# POLLUTION

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## ON THE ISSUE OF SORPTION OF MICROORGANISMS IN A SOLITARY PORE SYSTEM OF A CARBON SORBENT

Research article

**Abstract**

The article discusses the sorption of microorganisms on a carbon sorbent. The study of samples of recycled and purified waters was carried out using a luminometer and a turbidometer-nephelometer. Microorganisms immobilized in the pores were studied using light and electronic optics. With the help of bioinformatic interpretation, the sorption interaction of some types of microorganisms divided by size factor into blue-green algae and protozoa, bacteria and viruses with a solitary pore system consisting of three types of subsystems: macro-, meso- and micropores is modeled. Initially, for a theoretical description of the reduced system, an oriented graph was constructed using network theory. In the future, with the help of generating and exponential functions, a method for classifying microorganisms in accordance with the size factor is given, and the question of describing the number of ways of placing microorganisms in the presented pore system is considered, on which, ultimately, the total sorption depends. And since the latter is a reversible equilibrium phenomenon, in conclusion, the reverse process is also predicted – desorption, calculated using the Bayes theorem, often used in bioinformatics.

**Keywords:** microorganisms, recycled water, sorption purification, carbon sorbent, solitary pore system, macro-, meso-, micropores, digraph, generating and exponential functions, Bayes theorem.

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## К ВОПРОСУ О СОРБЦИИ МИКРООРГАНИЗМОВ В УЕДИНЕННОЙ ПОРОВОЙ СИСТЕМЕ УГЛЕРОДНОГО СОРБЕНТА

Научная статья

**Аннотация**

В статье рассматривается сорбция микроорганизмов на углеродном сорбенте. Исследование образцов оборотных и очищенных вод выполнено с помощью люминометра и мутномера-нефелометра. Микроорганизмы, иммобилизованные в порах изучены с помощью световой и электронной оптики. С помощью биоинформационной интерпретации смоделировано сорбционное взаимодействие некоторых видов микроорганизмов, подразделяемых по размерному фактору на сине-зеленые водоросли и простейшие, бактерии и вирусы с уединенной поровой системой, состоящей из трех типов подсистем: макро-, мезо- и микропор. Первоначально, для теоретического описания приведенной системы, с помощью теории сетей построен ориентированный граф. В дальнейшем, с помощью производящих и экспоненциальной функций приведен способ классификации микроорганизмов в соответствии с размерным фактором, а также рассмотрен вопрос описания количества способов размещения микроорганизмов в представленной поровой системе, от которых, в конечном итоге, зависит общая сорбция. А так как последняя есть обратимое равновесное явление то, в заключении, также спрогнозирован обратный процесс – десорбция, вычисленный с использованием часто употребляемой в биоинформатике теоремы Байеса.

**Ключевые слова:** микроорганизмы, оборотные воды, сорбционная очистка, углеродный сорбент, уединенная поровая система, макро-, мезо-, микропоры, орграф, производящая и экспоненциальная функции, теорема Байеса.

## 1. Introduction

Recycled (waste) water as a habitat for numerous microorganisms (blue-green algae, protozoa, bacteria, viruses) it causes many harmful phenomena, such as turbidity and unpleasant odor, corrosion of metals and alloys, even such as stainless steels, and also, due to the transfer of a number of serious diseases, it poses a real threat to human health. Municipal wastewater as a whole is an excessive nutrient medium for the development of algae and protozoa, as well as bacteria and viruses. Thus, due to the widespread use of synthetic detergents containing phosphates in high concentrations in everyday life, the growth and reproduction of blue-green algae occurs in wastewater, causing its active flowering, accompanied by a fall in water dissolved oxygen [1]. When the dissolved oxygen content decreases to critical values, many aquatic inhabitants (for example, fish) begin to die, so flowering can lead to the formation of overseas zones. One of the most effective methods of wastewater treatment from such pollutants is the use of carbon sorbents. Special attention is paid to the study of the nature of the adsorption interaction, porosity, as well as the specific surface area of sorbents, since the strengths of the use of these substances are their high absorbing and brightening ability, repeated use, as well as availability and cheapness [2].

## 2. Experiment and methods

Initially, the synthesis of carbon sorbents was developed and adjusted, with the development of technology for their use for wastewater treatment according to the method [3]. Then the porosity of the obtained sorbents was studied according to the method [4]. Thus, the average size of macropores was about 6-10 microns, mesopores had size indicators comparable to 1,0-0,6 microns, and the size of micropores (determined by electron microscopy) was assumed to be 0,05-0,2 microns. Sorption purification of recycled water from bio-contamination consisted in their passage through a column with a carbon sorbent and analysis of the degree of their purification upon completion of the filtration process (Fig. 1).

An important indicator of the quality of water used for almost any purpose is its transparency. Therefore, for an objective assessment of qualitative indicators during tests of carbon sorbent, the turbidity of circulating waters was studied with a Milwaukee MI-415 nephelometric turbidimeter [5]. The wastewater delivered for the experiment visually had a dirty yellow-green color and, therefore, showed a very high turbidity taking the value of 60 FNU. When studying this water that has been filtered through a sorbent, the turbidity became equal to 0,22 FNU. Thus, turbidity after filtration through the sorbent decreased by more than 270 times and, according to this criterion, assumed a value very close in transparency to the indicator of tap water (0,0-0,25 FNU).

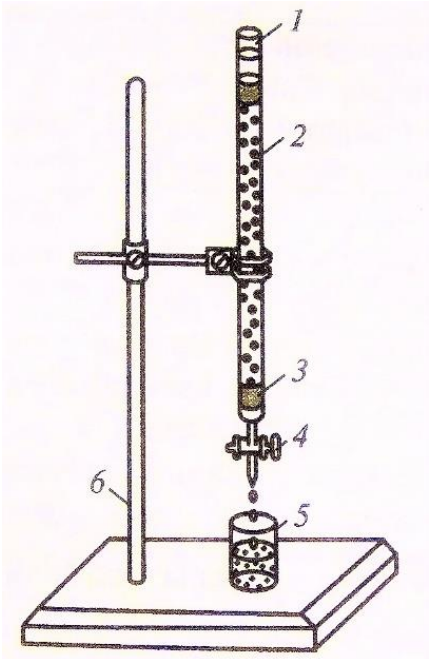


Fig. 1 – Filtration column with carbon sorbent:
*1* – glass burette; *2* – sorbent layer; *3* – glass wool or fiberglass layer; *4* – a tap to adjust the filtration rate;
*5* – a glass for collecting filtrate; *6* – metal tripod with foot

To determine the microbiological contamination of wastewater samples treated with carbon sorbent, a BIOLUM III luminometer was used, which is a device that works with test systems specially created for it that determine the biological purity of water samples by quantifying ATP based on the phenomenon of bioluminescence. Under the influence of the enzyme luciferase, ATP present in the sample accelerates oxygen oxidation of a special luciferin peptide with the release of a quantum of light (Fig. 2). The reaction occurs so fast that it allows you to get results in real time according to the following scheme: luciferin + $O_2$ + ATP → oxidized luciferin + $CO_2$ + $H_2O$ + ATP + $P_2O_7^{4-}$ + hυ [6]. In biology and medicine, methods using luciferase are also in demand, for example, immunoprecipitation for the detection of antibodies in autoimmune and infectious diseases, the study of the immune response in Ebola fever and the pathogenesis of herpesvirus infection, cytotoxicity research, etc.

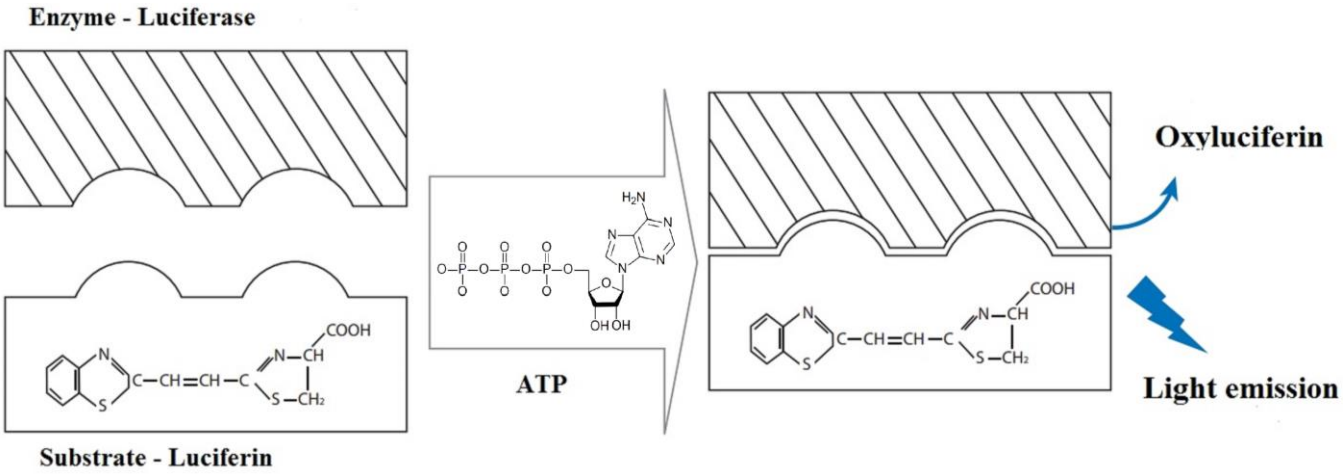


Fig. 2 – The principle of operation of the luminometer

Measurements showed that the wastewater samples had a bio-contamination equal to 905 RLU (relative light units). This indicator repeatedly exceeded the maximum permissible purity threshold for public water. Thus, the biointerpretation indicates that water having the maximum permissible concentration of microorganisms (viruses, bacteria, protozoa and algae) should be equal to the value of 30 RLU [7], [8], [9]. Purification of wastewater samples using an organomineral sorbent allowed to reduce bio-contamination to a value of 50 RLU, i.e. more than 18 times.

Upon completion of the filtration process, the carbon sorbent was drained under vacuum and frozen in a Dewar vessel to the temperature of liquid nitrogen. Then thin sections were obtained from its surface to expose pore systems. After that, optical and electron microscopy of their surfaces was carried out, first at a relatively low resolution, and then at the limit of electronic optics (Fig. 3).

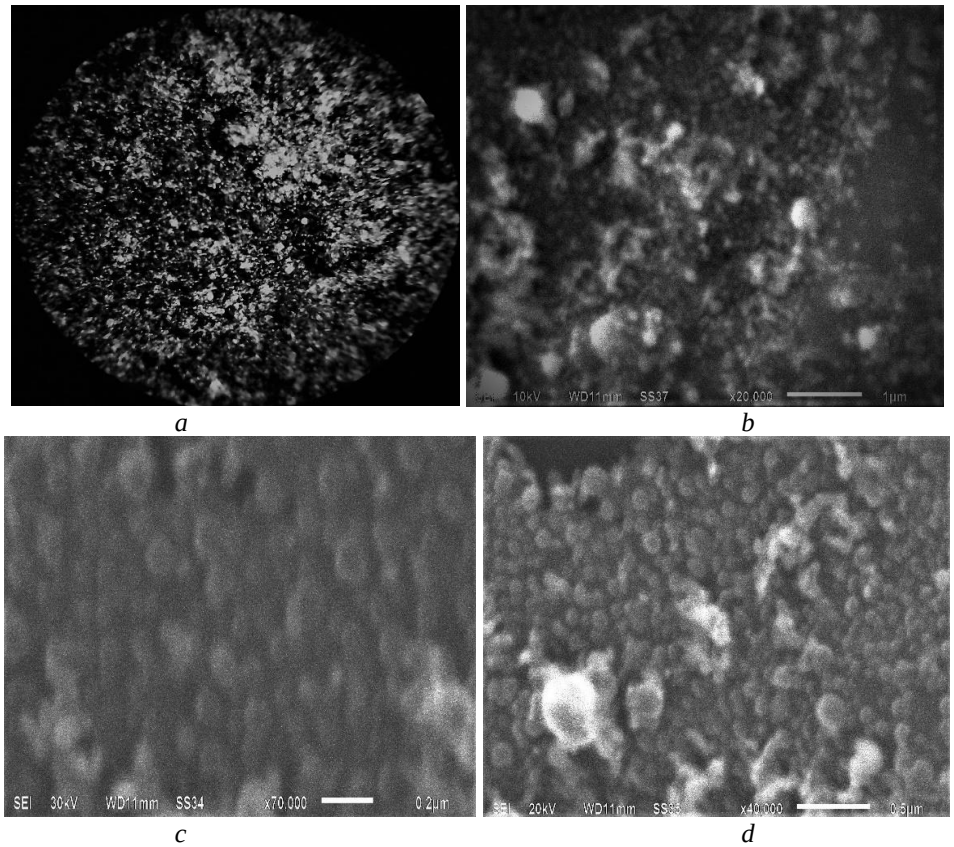


Fig. 3 – Optical (luminescence) and electronic micrographs microorganisms localized in the pore system:
*a* – localization of the biofilm on the surface of the sorbent (magnification X1000); *b* – a section of macropores, algae + protozoa + large bacteria (an increase of X20,000); *c* – a section of mesopores, large and small bacteria + viral particles (an increase of X40,000); *d* – a section of micropores, a colony of viral particles in the form of a dense package is visible (an increase of X70,000)

Thus, the experimental data obtained during the study of recycled water samples, after their passage through the sorbent layer, had high bio-purification rates.

### 3. Calculation algorithm and discussion of the results

When carrying out all calculations, the main condition of the described processes is that sorption (immobilization) in this case assumes an exclusively physical (dimensional) character, i.e. retention of such microbiological particles as blue-green algae, protozoa, bacteria, viruses, etc. in a solitary pore system, without destroying the shaped (membrane) integrity of these microorganisms.

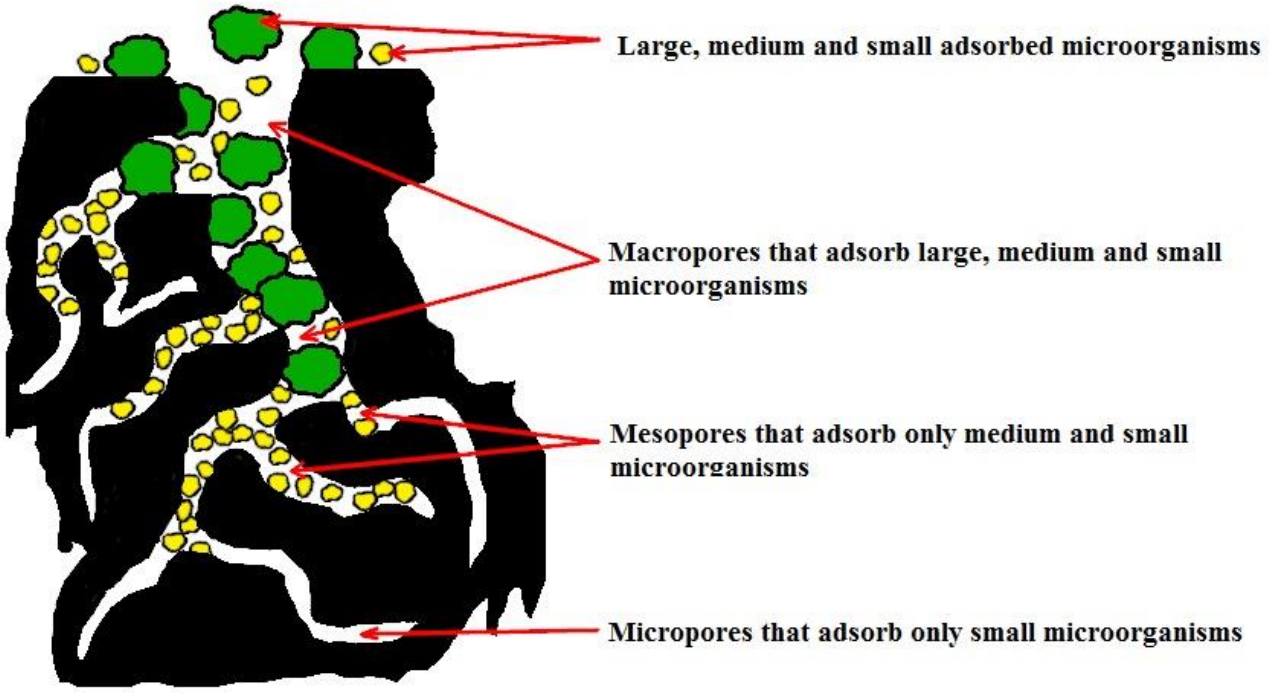


Fig. 4 – Model of a solitary pore system

Consider a solitary pore system consisting of subsystems such as macro-, meso- and micropores (Fig. 4). Now imagine it as a transporting system through whose capillaries water contaminated with microorganisms (blue-green algae and protozoa, bacteria and viruses) flows, passing from one point of the subsystem to another. Using this representation, using network theory, we will represent this transporting system in the form of an oriented graph, the edges of which are microcapillaries between points (subsystems of pores), in turn, represented by the vertices of the graph (Fig. 5) [10], [11]. We introduce the concept of flow as the number of microorganisms passing through the capillaries of a solitary pore system for their retention (sorption), and the flow in question will be directed only in one direction (from the liquid to the pores) and has constancy. Thus, there is some fixed flow, the source of which is the entrance (A) to the pore system through the macropore, the mesopore (B, D, E) will be an intermediate (connecting) link, and the micropore (C, F, Z), in turn, will become a drain. Then it becomes obvious that the amount of flow cannot exceed the throughput capacity of micropore capillaries. Thus, sorption in the most general case is limited by the filtration rate in micropores.

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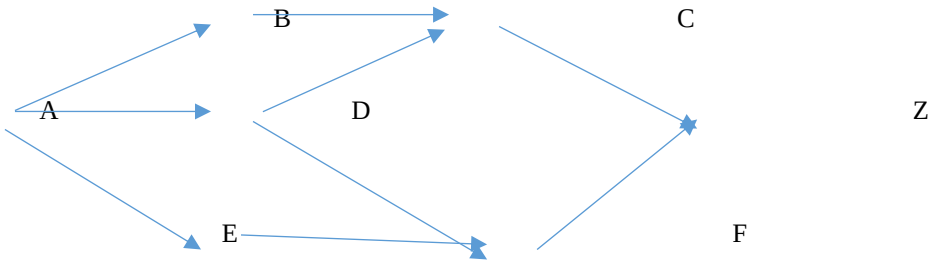


Fig. 5 – Digraph describing a solitary pore system

Further, in the sorption process, we will consider a very important question about the number of ways to place microorganisms in a solitary pore system, on which their total presence in the sorbent ultimately depends. So, we predict such placements. Let all microorganisms be classified according to the size factor of the solitary pore system in which they are retained (sorbed). In general, we will need to find a generating function describing the total number of different placement methods that can classify n-microorganisms in k-pores in such a way that none of the pores will be empty [12].

$$x^k\,(1+x+\,x^2+\cdots)(1+\,x^2\,+\,x^4+\cdots)(1+\,x^3+\,x^6+\cdots)\ldots(1+x^k+x^{2k}+\cdots)\text{ or }\frac{x^k}{(1-x)(1-x^2)(1-x^3)\ldots(1-x^k)} \quad (1)$$

And since the solitary pore system itself as a whole consists of only 3 subsystems (macro-, meso-, micro-), then the n-th number of microorganisms in it takes a very simple form:

$$\frac{x^3}{(1-x)(1-x^2)(1-x^3)} \quad (2)$$

The next step is to find a generating function describing the number of ways to place n-microorganisms in the three subsystems indicated, while accepting the condition that each of the subsystems can contain at least one (for example, algae or protozoa) but no more than n (bacteria + viruses) microorganisms. This will require the use of the basic property of ordinary exponential functions [13], [14]. Then, the desired exponential generating function will take the following form:

$$f_{(x)}=(\tfrac{x}{1!}+\tfrac{x^2}{2!}+\tfrac{x^3}{3!}+\cdots+\tfrac{x^n}{n!})\times(\tfrac{x}{1!}+\tfrac{x^2}{2!}+\tfrac{x^3}{3!}+\cdots+\tfrac{x^n}{n!})\times(\tfrac{x}{1!}+\tfrac{x^2}{2!}+\tfrac{x^3}{3!}+\cdots+\tfrac{x^n}{n!})$$
$$\text{or simplifying } f_{(x)}=(\tfrac{x}{1!}+\tfrac{x^2}{2!}+\tfrac{x^3}{3!}+\cdots+\tfrac{x^n}{n!})^3 \quad (3)$$

The final step in predicting the ways of placing microorganisms was the exponential function of placing microorganisms in 3 subsystems, provided that one protozoan is retained in the macropore, and the number of microorganisms in meso- and micropores is taken for odd and even numbers for simplicity. Then the placement function will be set by the following expression:

$$f_{(x)}=\left(\frac{x}{1!}+\frac{x^2}{2!}+\frac{x^3}{3!}+\cdots\right)\times\left(\frac{x}{1!}+\frac{x^3}{3!}+\frac{x^5}{5!}+\cdots\right)\times\left(\frac{x^2}{2!}+\frac{x^4}{4!}+\frac{x^6}{6!}+\cdots\right)=(e^x-1)\frac{e^x-e^{-x}}{2}\times\frac{e^x+e^{-x}}{2}$$
$$=(e^x-1)\frac{e^{2x}-e^{-2x}}{4}=\frac{1}{4}(e^{3x}-\,e^{-x}-e^{2x}+e^{-2x}), \quad (4)$$

therefore, the coefficient at $\frac{x^n}{n!}$ will be equal to: $\frac{1}{4}((3)^n-\,(-1)^n-(2)^n+(-2)^n)$.

Since many millions of such pores (solitary pore systems) are present in one gram of carbon sorbent, it seems that the described number of ways to place these microorganisms (algae, protozoa, bacteria, viruses) in them takes place.

Unfortunately, sorption is an equilibrium phenomenon, always accompanied by the reverse phenomenon of desorption. Therefore, some of the microorganisms retained in the pore system (due to independent reasons) will inevitably be lost in the filtrate. To judge the probable degree of desorption of microorganisms in a solitary pore system, we will use Bayes' theorem to study the effect and determine this cause [15]. So, this theorem is generally recognized today and is often used in bioinformatics, as it is very useful for determining the causes of many serious diseases (for example, cancer), as well as prognoses of their treatment and recovery [16].

As the basis of calculations, we take equally possible events B1, B2, B3 .... Bn, for P(B1) = P(B2) = P(B3) = P(Bn). Then the relation for $P(B_i|A)$ will be reduced to the form:

$$P(B_i|A)=\frac{P(B_i|A)}{P(A|B_1)+\,P(A|B_2)+P(A|B_3)+\cdots+P(A|B_n)} \quad (5)$$

The problem of calculating the probability of desorption takes a very simple form, under the intuitive condition that the vast majority of the largest microorganisms are concentrated in macro- and mesopore subsystems, and the smallest viral particles are localized mainly in micropores. For clarity of the sorption-desorption process, we will take well-defined, obtained using electromagnetic optics, during the experiment, digital values of the number of microorganisms retained in a solitary pore system. So, in the available qualitative composition of microorganisms during sorption in a solitary time, there is such a alignment of disjoint events B1, B2 and B3 that break up the sample space, and it is clear that event A has been realized. In the experiment, as a result of counting, it was obtained that the macropore contained 3 protozoa, 30 different bacteria and 100 viral particles; the mesopore contained 10 bacteria and 50 viral particles; and, finally, the micropore contained only 30 viruses. Then suppose that microorganisms were desorbed from an arbitrarily selected pore in the pore system. If these were the smallest viral particles, then we will predict and calculate the probability that a micropore was selected. Let B1 be the event that a macropore was selected; B2 is the event that a mesopore was selected; and B3 is the event that a micropore was selected. Let R be the event that viral particles have been desorbed. Since the choice of pores is random, let's assume that P(B1) = P(B2) = P(B3). Therefore, a

simplified formula can be used. We have: $P(R|B_1)$ = 100; $P(R|B_2)$ = 50; $P(R|B_3)$ = 30. Therefore $P(B_3|R) = \frac{30}{100+50+30} = \frac{1}{6} =$ 0,16.

Thus, we obtained a probability of desorption of viral particles from the micropore of 0.16 out of 1.0.

**4. Conclusion**

From the above, it follows that the use of a carbon sorbent allows you to obtain sufficient results in the bio-treatment of wastewater, in order to discolor them, remove various pollutants (which are nutrient media) and microorganisms for the possibility of reuse of recycled water. Carbon sorbents are highly efficient, environmentally friendly systems to prevent water blooming. The consequence of their use is a successful fight against microorganisms, increasing the level of environmental safety to the maximum possible. The sorbent itself is not an expensive reagent and, if necessary, can be installed in a replaceable cartridge directly into the pipeline with contaminated water.

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**Conflict of Interest**

None declared.

**Конфликт интересов**

Не указан.

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