TOWARDS MODELS COMPLEXITY IN WATER USAGE AND TREATMENT OPTIMISATION PROBLEMS

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The paper addresses water recycling in process industry, inter alia, the issues of mathematical models’ complexity problem in the “process integration”-based structural optimization of sustainable water usage and treatment networks. The nature of addressing structural optimization problems requires iteratively querying individual process models, which are incorporated as objective functions and constraints within the optimization model, throughout the process of finding a solution, therefore the goal was to explore the intricacy of mentioned models. Within the framework of the research, the impact of complexity of water network constituent parts models on the optimization performance was investigated by Monte Carlo method for one step of the optimization procedure, as well as for the optimization procedure as a whole. Units’ models in form of algebraic equations (for direct equation calculation case), algebraic equations (for root search), ordinary differential equations (for Cauchy initial value problem with a case of two differential equations), ordinary differential equations (for boundary value problem), and partial differential equations (for two spatial variables) were examined with an analysis of their applicability for optimization purposes. The justification for employing both deterministic "counter-current mass transfer" models and statistical polynomial "input-output" steady-state algebraic models were established for addressing the specific problems under investigation. As the case study, special polynomial model was constructed based on the experimental design / response surface methodology and the dynamics simulation results on adsorption wastewater treatment within the packed bed column filled with activated carbon. Central composite rotatable design was formulated and subsequently executed using computational experimentation methods for the parametric identification of a nonlinear polynomial model. The evaluation confirmed that the constructed model exhibits satisfactory predictive accuracy.

Key words: *adsorption, model, optimization, process integration, simulation, superstructure, water usage and treatment network*

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1. Introduction

The practice of water recycling and resource recovery in process industry, in particular, the issues of designing industrial plants in chemical engineering and other fields focuses on creating efficient systems that offer cost benefits. The designed technologies aim to achieve maximum output, minimize environmental impact, reduce resource consumption (including nonrenewable resources), minimize waste production, and provide a safe working environment. The fundamental concept known as “process integration” in water usage and treatment context (Wang & Smith, 1994) serves as a guiding principle to ensure the desired level of energy and resource

efficiency in project facilities. Process integration entails viewing the projected chemical-engineering system as a cohesive entity, taking into account the interplay of processes, devices, and the flow of mass and energy within the system. The process integration opposes the approach of independently optimizing the design of individual components of the chemical-engineering system. Process integration enables the utilization of “internal reserves” within the technology, such as utilizing excess heat from reaction products to heat the reagents.

As the concept of sustainable development continues to gain traction, the focus and priorities of designing industrial facilities have undergone a shift. The notion of “designing chemical-engineering systems based on the principles of sustainable development” or “sustainable design” now encompasses a set of project activities aimed at achieving economic growth, environmental preservation, and social advancement for the present generation, while also safeguarding the potential for future generations (El-Halwagi, 2017).

Within the framework of process integration, resource conservation measures, such as reducing freshwater consumption, are implemented by redirecting “partially contaminated” water from the output of one technological unit to the input of another, with the option of diluting it with freshwater. The current trend in optimizing water networks, based on the principles of process integration, involves static structural optimization. Such an approach focuses on finding the optimal redistribution of water flows to maximize water utilization under stationary conditions. Once the maximum potential for direct reuse has been exhausted, the "partially contaminated water" stream can undergo partial treatment, enabling its further reuse (Takama et al., 1980). Changes in productivity and operating modes within chemical technology networks, influenced by external factors or periodic production shutdowns for maintenance, can result in variations in mass flow rates and the composition of wastewater entering the treatment system. To ensure the efficient operation of wastewater treatment networks amidst changing loads, it is advisable to conduct structural optimization of water usage and treatment networks whenever significant load changes occur (Shakhnovsky & Kvitka, 2019). This enables the adaptation of the treatment process structure and mode to the altered external conditions.

In order to formulate the optimal structural objective for water usage and treatment networks, it is necessary to consider certain assumptions (Poplewski & Foo, 2020). These assumptions take into account that the water usage and treatment networks have already undergone both “organizational” and “parametric” optimization, ensuring that all processes within the network are optimized in terms of water consumption. “Organizational” optimization involves activities such as regular accounting and reporting of water usage and treatment network balances, providing incentives to individual staff members for practicing water conservation and addressing and eliminating unplanned water leaks. Furthermore, "parametric" optimization focuses on making resource-saving technological changes, such as replacing water-consuming devices with more efficient alternatives (for instance, replacing water cooling systems with air cooling systems). All the changes described above are intended to optimize the water usage and

treatment network by adopting more efficient technologies.

Numerous mathematical programming methods have been devised to optimize the structure of water networks. In particular, Takama et al. (1980) were the first to suggest a continuous nonlinear programming problem (NLP) for industrial water networks by creating a "generalized network" (also known as a superstructure), encompassing water treatment and usage components. Subsequently, several improvements were proposed for the superstructure approach to address situations involving water partial treatment and water loss (Huang et al., 1999), the recycling of water around specific usage units (Shakhnovskij et al., 2004), and also other factors. A series of publications by Bagajewicz et.al. (in particular, Savelski & Bagajewicz, 2003, etc.) presented mathematical optimization models based on essential conditions of optima, effectively addressing the challenges associated with reuse and recycling in water networks dealing with multiple contaminants. Wałczyk et. al (2007) explored the structural optimization of water networks with heat exchange. Deng et al. (2018) developed specialized flexible superstructural optimization routines that considered different water sources, including utility water and water used within the system. Fan et al. (2019) explored a subnetwork for water reuse and treatment, focusing on incorporating viable recycling streams. Yang et al. (2020) proposed an iterative technique for designing water networks that involved multiple partial treatment units.

All of the above-reported studies are based on unit models (of water users, water treatment processes, and flow redistributors) as constituent parts of the superstructure optimization problem. Hence, it is pertinent to explore the intricacy of mentioned models, which constitutes the main focus of this article.

2. Modeling of individual processes in water usage and treatment networks

Computer modeling of natural water and wastewater treatment processes involves the use of mathematical models and computational methods to simulate and analyze the behavior of these processes. Computer models aim to represent the physical, chemical, and biological processes that occur in natural water and wastewater treatment systems. Models use mathematical equations and algorithms to describe the behavior and interactions of processes under study, including mass and energy balances, transport phenomena, kinetics, and also to system performance evaluation, sensitivity and uncertainty analysis, design of the processes, real-time control circuits synthesis, etc.

In particular, the system of ordinary differential equations with initial conditions can be used for a simplified description of the biocenosis in bioreactors during the treatment of highly concentrated wastewater (Kyrychenko & Sabliy, 2023), as well as for modeling the process of gravity settling with coalescence (García & Betancourt, 2019). Systems of ordinary differential equations (or combined sets of algebraic and differential equations) are commonly used for modeling of anaerobic reactors treating wastewater (Batstone, 2006).

The boundary value problem for ordinary differential equations describes the stationary process of water purification in a

heterophase bioreactor with a fibrous carrier (Vlasyuk et al., 2022). Also, a system of differential and algebraic equations (which provides the hydrodynamic and kinetic description of concentration changes in the form of a boundary value problem of an ordinary differential equation, as well as an algebraic description of the adsorption isotherm and material balance of the process) helped describe the process of treating wastewater by removing organic impurities using a fluidized bed of adsorbent (Boyko 1993). The boundary value problem (namely, a mixed system of partial differential equations and ordinary differential equations) provided a detailed depiction of the activated sludge treatment process (Diehl & Farås, 2013). The partial differential equations model represented an adsorber with a fixed adsorbent bed (Givlyud et al., 2022), and also an emergency treatment of water by industrial-scale fluidized bed adsorption (Zheng et al., 2016).

The combination of the system of partial differential equations with the system of algebraic equations of equilibrium and equimolarity of the system was used as a model of ion exchange in the wastewater treatment system (Boyko, 1993, Ochando-Pulido et al. 2020).

The authors of the presented publications testify that the mathematical models used by them describe the processes under study with sufficient accuracy.

However, the nature of solving structural optimization problems necessitates making multiple queries to the individual process models, represented as objective functions and constraints within the optimization model, throughout the solution-finding process.

The computational capability required for handling these multiple requests varies considerably depending on the type of models used to represent the units of the water network within the optimization model, that is, whether models in the form of algebraic equations are used in the objective function and constraints, or models of other types (in particular, differential equations of various types, neural networks, etc.).

3. Exploring the impact of the complexity of water network constituent parts models on the optimization performance

Computational experiments were carried out to study the influence of the degree of complexity of individual process models on the performance of the water usage networks and treatment structural optimization procedure.

Due to the considerable variability observed in the performance parameters under study, the statistical Monte Carlo method (Ortega & Rovira, 2020) was applied to simulate and assess actual relationships in the evaluation process.

The performance of the optimization procedure was evaluated using the normalized values of the number of calculations, which were compared to the number of substitutions in the algebraic function.

3.1. Evaluating the computational resource demands per one step of the optimization routine

Figure 1 graphically represents the simulated estimation of computational resource requirements for each step of the optimization routine, considering mathematical models of different types.

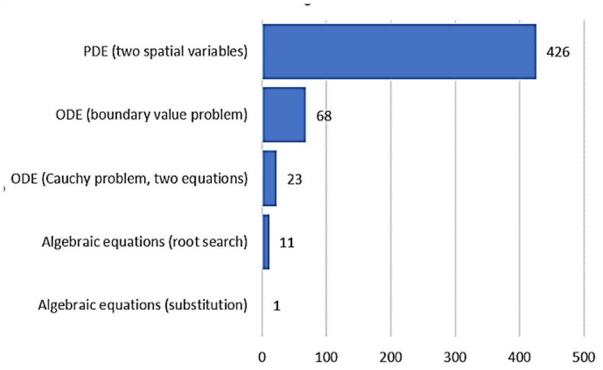

Fig. 1. *Average number of calculations per one step of the optimization routine*

Fig. 1. shows the average number of calculations for different types of models, including algebraic equations (direct equation calculation case, taken as a unit), algebraic equations (for root search), ordinary differential equations (for Cauchy problem, a simple case of two equations), ordinary differential equations (for boundary value problem), and partial differential equations (for two spatial variables).

The simulation results (Fig. 1) reveal that the number of calculations significantly increases for different types of models. Specifically, when using models represented as algebraic equations (root search), ordinary differential equations (Cauchy problem, two equations), and ordinary differential equations (boundary value problem), the number of calculations increases by one order of magnitude. Moreover, for models represented as partial differential equations (two spatial variables), the number of calculations increases by two orders of magnitude.

3.2. Assessing the overall computational resource requirements for the optimization routine procedure

The estimation of computational resource requirements for the optimization routine as a whole is conducted through simulations using the outcomes from a previous series of computational experiments (i.e., from the computational resource demands per one step of the optimization routine).

In Table 1, the average number of calculations is presented for various types of mathematical models, including algebraic equations (direct model calculation), algebraic equations (equation's root search), ordinary differential equations (Cauchy problem and boundary value problem), and partial differential equations (two spatial variables).

The value N was taken (Jung et. al., 2019) as the lower limit of the number of optimization procedure steps when solving a continuous non-linear programming problem (Takama et al., 1980) with “step-by-step” optimization routine:

$$N \cong 50 \cdot n^2, \qquad (1)$$

where n is the dimension of the optimization problem.

Figure 2 displays the detailed graphical representation of the normalized average number of calculations for mathematical models of various types (estimated for optimization routine as a whole).

The computational experiments (Table 1 and Fig. 2) reveal a notable increase in the required number of calculations as the level of detail in the model increases.

The field of structural optimization of networks often involves optimization models that surpass the complexity of continuous NLP and optimization routines that go beyond simple "step-by-step" methods (in particular, such “complex” cases include mixed-integer nonlinear optimization problems as well as global optimization procedures – see e.g., Poplewski & Foo, 2020).

Consequently, there is a demand to simplify (within reasonable limits) mathematical models in order to tackle these challenges effectively.

4. Investigation of the units' models complexity for optimization purposes

In the majority of superstructural approaches, water-using operations are typically represented as straightforward counter-current mass transfer processes, known as "fixed load" operations. In fixed load operations, the mass loads of contaminants and the maximum allowable concentrations at the process inlet and outlet are predetermined and provided in the data. The flowrate of the water stream, as well as the concentrations of contaminants at both the inlet and outlet, are treated as variables.

However, certain water-using operations, such as boiler blowdown or chemical reactions involving water as a reactant or product, cannot be accurately modeled solely as mass-transfer processes. In the context of water networks' structure optimization, water treatment processes are typically categorized into two groups (Huang et al., 1999).

The first group consists of processes such as extraction and water thermal treatment, which exhibit a fixed concentration $C_{C,out}^{trt}$ at the outlet. This concentration corresponds to a specific equilibrium value $C_{C,out}^{*}$:

$$C_{C,out}^{trt} = C_{C,out}^{*}, \quad c = \overline{1; Nc}, \qquad (2)$$

where Nc is the number of contaminants.

In the case of the second group of treatment processes, such as mechanical and biological treatment, the concentration at the outlet remains independent (within a specified range of mass flow values) of the water's mass flow.

Table 1. *The average number of calculations required to the optimization procedure as a whole*

	Models' type				
	Algebraic equations (substitution)	**Algebraic equations (root search)**	**ODE (Cauchy problem, two equations)**	**ODE (boundary value problem)**	**PDE (two spatial variables)**
Number of calcs. per step / **Number of units in water usage and treatment network**	**1**	**11**	**23**	**68**	**436**
5	1.00E+04	1.21E+06	5.29E+06	4.62E+07	1.90E+09
10	4.00E+04	4.84E+06	2.12E+07	1.85E+08	7.60E+09
20	1.60E+05	1.94E+07	8.46E+07	7.40E+08	3.04E+10
30	3.60E+05	4.36E+07	1.90E+08	1.66E+09	6.84E+10
50	1.00E+06	1.21E+08	5.29E+08	4.62E+09	1.90E+11
60	1.44E+06	1.74E+08	7.62E+08	6.66E+09	2.74E+11
70	1.96E+06	2.37E+08	1.04E+09	9.06E+09	3.73E+11

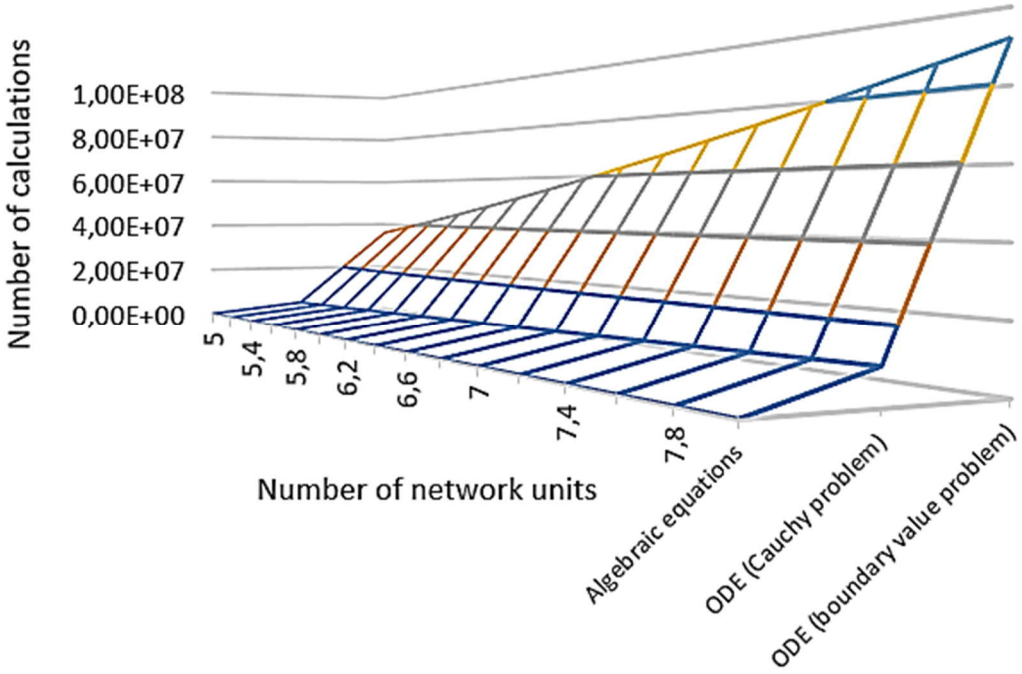

Fig. 2. *Average number of calculations for water network's structure optimization*

However, the concentration at the outlet is determined by two factors: 1) the input concentration $C_{C,in}$ and 2) the known removal ratio r_c for the given contaminant:

$$C_{C,out}^{trt} = C_{C,in} \cdot (1 - r_c), \quad c = \overline{1; Nc}, \quad (3)$$

where Nc is the number of contaminants.

In the majority of cases, models (2) and (3) are suitable for their intended purpose in optimizing the structure of a static network.

Nevertheless, these models do not incorporate certain specific parameters of treatment processes, including water loss, variations in viscosity as the concentration level rises, etc.

As an alternative approach, polynomial experimental-statistical models can be proposed for modeling individual components of water usage and treatment networks. This method allows for the development of straightforward "black box" models that differ from (2) and (3) by considering multiple parameters instead of just one.

The process of constructing experimental-statistical models in this study involved the following stages:

1. Establishing the dimensionality of the factor space, selecting the model type, and designing an experimental design.

2. Executing the experimental design as outlined.

3. Identifying the parametric model and conducting an "analysis of variances" (ANOVA) to verify the model's validity.

The presented methodology is exemplified through the following case study, which aims to acquire a model for the steady-state approximation of the adsorption process within a water usage and treatment network.

Table 2 showcases the primary parameters associated with the adsorption process in a fixed bed for water treatment, including the type of adsorbent and the characteristics of the treated water. In order to derive the model, a central composite rotatable experimental plan was formulated

and executed, as depicted in Table 3. The values of the intervals of variation for the factors X_1,· X_2 are presented in Table 2.

Table 2. *Certain parameters of the process of adsorption water treatment*

Parameter	Value
Wastewater flowrate*, m^3/hr	70..100
Inlet concentration of contaminants*, $mg\ O_2/dm^3$	200..400
Longitudinal mixing coefficient in liquid, m^2/hr	1.5
Effective diffusion coefficient of contaminants, m^2/hr	0.000007
Bulk density of the adsorbent, kg/m^3	760
Porosity of the adsorption layer	0.4
Vessel diameter, m	2.0
Adsorption layer length, m	2.0

Note. *Variable parameters.

Wastewater flowrate (x_1) and inlet concentration of contaminants (x_2) were chosen as input variables for the model. The pollutant concentration at the outlet of the adsorption layer (y) was taken as the output variable for the model. The plan included nine experiments and also reference points to check the adequacy of the model.

The experimental values of y were obtained using the Ecology software package developed at the Department of cybernetics of chemical-technological processes of Igor Sikorsky Kyiv Polytechnic Institute.

Upon analyzing the experimental outcomes, a mathematical model (4) was derived, exhibiting a significant resemblance to linearity.

$$\hat{y} = 0.2121 + 0.0014 \cdot X_1 - 6.9 \cdot 10^{-6} \cdot X_1^2 - 5.3 \cdot 10^{-7} \cdot X_1^2 - 7.5 \cdot 10^{-7} \cdot X_1 \cdot X_2. \quad (4)$$

It should be noted that the mathematical model (4) is presented here in its natural (rather than coded) form.

After the standard ANOVA procedure, the model was tested on randomly taken points of the factor space (Table 4).

Table 3. *Data for mathematical model parametric identification*

Run No	X_1 – wastewater flowrate, m^3/hr	X_2 – inlet concentration of contaminants, $mg\ O_2/dm^3$	y – the concentration of contaminants at the outlet of the adsorbent layer (COD), $mg\ O_2/dm^3$
1	100	400	4.5933
2	70	400	4.6023
3	100	200	2.2966
4	70	200	2.3011
5	106.213	300	3.3048
6	63.787	300	3.5354
7	85	441.42	5.0527
8	85	158.58	1.8152
9	85	300	3.4339
R1*	77.5	400	4.733703
R2*	100	250	2.870805
R3*	92.5	250	2.760181

Note. *Reference points

Table 4. *Assessing the predictive performance of the mathematical model*

X_1 – wastewater flowrate, m^3/hr	**X_2 – inlet concentration of contaminants, mg O_2/dm^3**	**y – the experimental concentration value of contaminants at the outlet of the adsorbent layer (COD), mg O_2/dm^3**	**$\hat{y}$ – the calculated concentration value of contaminants at the outlet of the adsorbent layer (COD), mg O_2/dm^3**
71.5	390	4.62075	4.50837
73	380	4.41192	4.38859
82	320	3.58281	3.67199
88	280	3.25299	3.19621
89.5	270	3.15176	3.07751
95.5	230	2.52738	2.60368
97	220	2.56085	2.48547
71.5	390	4.62075	4.50837
73	380	4.41192	4.38859
82	320	3.58281	3.67199

As evident from the data presented in Table 4, the resulting model demonstrates satisfactory prediction accuracy: the average squared deviation between the calculated values and the original values did not exceed 1.20 %.

4. Conclusions

The addressed mathematical models' complexity problem for "process integration"-based structural optimization of sustainable water usage and treatment networks is of quite importance.

The use of complex adequate network units' models leads to a critical increase in computational needs and, as a result, to the impossibility of structural optimization of large systems. On the other hand, excessive simplification of models critically reduces the accuracy of optimization.

Under these circumstances, the use of deterministic "counter-current mass transfer" models as well as statistical polynomial "input-output" steady-state algebraic models may be desirable.

As the case study, a specialized polynomial model was developed for adsorption wastewater treatment within a packed bed column. The model was constructed using a combination of response surface experimental design methodology, and dynamics' simulation results. To identify the parameters of the nonlinear polynomial model, a central composite design was formulated and implemented through computational experimentation methods.

The model obtained exhibits favorable predictive accuracy, as evidenced by an average squared deviation between the calculated values and the original values that remained below 1.20 %.

Future research plans involve investigating the feasibility of utilizing big data models within the superstructural optimization routines.

References

1. Batstone, D. J. Mathematical modelling of anaerobic reactors treating domestic wastewater: rational criteria for model use. *Reviews in Environmental Science and Bio/Technology*, **2006**, *5* (1), 57–71. https://doi.org/10.1007/s11157-005-7191-z

2. Boyko, T. V. *Modeling of ion exchange systems of industrial wastewater treatment: dissertation abstract*. (Kyiv, **1993**). [In Ukrainian].

3. Deng, Ch.; Jiang, W.; Zhou, W.; Feng, X. New superstructure-based optimization of property-based industrial water system. *Journal of Cleaner Production*, **2018**, *189*, 878–886. https://doi.org/10.1016/j.jclepro.2018.03.314.

4. Diehl, S.; Farås, S. Control of an ideal activated sludge process in wastewater treatment via an ODE–PDE model. *Journal of Process Control*. **2013**, *23* (3), 359–381. https://doi.org/10.1016/j.jprocont.2012.12.011

5. El-Halwagi, M. *Sustainable Design Through Process Integration*: *2nd Edition*. (Amsterdam-Oxford-Cambridge: Elsevier. **2017**).

6. Fan, X.-Y.; Klemeš, J. J.; Jia, X.; Liu, Zh.-Y. An iterative method for design of total water networks with multiple contaminants. *Journal of Cleaner Production*, **2019**, *240***,** 118098. https://doi.org/10.1016/j.jclepro.2019.118098.

7. García, A.; Betancourt, F. Conservative mathematical model and numerical simulation of batch gravity settling with coalescence of liquid-liquid dispersions. *Chem. Enging. Sci.*, **2019**, *207*, 1214–1229. https://doi.org/10.1016/j.ces.2019.07.034

8. Givlyud, A. M.; Humnytskyi, Y. M.; Ruda, M. V. *Purification of wastewater from the dairy industry by the adsorption method: monograph*. («Mizhnarodna naukova hil′diya», **2022**). URL: https://liegudzyk.com/ochyshchennya-stichnykh-vod-molochnoyi-promyslovosti-metodom-adsorbtsiyi. [In Ukrainian].

9. Huang, C.; Chang, C.; Ling, H.; Chang, C. A mathematical programming model for water usage and treatment network design. *Ind Eng Chem Res.*, **1999**, *38* (7), 2666–2679. https://doi.org/10.1021/ie990043s

10. Jung, D.; Lee, S.; Hwang, H. Optimization difficulty indicator and testing framework for water distribution network complexity. *Water*, **2019**, *11* (10), 2132. https://doi.org/10.3390/w11102132

11. Kyrychenko, K. C.; Sabliy, L. A. Calculation of optimum parameters of biological wastewater treatment based on the GPS-X program. *17th International Scientific and Practical Conference "Biotechnology of the 21st Century"*, **2023**, 228–230. [In Ukrainian].

12. Ochando-Pulido, J. M.; Vellido-Pérez, J. A.; González-Hernández, R.; Martínez-Férez, A. Optimization and modeling of two-phase olive-oil washing wastewater integral treatment and phenolic compounds recovery by novel weak-base ion exchange resins. *Separation and Purification Technology*, **2020**, 117084. https://doi.org/10.1016/j.seppur.2020.117084

13. Ortega, G.; Rovira, A. A fast and accurate methodology for the calculation of the shading and blocking efficiency in central receiver systems. *Renewable Energy*. **2020**, *154*, 58–70. https://doi.org/10.1016/j.renene.2020.03.005

14. Poplewski, G.; Foo, D. C. Y. An extended corner point method for the synthesis of flexible water network. *Process Safety and Environmental Protection*, **2020**, *148* (2), 210–224. https://doi.org/10.1016/j.psep.2020.09.050

15. Savelski, M. J.; Bagajewicz, M. J. On the necessary conditions of optimality of water utilization systems in process plants with multiple contaminants. *Chem Eng Sci*., **2003**, *23–24*, 5349–5362. https://doi.org/10.1016/j.ces.2003.09.004.

16. Shakhnovskij, A.; Jeżowski, J.; Kvitka, A. et al. Optymalizacja sieci wody procesowej przy zastosowaniu programowania matematycznego. *Inżynieria Chemiczna i Procesowa*, **2004**, *25* (3), 1607-1612.

17. Shakhnovsky, A.; Kvitka, O. Design of sustainable industrial water networks: 1. Genesis of the systematic methods. *Water and water purification technologies. Scientific and technical news*, **2019**, *24* (1), 34–44. https://doi.org/10.20535/2218-93002412019172907.

18. Takama, N.; Kiriyama, T.; Shiroko, K.; Umeda, T. Optimal water allocation in a petroleum refinery. *Computers & Chemical Engineering*, **1980**, *4* (4), 251–258. https://doi.org/10.1016/0098-1354(80)85005-8

19. Vlasyuk, A. P.; Zhukovsky, V. V.; Zhukovska, N. A. *Mathematical and computer modeling of mass transfer during filtration of salt solutions in porous and nanoporous media: monograph* (Rivne: NUVHP. **2022**). [In Ukrainian].

20. Wałczyk, K.; Poplewski, G.; Jeżowski, J. et. al. Optimization of water network with models of non-

mass transfer processes. *Chem. Proc. Enging.,* **2007**, *28*, 515–525.

21. Wang, Y.-P.; Smith, R. Wastewater Minimization. *Chem. Eng. Sci.*, **1994**, *49* (7), 981–1006. https://doi.org/10.1016/0009-2509(94)80006-5.

22. Yang, F.; Fan, X.-Y.; Jia, X.; Klemeš, J. J., Liu, Zh.-Y. An iterative design approach for water networks with multiple regeneration units. *Journal of Cleaner Production*, **2020**, *271***,** 122483. https://doi.org/10.1016/j.jclepro.2020.122483.

23. Zheng, T.; Du, Z.; Cao, H.; Jiang, J. et. al. Development of a novel mobile industrial-scale fluidized adsorption process for emergency treatment of water polluted by aniline: CFD simulation and experiments. *Advanced Powder Technology*, **2016**, *27* (4), 1576–1587.
https://doi.org/10.1016/j.apt.2016.05.021

ДЕТАЛЬНІСТЬ МАТЕМАТИЧНИХ МОДЕЛЕЙ У ЗАДАЧАХ ОПТИМІЗАЦІЇ СХЕМ ВОДОСПОЖИВАННЯ ТА ВОДООЧИЩЕННЯ

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Стаття присвячена дослідженню проблем складності математичних моделей для потреб структурної оптимізації схем сталого водоспоживання та водоочищення на засадах «інтеграції процесів». Природа вирішення проблем структурної оптимізації вимагає багаторазового розрахунку окремих моделей процесів у складі цільові функції та обмежень задачі оптимізації протягом усього процесу пошуку рішення, тому метою було дослідити складність згаданих моделей. В рамках дослідження оцінено із використанням методу Монте-Карло вплив ступеню складності моделей складових частин схеми водоспоживання та водоочищення на ефективність оптимізації як для одного кроку процедури оптимізації, так і для процедури оптимізації в цілому. Були розглянуті та проаналізовані в контексті застосовності для цілей оптимізації математичні моделі у формі алгебраїчних рівнянь, звичайних диференціальних рівнянь (для задачі Коші у випадку двох диференціальних рівнянь та для крайової задачі), а також у вигляді диференціальних рівнянь в частинних похідних (для випадку двох незалежних просторових змінних інтегрування). Було обґрунтовано використання в математичній постановці задач структурної оптимізації схем водоспоживання та водоочищення математичних моделей спеціального вигляду: детермінованих моделей протиточного масообміну та експериментально-статистичних поліноміальних алгебраїчних моделей «вхід-вихід». В якості прикладу була побудована спеціальна поліноміальна модель процесу адсорбційного очищення стічних вод у нерухомому шарі адсорбенту на основі методології планування експерименту та результатів комп'ютерного моделювання динаміки процесу. Для параметричної ідентифікації нелінійної поліноміальної моделі був сформований та реалізований центральний композиційний рототабельний план активного експерименту. Стастична перевірка отриманої моделі показала, що побудована модель є адекватною та забезпечує достатню точність прогнозу.

Ключові слова: *адсорбція, інтеграція процесів, комп'ютерне моделювання, модель, оптимізація, схема водоспоживання та водоочищення*