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Modeling of Sewage Bioremediation as a Modified Petri Net

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Abstract: The article discloses the mathematical basis of Petri nets used in the modeling and design of the module bioremediation of hydrocarbon wastewater. There described the technique of two-tier system of the modeling process of biochemical treatment of oily wastewater, as well as a model developed by the authors in the form of a modified Petri nets and software package management system of biochemical treatment of wastewater.

Key words: Modified Petri nets · Wastewater bioremediation · Biochemist technology system · Hierarchical structural model · System modeling.

INTRODUCTION

Modern production lines and biotechnology industries are characterized by a complex multi-level structure, they can therefore be regarded as a complex cybernetic systems. Studying them, there used a strategy of system analysis. Due to the complexity of the modeling and analysis of such systems, there is a need to attract modern methods of mathematical and computer modeling [1,2,3].

The purpose of this research is modeling of biological treatment of wastewater (BTW) in order to increase its efficiency based on the strategy of system analysis [4]. The complete mathematical model of a biochemical process system (BChP) can be represented in a hierarchical structural model using the apparatus modified Petri nets (MPN) [5].

MATERIALS AND METHODS

When solving the problems in the research there are used methods of system analysis, computer modeling, Petri nets theory [6] and graphs, numerical methods for solving equations. Computer simulation is implemented within the concept of a new information technology based on object-oriented approach to creating software using SCADA-technology [7].

Results of the Research: An important issue is to protect the ecological safety of water basin from the release of contaminated wastewater by industries. Cleaning of effluent is a prerequisite maintain the ecological balance of the environment. However, the existing wastewater treatment technology are not sufficiently advanced and don’t ensure its efficiency level. Modern wastewater treatment plants of large petrochemical enterprises are structurally complex systems. Therefore, a substantial interest is attracted by the conditions of their freelance operation, in which the wastewater have dynamically varying parameters such as the composition and flow rate, up to the indicators of volley dump. The efficiency of such systems can be achieved by using modern methods of information processing using the methods of system analysis of complex objects based on the mathematical description of the process [8].

The system analysis is a sequence of actions to establish the structural relationships between variables or elements of the studied system which is based on the consideration of objects as systems with a given degree of consistency and independence [9]. The concept of a complex system is that the latter can be split into a finite number of subsystems. Each subsystem, in turn, can be split into a finite number of smaller subsystems to obtain such elements of a complex system, which under the conditions of the problem can not be further

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dismemberment. Elements of a complex system interact. The properties of one element depend on the conditions defined by the behavior of other elements. Properties of a complex system as a whole are determined not only by the properties of its elements, but also the nature of their interaction [10].

In accordance with the principles of system analysis, an industrial plant of BTW represents BChP comprising a set of interrelated material, thermal and flow of information devices, each of them has a hierarchical structure [1]. Processes in individual units of BTW should be considered as a multiphase, multicomponent environ distributed in space and time in which proceeds the set of elementary processes [11]. The increased efficiency of BTW is possible at different levels of the hierarchy of its installation: cells, cells agglomerates of activated sludge (flocculation), ensemble of flocculation, apparatus bioremediation, bioremediation unit, BTW system as a whole.

BTW can be subdivided into interrelated subsystems characterized by a hierarchical structure [12]. The first stage of the hierarchical structure is model biochemical processes and local governance, mainly the automatic control system. The second stage is aggregates and complexes representing an interrelated set of standard processes and apparatus implementing a particular operation. At this stage there is used an automated control system of technological processes. The third stage is BWT system allowing to obtain purified water. Here we use an automated control system (ACS) of technological and organizational functioning of production (ACS second level). The fourth stage is an enterprise as a whole. At this stage there is applied an automated enterprise management system.

Management tasks at each level of the hierarchy of production are different, but the general objective is to wastewater treatment given quality with maximum efficiency. Thus, the objectives of optimum local control are interconnected with a common purpose, aimed at increasing the efficiency of production as a whole.

A major step in the study of complex systems is a programming and mathematical modeling of the object [13]. Modeling and computer experiments with model - replacement facility are an effective means to create a management system, consider the behavior of the object in emergency situations, to evaluate its structure and control laws, as well as to take into account the stochastic nature of disturbances [7, 14]. There are two approaches to the modeling of real objects. In the first approach the object is represented as a dynamic system with continuous variable [15]. The functional mathematical model of the object is a system of ordinary differential equations, partial differential equations and algebraic polynomials obtained by the regression analysis to characterize the input (output) of the system. This approach is widely used in modeling chemical processes with a continuous organization of the process [16, 17, 18] provided that it is stationary and the immutability of physical and chemical parameters. In the second approach, the object is represented as a dynamic system with discrete events (DSDE) [15], which can not be described by conventional methods. These include manufacturing systems, assembly lines, computer networks. Such systems depend on a complex interaction of discrete events (incoming signal, the start or the end of a message) [19]. The problem of constructing models of DSDE is to determine the set of states of the system and to establish patterns of change of its states. We distinguish the following features, which must be satisfied by DSDE as a piecewise constant function: the discrete nature of events and the phase trajectory; continuous nature of the objective function (optimization criterion); stochastic formulation of a problem, a sequence of actions to establish the structural relationships between variables or elements of the system studied, reflecting the dynamics of internal operation of facilities; feasibility of computer calculations including combinatorics dependencies of DSDE number of states on the number of items that should not condition the progressive increase in the dimensions of the model as it complicates its practical applicatin.

This DSDE class also includes discrete-continuous biochemist technological systems. Solving problems of management organization of such discrete dynamical systems requires the use of special mathematical methods. Traditionally, for this purpose there are used methods of finite automata, logical-linguistic and simulation models, as well as of the theory of graphs and networks, Petri nets (PN) [20]. We have performed a comparative analysis of these methods applied to the problems of DSDE modeling. On this basis, as the main mathematical modeling of the theory is selected the PN, which is an important mathematical tool in solving such problems [20]. The PN allow you to simulate discrete concurrent asynchronous processes [20], to obtain a graphical representation of the network, describe the system at different levels of abstraction, present the system hierarchy [6], analyze models using modern application package.

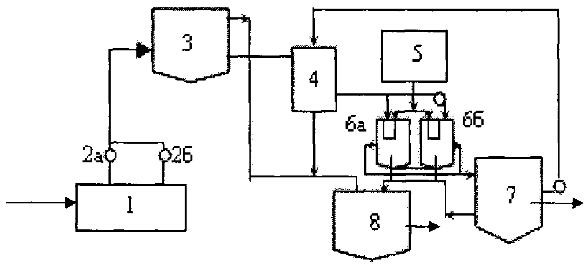

Fig. 1: Block diagram of Bioremediation of oily wastewater (OW) installation Block diagram of the apparatus includes: 1 - drive effluents; 2a and 2b - pumps, 3 - primary clarifier; 4 - averager; 5 - capacity for micro-organisms and bio-stimulants; 6a and 6b - jet settlers; 7 - secondary settling tank; 8 - slurry tank

Thus, the application of system analysis methods allow the development of a control system of wastewater treatment installation of petrochemical plants, which includes the construction of a mathematical model of the lower and upper levels of functioning. On the lower level of functioning there is determined an analytical model of the bioreactor. This allows you to provide wastewater treatment to the maximum allowable concentration. On the upper level of functioning, network models are built in a joint venture that provides flow control to install.

Block diagram of Bioremediation of oily wastewater (OW) installation is shown in Figure 1.

Upper level of bioremediation process of OW in industrial plants can be efficiently described by PN [21]. To describe this system, we propose the use of N-schemes based on mathematical apparatus PN [22], one of its advantages is the possibility of representing the network model in analytical form to automate the process of analysis and graphical form for clarity of models [20].

In the analysis of chemical-engineering or a biochemical process flow diagrams there should be considered the main limitation of the formalism of N-schemes which consists in the fact that they do not consider the temporal characteristics of the simulated systems, since the response time of transition is considered to be zero. Given these conditions, we propose to use MPN - PN of the form $C=\langle P,T,I,O,M,\tau_1,\tau_2\rangle$ [21],

where $T=\{t_j\}$ - finite nonempty set of symbols (transitions) estimated from the number of servings of conventional products with a continuous feeding in the apparatus of the flowsheet;

- $P=\{p_i\}$ - finite nonempty set of symbols (position) which are understood many devices flowsheet;
- $I: PxT \to \{0, 1\}$ - input function which gives the set of its position $p_i \in I(t_j)$ for each transition t_i;
- $O: PxT \to \{0, 1\}$ - output function which displays a transition to a set of output positions $p_i \in O(t_j)$;
- $M: P \to \{1, 2, 3...\}$ - function labeling (marking) network which assigns to each position a non-negative integer equal to the number of labels in this position, changing in the process of the network.

Actuation of the transition instantaneously changes the markup $M(p)=(M(p_1), M(p_2), M(p_3)\ldots M(p_n))$ for marking $M^{/}(p)$ by the following rule:

$$M^{/}(p) = M(p) - I(t_j) + O(t_j) \quad (1)$$

Equation 1 indicates that a transition t_j removes one of each tag of its input position and adds one tag to each of the output positions.

τ_1: T→N и τ_2 : P?N functions that define the time-delay at the transition and time delay in the position.

The dynamics performing MPN is defined by the marks movement simulating traffic flows of discrete intermediates.

The considered PN modification allows to analyze the functioning of the system units under emergency situations, switching the control at the network layer, as well as technological schemes discrete-continuous processes for sustainable, stable system state.

Here we consider the modeling process of the degradation of petroleum hydrocarbons by oxidizing microorganisms in jet settlers (JS) on the lower level. Waste liquid balanced in preparation for salts, nutrients, biokataliziruschim compounds, pH, temperature oxidizing microorganisms served in the jet settlers through the jet element. The technological process of bioremediation OW is carried to the column continuous or bolus settlers. To construct a mathematical description of the flow structure in JS, the entire volume of the device is divided into three zones: the upper part of the column - the mixing zone, where is the basic process of decomposition of hydrocarbons; the medium part of the unit - the zone of subsidence, where is the further process of OW bioremediation from pollution; the lower part of the machine - the zone of sludge where ends the process of decomposition of hydrocarbons (Fig. 2).

The mathematical model of the process in the mixing zone (zone I) is written as a model of ideal mixing (2, 3):

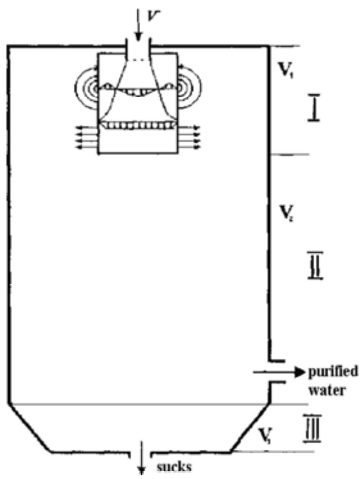

Fig. 2: Jet settlers

$$V\frac{dB^{(1)}}{dt}=\left(B^{(0)}-B^{(1)}\right)*\upsilon+q_B V \quad (2)$$

$$V\frac{dS^{(1)}}{dt}=\left(S^{(0)}-S^{(1)}\right)*\upsilon-q_S V \quad (3)$$

Initial Conditions:

$$B^{(0)}=const, S^{(0)}=const \quad (4)$$

where $B^{(0)}$, $B^{(1)}$ - concentration of microorganisms, respectively, in the input stream and the mixing zone; $S^{(0)}$, $S^{(1)}$ - concentration of hydrocarbons of oil, respectively, in the input stream and in the mixing zone; q_B - growth rate of the microorganisms; q_S - rate of oil oxidation by microorganisms; V - volume of a zone of the apparatus; υ - flow rate.

Kinetic characteristics of the process q_B and q_S are determined by empirical relations 5 and 6:

$$q_B=\frac{m_{\max}SB}{(1+H^+/K_1+K_2/H^+)(K_S+S)\exp[(t^0_{opt}-t^0)^2/d](1+C_{???}/K_{???1}+K_{???2}/C_{???})}-K_d B \quad (5)$$

$$q_S=-\frac{1}{Y_S}\frac{m_{\max}SB}{(1+H^+/K_1+K_2/H^+)(K_S+S)\exp[(t^0_{opt}-t^0)^2/d](1+C_{???}/K_{???1}+K_{???2}/C_{???})} \quad (6)$$

where m_{max} is maximum specific growth rate of microorganisms; K_d is rate constant of microorganisms dying; Y_s is coefficient for substrate binding amount of biomass and amount of the past on its growth substrate (hydrocarbons); K_s is half-saturation constant (affinity constant to the substrate), K_1 and K_2 are inhibition constants by hydrogen ions (K_1 describes inhibition in acidic region ($Í^+$>>K_1)); K_2 describes the inhibition in the alkaline region (K_2>>H^+); H^+ is hydrogen ions concentration; $t°_{opt}$ is temperature optimal for microbial growth; t° is current temperature; d is temperature range; $C_{Kàт}$ is concentration of biocatalysts compounds; $K_{Kàт1}$ and $K_{Kàт2}$ are effective inhibition constants - activation in their respective fields, pK_1 and pK_2 are dissociation constants.

Identification of kinetic parameters of the reaction rate q_B and q_S was based on data obtained in the Biotechnology laboratory of Kazan (Volga Region) Federal University: m_{max} = 0,7; K_S = 10; pK_1 = 4; K_1 = -lg(pK_1); pK_2 = 9; K_2 = -lg(pK_2); $K_{Kàт1}$ = 5; $K_{Kàт2}$ = 50; $t°_{opt}$ = 28°C; d = от 14°C до 30°C; K_d = 0,02; Y_S = 1.

The system of equations 2 and 3 is solved together with the equations of the kinetics of biochemical transformation 5, 6 by Runge-Kutta method, which allows to obtain reliable and accurate numerical evaluation of OW [23].

Mathematical model OW biorefining in the sedimentation zone (zone II) is defined with the proviso the bioprocess is accompanied by gradual deposition of sputtered particles flux, allowing to record the process in a diffusion-parameter model represented by demonstrations 7 and 8:

$$f\frac{\partial B^{(2)}}{\partial\tau}=-\upsilon\frac{\partial B^{(2)}}{\partial x}+fD_L\frac{\partial^2 B^{(2)}}{\partial x^2}+q_B f \quad (7)$$

$$f\frac{\partial S^{(2)}}{\partial\tau}=-\upsilon\frac{\partial S^{(2)}}{\partial x}+fD_L\frac{\partial^2 S^{(2)}}{\partial x^2}+q_S f \quad (8)$$

where $B^{(2)}$ is concentration of microorganisms in the displacement zone; $S^{(2)}$ is concentration of hydrocarbons in the displacement zone; $\tau_{Cð2}$ is average residence time of a flow cell in the displacement zone; D_L is longitudinal mixing ratio during the deposition of sputtered flow particles, l is length of the deposition zone, υ- volumetric flow rate of oily wastewater (OW), f is cross section of the machine.

For the system of equations 7, 8 we formulate the range of initial and boundary conditions in the zone of variables:

$$\tau\in[\tau_{cp1};\tau_{cp1}+\tau_{cp2}]\ x\in[0;l] \quad (9)$$

Initial conditions: $\tau_{Cð1}<\tau<\tau_{Cð1}+\tau_{Cð2}$, $B^{(2)}|_{\tau=\tau Cð1}=B^{(1)}$, $S^{(2)}|_{\tau=\tau Cð1}=S^{(1)}$; (10)

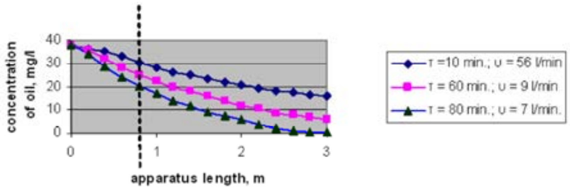

Fig. 3: Changing the concentration of oil along the length of the apparatus

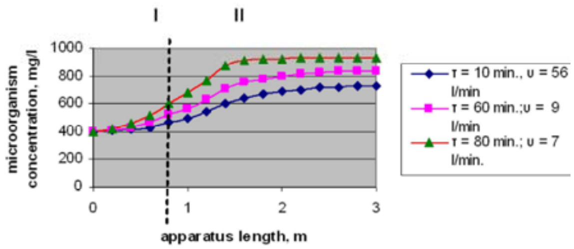

Fig. 4: Changing the concentration of microorganisms on the length of the apparatus

Boundary conditions:

$$B^{(2)}(0;\tau)=B^{(1)}\; S^{(2)}(0;\tau)=S^{(1)}\; \frac{\partial B}{\partial x}\Big|_{x=l}=0\; S^{(2)}(l;\tau)=S^{???} \tag{11}$$

The system of equations 7 and 8 is solved together with the equations of the kinetics of biochemical conversion of 5, 6. This system of differential equations is an important tool in analytical calculations [24, 25]. It describes the process of in the settling area and solved using the finite difference method for the implicit scheme.

Model calculations are performed on an example of Jet settlers. They showed that the permissible degree of OW bioremediation achieved at flow rates in the range of 7 l / min (Fig. 3).

At flow rates in the range of 7 l / min epy number of microorganisms increased twice, which increases the efficiency of the bio-oxidation process in the JS (Fig. 4).

Thus, we developed a mathematical model of the process of OW bioremediation in JS, which is the basic model to describe this process [4], defines the operation of the plant of OW cleaning with an neutralization efficiency of petroleum products to the maximum allowable concentration for 1.2 hours of cleaning and it allows to intensify this process for temporary parameter.

To manage the process of OW bioremediation on the upper level, a mathematical model of the technological scheme and its software implementation is developed. The mathematical model of OW bioremediation is developed as MPN which implementation helped to explore the communication system and the laws of functioning of the unit as a whole. Also there are constructed the models of the main devices implementing OW bioremediation process [21]. Of the PN models of typical devices was synthesized a model of the entire system (Fig. 5).

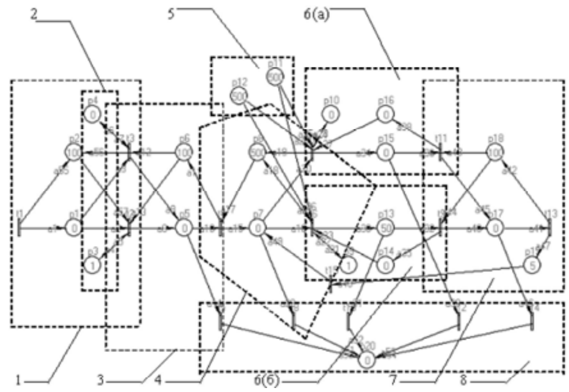

Fig. 5: Model of the process module as MPNFig. 5. Model of the process module as MPN

Using the PN model we have developed a software package of the technological feasability of OW bioremediation module simulating the operation of bioremediation in virtual time. With SCADA- technology means TRACE MODE was designed software package of process control system of biological OW treatment [26, 27]. An essential feature of the developed software process control system is its ability to adapt to technological feasability module of OW bioremediation of any capacity, as for installation in a separate gas station (tanker) and water treatment systems of large petrochemical industries [28].

The process control system allows to perform the supervisory control of the main elements of the management system, stop the system of OW bioremediation and analyze its feasability as a whole and to predict the development of emergency situations [13].

CONCLUSION

In the analysis of chemical-engineering (biochemical process) systems there was defined the basic restriction formalism of N- schemes which is the lack of accounting of temporal characteristics of the simulated systems by N-schemes [20]. This necessitates the use of MPN oriented to the modeling and analysis of discrete-continuous BchP by incorporating priority transitions and timing the delaying marks in the positions and transitions. The technique of two-level modeling system of biochemical OW purification process allows the analysis of the functioning of industrial installations of OW bioremediation in a dynamically changing process parameters [29] and benefit at the meso and macro levels [13].

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