ions can be neglected, at pH = 7 the content of $H_2S$ and $HS^-$ is approximately the same, at pH = 4 $H_2S$ is almost entirely (99.8 %) in the form of $H_2S$.

At the same time introduction of an additional oxidizer $H_2O_2$ promptly stabilized the technological situation (Table 2).

The results obtained (Table 2) demonstrate the positive technological effect of using AOPs approaches in biological water treatment – the process of swelling of AS was stopped, and its regeneration began.

At the same time several other solutions can be used to prevent bloating of AI: when the concentration of dissolved oxygen in the aerobic zones of the aeration tank is less than 1.0 mg/l – to use the maximum available capacity of the aeration system and ensure a dissolved oxygen concentration not lower than 1.0 mg/l; when pH values of sludge mixture are less than 6.0–6.5 – provide the possibility of pH regulation; when volley discharge of toxic substances and/or oil products to the treatment plant – increase the air supply to the aeration tanks to ensure the concentration of dissolved oxygen in the tank.

However, all such operations require maximum automation of the process, taking into account normal and abnormal situations, and to date, the wastewater treatment process using activated sludge is uncontrollable (very poorly controlled) in real-time. In the design of sewage treatment plants, this process is considered self-organizing. At the same time, with the emergence of new factors that lead to the death of AS, the natural process of self-regulation can not, in some cases, ensure the survival of activated sludge.

Accordingly, there is a problem with creating a process control system. And, in modern conditions, the primary process in this system must be an automatic control system (ACS).

Table 1 – Species composition of AS before and after application of $H_2O_2$ (3 % solution)

| Active peroxide treatment (3 % concentration) | | Species composition of the initially AS |
|---|---|---|
| Active peroxide treatment (3 % concentration) | Species composition after peroxide application (3 % concentration) | |
| 0.5 | Nitrous; Opercularia sp; Vorticella; Aspidisca; Carchesium (singular); Amoeb shell cysts<br><br>In the silt, Vorticella, attached colonials are mainly present. Vagrants are observed. Protozoa cysts are present.<br>Cottonwood of moderate size, dark brown color | Nitrous; Carchesium; Opercularia sp; Vorticella (разнообразные); Pamphagus; Aspidisca.<br><br>A relatively large number of attached infusoria, solitary forms, and colonial forms are observed. The activity of the attached ones is satisfactory. The number of bacteria not associated with the active sludge is moderate. Gastropod infusoria appeared occasionally. Small filamentous are present in sludge flakes. Diversity in attached infusoria. Sludge flake of moderate size |
| 1.0 | Nitrous; Opercularia; Vorticella; Carchesium.<br><br>Sludge flakes are finer, the number of attached ones decreased, single attached (Vorticella) jug-shaped, attached infusoria are smaller. The number of filamentous bacteria not associated with activated sludge flakes has decreased. No other species diversity was observed | Nitrous; Euglypha; Opercularia (with a closed eyelash disc); Oligohymenophora; large free-floating infusoria; Vorticella; several species are found in the mud funnel-shaped and with a narrow peristome; Carchesium (colonial infusoria); Opercularia coarctata.<br><br>Cotton silt of moderate size, pervaded by many small filamentous bacteria. Little diversity of protozoa by species. The silt is dominated by attached infusoria |
| 1.5 | Small filamentous;<br>- Carchesium;<br>- Opercularia;<br>- Vorticella;<br>- Shell corneocytes;<br>-Equal-crested infusoria.<br><br>Attached are found in a depressed state. Protozoan cysts are found. The total number decreased, the cotton was more fragmented. Water over silt has non-sedimentary turbidity | Small filamentous; Archesium; Opercularia; Vorticella; Shell cornicles; Equinocular infusoria.<br><br>Cottonwood silt of moderate size,<br>a variety of attached infusoria both solitary and colonial forms is observed. Mostly moderately active, but there are also with a closed ciliated disk.<br>Equiaceous ciliated infusoria appeared, shell amoebae - singularly.<br>The number of free-floating bacteria decreased |

Table 2 - AS states at increased concentrations of reduced sulfur compounds and with the addition of an additional oxidizer $H_2O_2$

| The total concentration of sulfide ions and hydrogen sulfide | Without hydrogen peroxide | | After a dose of 1 ml/l of peroxide (3 % concentration) | |
|---|---|---|---|---|
| | Transparency, cm | Dissolved oxygen concentration, mg/l | Transparency, cm | Dissolved oxygen concentration, mg/l |
| 2.80 | 0.7 | 1.3 | 6.8 | 2.3 |
| 1.36 | 1.1 | 1.5 | 5.1 | 3.4 |
| 2.06 | 0.9 | 1.1 | 7.1 | 2.5 |

### 4.2 Formalization of mathematical models

In the procedure of ACS synthesis, the first step is the synthesis of the mathematical model of the control object (CO). In this process, the control object is the AS itself, located inside the technological equipment.

Therefore, the following hierarchical structure of the solution of the complex problem is built.

– Problem 1 (global). Preventing the death of activated sludge at sewage treatment plants.

Solution of the problem 1. Creation of a process control system.

– Problem 2 (consequence). An adequate mathematical model of the process is needed to create the ACS.

Solution of problem 2. Studying the process, in the course of experimental researches, with its subsequent formalization.

– Problem 3. Formalization of the process implies the introduction of process quality criterion as a numerical expression of control objective.

Solution of problem 3. Formation of a control quality criterion by setting its physical meaning, designation, and scale.

– Problem 4. Both the study of the control object, to synthesize a mathematical model, and the control process require the automatic definition of a global criterion. The input quality criterion cannot be determined automatically by direct measurement.

The solution to Problem 4. Application of indirect measurement by determining the global quality criterion through the quantities available for direct automatic measurement.

– Problem 5. At present, no adequate models are defining the connection of global criterion with output parameters available for direct automatic measurement.

The solution to Problem 5. Carrying out experimental researches on the determination of relation of values available for direct automatic measurement and global criterion, with its further formalization in the form of a mathematical model.

A global criterion must be connected with a control purpose to solve a global problem. At the same time, it must be an adequate numerical expression of the goal, i.e., the assessment of the state of the AS biocenosis.

It should be noted that there are many techniques for assessing the viability of AS [11, 15–18]. They are based on studying the qualitative and quantitative composition of its biocenosis. The quantitative composition of microorganisms has a direct relationship with the incoming wastewater flow rate. After counting all microfauna, the following is calculated: number of species, the ratio of attached microorganisms to free-floating (K coefficient), percentage of sensitive microorganisms to resistant ones, Cuba index (it contains information both on the number of species and their numerical distribution by species) and the number of microorganisms per dose of sludge. These quantitative indices serve to assess the biocenosis of activated sludge. For example, according to them, one can judge whether it has a good species composition if all the indices are normal [15, pp. 195–203].

Thus, in [16–18], approaches to the systematization of filamentous microorganisms are outlined. These techniques for assessing the AS biocenosis are rather labor-intensive. Therefore, we proposed to use a simplified expert evaluation scheme as a global criterion for the quality of the management process with the characteristics presented in Table 3 for express evaluation.

For example, it is proposed to use ORP (redox potential) and pH as parameters available for direct automatic measurement.

As a first approximation, the following regression equation for determining the global criterion for the wastewater treatment plants understudy is proposed:

$$\alpha = a_1 \cdot (ORP_1 - ORP_2) + a_2 \cdot (pH_1 - pH_2) + a_3 \cdot ((ORP_1 - ORP_2) \cdot (pH_1 - pH_2))$$

where $a_1$, $a_2$, $a_3$ – regression coefficients; $ORP_1$, $ORP_2$ – readings of potential redox sensors at the inlet and outlet of aeration tank (digester), respectively; $pH_1$, $pH_2$ – readings of pH sensors at the inlet and outlet of the aeration tank, respectively.

Accordingly, such a mathematical model can be included in decision support systems for wastewater treatment process management (Figure 3).

Such pattern will allow providing water treatment systems with two-level hierarchical control:

– situational-operational in real-time with preventive response to emergencies;

– tactical with daily, as a minimum, forecasting of treatment facilities operation.

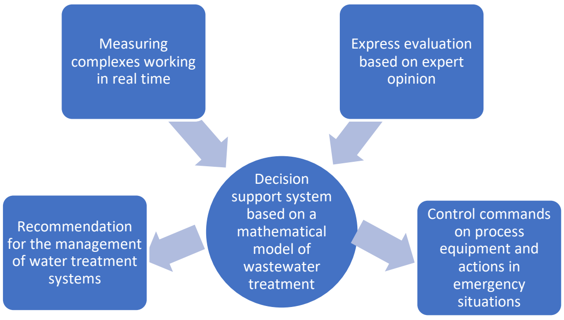


Figure 3 – Integration of the decision support system based on the proposed mathematical models with the existing water treatment system

## 5 Conclusions

The wastewater treatment plant is complex, multi-parameter, and non-linear to control the object, which is confirmed by the experimental studies on the effect on the activated sludge oxidant $H_2O_2$ (one of the approaches AOPs):

– under conditionally normal conditions, such influence is negative: exceeding technological standards of dissolved oxygen concentration in water solutions (3.04–13.68 mg/l), low transparency of the water column (1.4– 1.6 cm), higher concentrations of ammonia nitrogen and phosphorus

– with the appearance of a toxicant in the form of reduced sulfur compounds (total concentration of sulfide ions and hydrogen sulfide 1.38–2.80 mg/l), for which measurements in real-time there are no effective measuring instruments, on the contrary, the effect of the oxidant $H_2O_2$ has a positive effect on the biological water treatment: the concentration of dissolved oxygen increases to 3.4 mg/l. It stops bloating of AI with further regeneration.

Using the global criterion (criterion of AS vitality) associated with the purpose of management, as a form of solving the global problem of automation of wastewater treatment plants, as a tool for formalizing mathematical models, will create an appropriate decision support system with the functionality of operational regulation and tactical prediction even in emergencies.

Further research should be aimed at forming a knowledge base for creating mathematical models and checking their adequacy and technological compliance.

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