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MATHEMATICAL MODEL OF DIFFUSION PROCESS FOR SOLVING HYDROECOLOGICAL PROBLEMS

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МАТЕМАТИЧНА МОДЕЛЬ ПРОЦЕСУ ДИФУЗІЇ ДЛЯ ВИРІШЕННЯ ГІДРОЕКОЛОГІЧНИХ ЗАВДАНЬ

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The article discusses the actual tasks of adaptive control of local water treatment plants to ensure the rational use of water. The software solutions for modeling the diffusion process in a porous medium with the absorption of a diffusing substance on the pore surface are considered in detail.
Keywords: *simulation modeling, automated systems, wastewater, water purification, adsorption, software.*

The development of the productive forces of Ukraine is accompanied by an accelerated rate of water consumption. Taking into account the fact that, according to the international classification, Ukraine is among the European powers, the least endowed with its own water resources, the rational use of water becomes of paramount importance for it and is one of the most important tasks of ensuring environmental safety and sustainable development of the country's economy.

Optimal water supply can be achieved as a result of the introduction of water-saving technologies and technologies with low water consumption or as a result of improved water supply systems [1].

One of the effective ways of rational use of water resources is to protect them from pollution by improving systems and methods of wastewater treatment. The most current way to achieve the required quality of water purification are adaptive methods of managing the purification process. The implementation of adaptive control requires the creation and use of a mathematical modeling tool.

The article presents the results of solving problems of modeling water preparation processes. The adsorption purification method is considered. This method is used for deep treatment of wastewater from dissolved organic substances after biochemical treatment, as well as at local sewage treatment plants of industrial effluents, which are multicomponent mixtures [2]. In this method, the molecules of the dissolved pollutant are transferred from the solution to the surface of a highly absorbing substance (adsorbent) under the action of the force field of the surface. Based on the studies presented in [3], adsorption can be considered as a process of stationary diffusion with absorption on the surface of particles in regions with a fine-grained random boundary.

The purpose of the study is to improve the local wastewater treatment system based on adaptive control methods using simulation modeling of the diffusion process in a porous medium with absorption of a diffusing substance on the surface of pores.

The limiting model of diffusion in a porous medium with absorption on the pore surface is based on Dirichlet problem [4]:

$$\begin{cases} -D\Delta u(x)+C(x,u)=f(x), \ x\in\Omega, \\ u(x)=0, \quad x\in\partial\Omega \end{cases}, \qquad (1)$$

where D is the diffusion coefficient, Δ is the Laplace operator, C(x, u) describes the limiting absorption of the system, f(x) is the given function of external sources, Ω is the area of a substance that diffuses.

The required function u(x) sets the concentration of a substance that diffuses at every point of the Ω area.

The universal methods for the approximate solution of differential equations applicable to a wide class of equations in mathematical physics are numerical methods, in particular, the finite difference method (or the grid method).The finite difference method is as follows. The area of continuous change of arguments is replaced by a finite (discrete) set of points (nodes), called a grid with step division (h) by spatial variables (Fig. 1.).

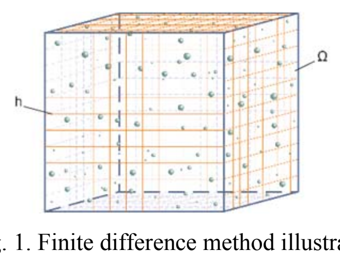

Fig. 1. Finite difference method illustration

Instead of functions of a continuous argument, functions of a discrete argument are defined, which are defined at the grid nodes and are called grid functions. Derivatives included in the differential equation are replaced (approximated) using the appropriate difference relations. The differential equation is replaced by a system of algebraic equations (difference equations). The initial and boundary conditions are also replaced by the difference initial and boundary conditions for the grid function.

The finite difference method was applied to the model (1), after which the system of difference equations acquired the following form (2).

$$\begin{cases} \frac{D}{h^2}[u(i-1,j,k)+u(i+1,j,k)+u(i,j-1,k)+u(i,j+1,k)+ \\ u(i,j,k-1)+u(i,j,k+1)-6u(i,j,k)-C(i,j,k,u)+f(i,j,k)]; \\ i=1,\dots,n_1-1; j=1,\dots,n_2-1, k=1,\dots,n_3-1; \\ u(0,j,k)=u(i,0,k)=u(i,j,0)=0; \\ i=0,\dots,n_1; j=0,\dots,n_2; k=0,\dots,n_3. \end{cases} \qquad (2)$$

Jacobi's iterative method is used to solve a system of difference equations. The computational algorithm of the method is that the new value at each grid point is determined as the average of the previous values of the four neighboring points (left, right, top and bottom). This process is repeated to the last point.

Computational algorithm was compiled for a system of difference equations (2). This algorithm consists of performing the following formal procedures:

1) Set $u^0[i,j,k]=0;\ i,j,k=\overline{0,\dots,n}$;
2) Calculate $u^1[i,j,k],\ u^2[i,j,k],\dots,u^n[i,j,k]$

bye $\left|u^{n-1}[i,j,k]-u^n[i,j,k]\right|<\varepsilon$,

where ε - accuracy is 0.001;

$$u^n[i,j,k]=\frac{1}{6}(u^{n-1}[i+1,j,k]+u^{n-1}[i-1,j,k]+u^{n-1}[i,j+1,k]+$$
$$+u^{n-1}[i,j-1,k]+u^{n-1}[i,j,k+1]+u^{n-1}[i,j,k-1])+$$
$$+\frac{h^2}{6}\left(C\left(x_1^i,x_2^j,x_3^k,u^{n-1}[i,j,k]\right)-f\left(x_1^i,x_2^j,x_3^k\right)\right);$$
$$u^n[0,j,k]=u^n[n,j,k]=u^n[i,0,k]=u^n[i,n,k]=$$
$$=u^n[i,j,0]=u^n[i,j,n]=0$$

The final stage of mathematical modeling is the development of a modeling tool - a set of programs that implement the presented methods and computational algorithms. A visual interface has been created to present the results of computational experiments using the Delphi development environment. This interface is convenient to use, buttons and windows are arranged so that they are easy to manipulate, related data is placed in one window, and moderate colors is used. One of four models is proposed for calculating the optimal amount of adsorbent: for moderate absorption, critical absorption, strong absorption, and for ultra-small particles.

The the program working window is shown in the figure (Fig. 2), where objects are indicated by numbers:

1. method selection switch;
2. input fields for diffusion parameters;
3. input fields for region parameters;
4. output field of the concentration matrix;
5. section layer illustration;
6. calculation start button.

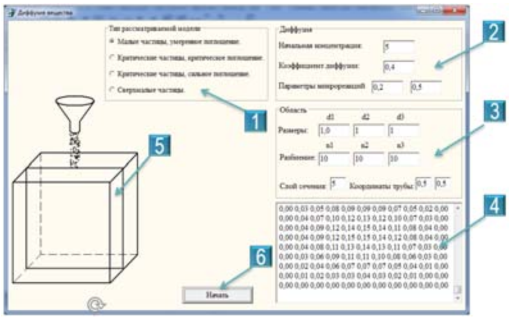

Fig. 2. The working window of the program

The results illustrate the effectiveness of the developed algorithms for determining the optimal parameters of the wastewater treatment process.

The introduction of the developed simulator into the control system of local water treatment plants will improve the accuracy of calculations of the required volume of the adsorbent, ensure the implementation of control system adaptation algorithms to the changing characteristics of wastewater, as well as obtain high quality water treatment.

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Гулевська К.В., Шумова Л.О., Мохонько В.І. Математична модель процесу дифузії для вирішення гідроекологічних завдань

У статті розглядаються актуальні завдання адаптивного управління локальними водоочисними спорудами для забезпечення раціонального використання води. Детально розглянуті програмні рішення для моделювання дифузійного процесу в пористої середовищі з поглинанням диффундирующего речовини на поверхні пір.

Ключові слова: *імітаційне моделювання, автоматизовані системи, стічні води, очищення води, адсорбція, програмне забезпечення.*

Гулевская К.В., Шумова Л.А., Мохонько В.И. Математическая модель процесса диффузии для решения гидроэкологических задач

В статье рассматриваются актуальные задачи адаптивного управления локальными водоочистными сооружениями для обеспечения рационального использования воды. Подробно рассмотрены программные решения для моделирования диффузионного процесса в пористой среде с поглощением диффундирующего вещества на поверхности пор.

Ключевые слова: *имитационное моделирование, автоматизированные системы, сточные воды, очистка воды, адсорбция, программное обеспечение.*

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