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Mathematical Modeling and Optimization of Contaminated Water Treatment Processes

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ABSTRACT: The aim of the study is to develop mathematical models and algorithms for solving stochastic and deterministic problems of purifying contaminated waters and establishing the ratio of duality and optimality, as well as a marginal relationship for these problems and determining the optimal cost of purifying contaminated waters in various purification schemes.

Keywords - wastewater; production wastes; environmental-economic model; mathematical modeling; treatment of contaminated waters

I. INTRODUCTION

Water is a valuable natural resource. It plays an exceptional role in the metabolic processes that form the basis of life. Water is of great importance in industrial and agricultural production. It is common knowledge that it is necessary for the domestic needs of humans, all plants and animals. For many living creatures, it serves as a habitat.

Freshwater shortages are already becoming a global problem. The increasing demands of industry and agriculture for water are forcing all countries, scientists of the world, to seek a variety of means to solve this problem.

During the development of civilization, the purification of natural water to obtain fresh water suitable for public use evolved from simple settling to filtration, disinfection, the use of physicochemical and biological technologies, which required increasing material energy and labor costs. In the limit, with the complete pollution of natural waters by civilization, the only method of its purification may be the natural process of purification with the help of evaporation and subsequent condensation (distillation.), I.e., water purification will take place on the basis of a natural thermodynamic cycle using the maximum amount of energy and significant social costs.

The main sources of pollution and clogging of water bodies are insufficiently treated wastewater from industrial and communal enterprises, large livestock complexes, production waste from the development of ore minerals; waters of mines, mines, processing and alloy of timber; water and rail transport discharges; primary flax treatment waste, pesticides, etc. Contaminants entering natural reservoirs lead to qualitative changes in water, which are mainly manifested in changes in the physical properties of water, in particular, the appearance of uppleasant odors, flavors, etc.); changing the chemical composition of water, in particular, the appearance of harmful substances in it, the presence of floating substances on the surface of water and their deposition at the bottom of water bodies.

The relevance and mathematical complexity of the problem leads to the need for the effective use of optimization methods and modern computer technology. The wide distribution and intensive use, as well as the rapid improvement of computers, significantly contribute to the accelerated pace of implementation of theoretical developments in optimizing environmental problems.

II. ANALYSIS OF CURRENT STATE OF METHODS OF MATHEMATICAL MODELING OF PROCESSES OF CONTAMINATED WATER TREATMENT.

A. Main process diagrams for the treatment of contaminated water.

At this stage we will focus on the problem of distributing a certain amount of contaminated discharge water to the process treatment circuits. By cleaning process circuit is meant a set of some cleaning devices arranged in series. The part of the discharge, allocated for cleaning according to some scheme, in the future should not fall on the cleaning devices of another scheme.



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The objective is to select such an acceptable combination of treatment technologies and distribution of contaminated water volume between them so that the cleaning costs are minimal and the concentration of impurities after cleaning at the control solution does not exceed the specified maximum permissible values. In reality, the task of water treatment is solved for a certain water treatment complex in the presence of several spillways and the concentration of controlled impurities at the control range depends on the quality of water protection measures at all spillway facilities.

When forming the task of optimizing water protection measures, it is essential to choose a model of a set of water protection measures that establishes the dependence between the amount of funds allocated to the water user for treatment and the quality composition of contaminated waters before discharging into the water body. Given this, an important task is to optimize the development of a set of contaminated water treatment complexes connected by a single hydrographic network at given restrictions on water quality in a water body.

B. Wastewater treatment methods.

Wastewater treatment methods can be divided into mechanical, chemical, physicochemical and biological, when they are used together, then the method of wastewater treatment and neutralization iscalled combined. The application of a method on a case-by-case basis is determined by the nature of the contamination and the degree of harm to the impurities.

III. DEVELOPMENT OF ALGORITHMS FOR ENVIRONMENTAL-ECONOMIC MODELING OF CONTAMINATED WATER TREATMENT PROCESSES.

A. Setting the objective and objectives of the study.

According to the available literature sources [6], dependencies reflecting the relation of the water user's costs for the implementation of water protection measures with the load volume of purification process circuits are concave functions and are well approximated by power functions with a fractional indicator.

The objective is to select such an acceptable combination of technologies and such a distribution of the volume of contaminated water between them so that the cost of purification is minimal and at the same time the concentration of impurities after purification at the control solution does not exceed the specified maximum permissible values. In reality, the task of water treatment is solved for a certain water treatment complex in the presence of several spillways and the concentration of controlled impurities at the control range depends on the quality of water protection measures at all spillway facilities.

Enter the following symbols:

- q_k the volume of contaminated water supplied to the treatment complex on the k-t spillway;
- X_{ki} volume of contaminated water, which will be treated according to the technological scheme of treatment on the k-

volume spillway. Thus, $X_k = \{x_{ki}\}, i = \overline{1, N}$, the vector of the distribution of the total amount of contaminated water among the treatment technologies on the k-t spillway;

 x_{ki}^{-} and x_{ki}^{+} - values limiting the production capacity of the i-th process diagram during volume discharge cleaning q_k ;

- C_{0kj} , C_{kj} concentration of j-type impurities respectively before purification and maximum permissible concentrations (MPC) after purification;

- P_{kii} the degree of cleaning of the j-th impurity according to the i-th purification technology on the k-t spillway;

- A_{ki} , λ_{ki} approximation factors of the cost function for contaminated water treatment according to the i-th process diagram on k- volume spillway ($A_{ki} \ge 0$; $0 \le \lambda_{ki} \le 1$, $k = \overline{1, L}$, $i = \overline{1, N}$).

We define an environmental-economic model reflecting the process of finding the best method of cleaning with minimum costs:



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$$F(x) = \sum_{k=1}^{L} \sum_{i=1}^{N} A_{ki} x_{ki}^{\lambda_{ki}} \to \min$$
(1)

$$\sum_{i=1}^{N} B_{kij} x_{ki} \le C_{kj}, \quad k = \overline{1, L}; \ j = \overline{1, M},$$
(2)

$$\sum_{i=1}^{N} x_{ki} = q_k, \ k = \overline{1, L}; \tag{3}$$

$$x_{ki}^{-} \le x_{ki} \le x_{ki}^{+} \quad , k = \overline{1, L}; \ j = \overline{1, M},$$

$$(4)$$

$$A_{ki} \ge 0, \quad 0 \le \lambda_{ki} \le 1, \quad k = 1, L, i = 1, N$$

Let us dwell on the economic content of the model (1) - (4). The objective function (1) reflects the total cost of the water user to carry out water treatment measures. It will be appreciated that the dependencies reflecting the relationship of cleaning implementation costs to the loading volume of cleaning technologies are concave functions. Minimizing the objective function even on the convex region presents increased complexity.

Constraints (2) to (4) specify the best solution search area. Limitation (2) means that in the control solution the concentration of j- of this type of impurity should not exceed the permissible one. The "clean ability" factor indicated is calculated as follows:

$$B_{kij} = C_{0kj} (1 - P_{kij})$$
(5)

Limitation (3) requires that the weight and volume of that discharge on that spillway be distributed to process diagrams. Limitation (4) means that the amount of contaminated water directed for treatment shall not exceed the production capacity of the process diagrams.

To solve this problem (1) - (4) we apply the algorithm proposed in operation [7]. Build the Lagrange function

$$L(x,u) = \sum_{k=1}^{L} \sum_{i=1}^{N} A_{ki} x_{ki}^{\lambda_{ki}} - \sum_{k=1}^{L} \sum_{i=1}^{N} (\sum_{j=1}^{M} u_{kj} B_{kij} - u_k, x_{ki}) + \sum_{k=1}^{L} \sum_{j=1}^{M} u_{kj} C_{kj} + \sum_{k=1}^{L} u_k q_k \quad (6)$$

If we know u * - the optimal solution of the dual problem to the problem (1) - (4), then we can consider its equivalent setting:

$$L(x, u^*) \to \min$$
 (7)

 $x \in X$ where X is a set of vectors satisfying conditions (2), (4).

From task (7) we obtain, taking into account (6), k-independent subtasks for each catchment

$$\sum_{k=1}^{L} \sum_{i=1}^{N} A_{ki} x_{ki}^{\lambda_{ki}} - \sum_{k=1}^{L} \sum_{i=1}^{N} \left(\sum_{j=1}^{M} u_{kj}^{*} B_{kij} - u_{k}^{*}, x_{ki} \right) \to \min$$

$$x \in X$$
(8)

IV. DEVELOPMENT AND IMPLEMENTATION OF DEVELOPED ALGORITHMS.

Now we are moving to our goal of directly designing the OCHISTKA_D software complex. Adding the letter D to the project name indicates that the visual object-oriented programming environment Delphi [12-16] is used as a tool.



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Fig. 1. Project Main Window Shape

E M	ain.pas						
Main	Ochistka OUTPUT PROLOG CALCUL CONTROL DataWindow DECLAR 🛛 🗧 🚽	\Rightarrow .					
	var Frmain: TFrmain;						
	implementation						
	CONTROL, PROLOG, OUTPUT, DataWindow, DECL&R (\$R *.dfm)						
	<pre>procedure TFrmain.Run1Click(Sender: TObject); hegin</pre>						
	Contrl; // Управление реализацией алгоритма вычислений end;						
	<pre>procedure TFrmain.ToolButton4Click(Sender: TObject); hegin</pre>						
	Contrl; // Управление реализацией алгоритма вычислений end;	-					
<u> </u>							

Fig. 2. Event Handler for Run Manage keyboard input

To organize the input of the source data, we create a special window, for which we add a new form to the project. In the upper part, we place an inscription explaining for which task the source data is entered. Below are four or five input groups, each of which provides a field for entering the value of this, and an explanatory signature on the purpose of the input of this with the indication of its dimension. The composition of each of the groups of input data is determined by the task or class of tasks for which the developed set of programs is intended. For example, for a linear optimization cleanup task, the input input window can be as shown in Figure 3.

сходные ,	данные				- -			
TabSheet1	TabShe	et2 TabSheet3	-					
ВВод исходных данных задачи								
L=2 • N= 4 • M= 6 •								
Коэффици	иенты зад	ачи Aki, lamki						
	i=1	i=2	i=3	i=4				
Aki,k=1	0	2723.76	3358.37	5037.55				
k=2	0	1750	2585.95	0				
lamki,k=1	1	1	1	1				
k=2	1	1	1	1				
- GroupBox - Методы р • Метод С Метод С Метод	5- решения з 1 решения 1 решения	адач очистки плинейной зада нелинейной за	чи дачи й зарачи	Параметры Число итер Точность в	итерация Эацияй 10 ынаколений 0.1			
			Ввод	Закрыть	Help			

Fig. 3.Window for input of source data against the background of the main window of the program Read source data from the file on disk.



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Implementation of the program complex of contaminated water treatment.

The city of Nukus is the capital of the Republic of Karakalpakstan, located on the right bank of the Amu Darya River within its name terrace. At the moment, the city is landscaped with mainly developed industry. The population of the city in 1.01.2007 is 263.034 thousand people. The main water artery that feeds irrigation systems and lakes is the Amu Darya River.

One of the largest in the adjacent territory to Nukus is the Kyzketken Canal, the waters of which are the source of water supply for the city. The total length of the channel is 25km; it originates 9 km south of the city of Nukus on the right bank of the river. Amu Darya. The existing water supply to the city of Nukus is carried out due to the surface waters of the canal and the water conduit from the Tuyamuyunsky reservoir. The water intake site has the following facilities:

- Onshore pumping station on the Kyzketken channel.
- Earthen horizontal sumps.
- 1st lift pump station.
- Clean water tank, tank. 10000 mZ -2 pcs.
- 2nd lift pump station.

Installed production capacity of water intake facility 65kmZ/day. Currently, work is underway on contract 30 "Reconstruction of the Nukus BOS" in accordance with program 5.1 "Uzbekistan clean water sanitation and health." The contract provides for:

- Repair of mechanical and electrical equipment at Onshore pumping station.
- New flow separation and mixing chamber.
- Repair of existing settling ponds.
- New flapping chambers.
- New clean water tank.
- Repair of mechanical and electrical equipment at the first lift pump station.
- New filter building.
- New administrative and control building.
- New reagent building.
- Repair of existing laboratory building with replacement of equipment.
- Repair of mechanical and electrical equipment at the second lift pump station.
- New cameras, tsumpipes.

After completion of reconstruction works, the production capacity of the facility will be 86 thousand mZ/day. To increase the productivity of the water intake facility, additional funds are expected to be allocated from the Iranian loan. In addition, work on the construction of an additional filter unit, settling tanks for pre-deposition of suspension is provided, installation of pumps to remove sludge from these settling tanks into the channel, According to the control data of the Kyzketken channel, the self-washing channel with the maximum channel capacity, the volume of discharge of deposited substances will be 0,758kg/second or 0.28% of the total volume, with an average throughput of 0,281 kg/second or 0.66%, with a minimum pass of 0.06kg/second or 2.5% (calculation of reset volume attached).



Fig. 4.Process diagram of Nukus treatment plant.



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Here the PK-receiving chamber, OP - pond sump, PP - starter pond, PK - cultivator pond, PB - biocogulator pond, PP - channel pond, VBR - pond with higher aquatic vegetation.

To improve reliability of compliance with KMK requirement 2.04.02-97, it is also envisaged to divide all earthen capacitance structures into two parallel operating sections, each of which is designed to pass 50% of the design flow in normal operation mode and 100% in forced operation.

Lean liquid clarified during 5 days is divided into two streams in accordance with 30% or 70%.

A smaller flow is passed through the cultivator pond for 6 days for the development of algal biomass and the accumulation of the sum of oxidants, after which it is mixed with the main flow. To accelerate cultivation, 10% of the flow is supplied to the cultivator - starter pond, from which it enters the cultivator after 4.5 days.

The resulting mixture continuously enters the biocogulator pond, where during 2 days a complex biocogulation process occurs, as a result of which the content of suspended and dissolved contaminants is reduced.

Next to the pond biocogulator treatment stage is aerobic treatment stage under flow conditions in the pond insolator, the main process of which is bacterial oxidation of dissolved organic and mineral components of waste water.

In the flowing pond, the waste liquid is located for 2 days, the MIC is brought up to 15 mg/liter. After biological treatment, water enters post-treatment ponds with the highest water vegetation, where the quality of the treated effluents is brought to the requirements that meet the rules of the Protection of Surface Waters from Pollution by Waste Water.

Approved PDS and waste water composition (discharge of substances not specified below is prohibited) according to the table.

		Table 1.			
	Indicators.	Reset conditions.			
		mg/liter	PDS g/hour.		
1	Suspended matter	140.0	53040,4		
2	BOD ₅	5,0	1894.3		
3	Mineral composition	2000.0	757720.0		
4	Chlorides	350,0	132601.0		
5	Sulphates.	500,0	189430.0		
6	Fats	5.5	2083.73		
7	Nitrate nitrogen	-	-		
8	Nitride Nitride	-	-		
9	Ammonium nitrogen	-	-		

Tables 2., 3. show the technical and economic characteristics of the wastewater treatment plant in the city of Nukus: throughput capacity, actual, permissible and even after the concentration of pollutants, as well as costs, codes of measures for wastewater treatment.

								Table 2
			Cle	aning efficiency				
No.	Name och and stny and	The capacity of the			Allo with	The concentration of (F to cal)		
	structures m e Tod	joint ventur	e on lities		tim to n			
	purification	cubic mete	rs / day		Tacility			
		Projections	Fact and	Ingredient	g/m -	ln %	Post at	Dischargeo
		so naya	Th with kaya				drank g/m ³	e but g/m
1	2	3	4	5	6	7	8	9
1	Station biological	65000.0	9092.6	Weighted Mr.	140.0	53.22	193.7	103.1
	treatment hozbyt			nye vesch e -				
	about O drains			OPERATION				
				BOD ₅	5,0	52.63	7.6	4.0
				Mineral s ny composition	2000.0	88.62	2769,0	2454.0
				Chlorides	350,0	79.91	712.5	569.4
				Sulphates.	500,0	70.32	404.4	284.4
				Fats	5.5	-	1	1
				Nitrogen Nitra t	20	52.23	47.1	24.6
				ny				
				Nitrogen nitrification d ny	0.02	52,5	0.08	0,042
				Nitrogen atm of Nij	0.1	52.75	0.91	0.48



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Water protection measures in accordance with formulas (2.2.1) - (2.2.4) are described as follows:

 $f_{1} = 9,67 \cdot 365 \cdot (x_{10} + 602.9 \cdot x_{11} + 741.5 \cdot x_{12} + 1083.6 \cdot x_{13}) = 3530 \cdot x_{10} + 2128237 \cdot x_{11} + 2617495 \cdot x_{12} + 3825108 \cdot x_{13};$

 $C_{12} = 7,6 \cdot x_{10} + 4 \cdot x_{11} + 1,4 \cdot x_{12} + 0,8 \cdot x_{13};$

.....

 $x_{11} + x_{12} + x_{13} + x_{10} = 1;$

The results of solving the problem of calculating the PDS formed substances and wholesale and mal in doohrannyh measures for their achievement, obtained with the help of "software package OCHISTKA », pref e listed in Table. 4 ..

Table 4.

Optimal water conservation measures to achieve MPP							
	Cipher measures about priyament	Wastewate	These of				
Reset		thousand m ³ /day	IN %	x _{1i} - dec	a waste, thous. UZS. / Year		
	No cleaning	0.7523	7.78	0,0778	274		
1	101	-	-	-			
1	202	8.9177	92.22	0.9222	2413792		
	206						
Total			one hundred	1.00	2414016		

The resulting solutions, it follows that to achieve acceptable performance concentration of a polluting substances necessary to clean mainly flow sheet 202, as when cleaning with y exists the template 101 some valid data are not achieved, for example m ineralnomu composition, chlorides and nitrogen. Comparing the cost of various purification tehn of logical e Skim integrated circuits and purification are shown in Table 4.

Table 5

÷	Comparison of the costs of cleaning different options						
	No.	Ingredients g/m ³	Without och and	CLEAR	Purification	Purification	Compl
			stock	DIR t ka	by cx e IU	by cx e IU	treatment for
				scheme 101	202	206	perm to n
							Center
	1.	Suspended vesch e -	193.7	103.1	34,4	20.6	140.0
		OPERATION					
[2.	BOD5	7.6	4.0	1.4	0.8	5,0
ſ	3.	Mineral with about	2769.0	2454	1454	1172	2000.0
		becoming					
Ī	4.	Chlorides	712.5	569.4	319.4	274.4	350,0
ſ	5.	Sulphates.	404.4	284.4	284.4	284.4	500,0
[6.	Fats	1	1	1	1	5.5
Ī	7.	Nitrogen Nitra t ny	47.1	24.6	4.4	2,4	20
Ī	8.	Nitrogen	0.08	0,042	0.02	0.02	0.04
		nitrification d ny					
t	9.	Ammonium	0.91	0.48	0.12	0.04	0.4
		nitrogen					
Ī	10.	Costs, thousand s	0	5830,0	7170.3	10478.4	6613.7
		for mov per day					

V. CONCLUSION

The protection of the environment and the rational use of natural resources are now of the utmost importance. In the interests of present and future generations, measures are being taken to protect and scientifically sound, rational use of land and its subsoil, water resources, plant and animal world, to preserve clean air and water, ensure the reproduction of wealth and improve the environment.



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In the age of technological progress, water is an important raw material on which the development of productive forces depends. Water consumption for industrial, agricultural and household needs increases annually. Intense water pollution poses a serious danger. Waste from industrial enterprises, falling into reservoirs, make them unsuitable for technological and household needs.

In modern conditions, special attention is paid to various ways of intensifying wastewater treatment processes, improving existing treatment technologies, as well as introducing new methods and technological methods that can improve the quality of wastewater treatment and reduce the anthropogenic impact on the ecosystem. For this purpose, it is advisable to use resource-efficient wastewater treatment technologies that save material and natural resources.

When forming the task of optimizing water protection measures, it is essential to choose a model of a set of water protection measures that establishes the dependence between the amount of funds allocated to the water user for treatment and the quality composition of contaminated waters before discharging into the water body.

Given this, an important task is to optimize the work of contaminated water treatment complexes using environmentaleconomic modeling and computer technology methods.

The key results of this work are as follows:

• Theoretical studies have been carried out to study and refine options for the environmental-economic model of treatment of contaminated waters;

• Research was carried out on the development of algorithms for solving multi-extreme problems.

• Algorithm for solution of stochastic environmental-economic model of contaminated water treatment built and investigated;

• Study of stability on the right side of the deterministic environmental-economic model of contaminated water treatment;

• Studies were carried out on theoretical issues of creating software tools for calculations on the environmentaleconomic model of treatment of contaminated waters.

• A software package was developed for calculations on the environmental-economic model of treatment of contaminated waters.

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