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SOME ISSUES ON COMPUTER SIMULATION AND OPTIMIZATION OF SORPTION-BASED TREATMENT OF FLUORIDATED WATER

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Abstract

The problem of fluoride contamination in natural water sources has become increasingly relevant, particularly in rural areas and regions with naturally elevated fluoride levels in groundwater. The lack or military destruction of centralized water treatment infrastructure in many such areas exacerbates the health risks associated with excessive fluoride intake. These challenges highlight the need for affordable and locally adaptable solutions for decentralized water purification. The study focuses on the neural network (NN) simulation and optimization of sorption-based water treatment processes aimed at the removal of fluoride compounds using iron-containing sorbents derived from water treatment waste. For the NN approximation of the sorption capacity of the sorbent and fluoride ion removal efficiency as well as for the subsequent search for a compromise optimum (simultaneous multigoal maximization), a Python-based program was developed.

To address the multi-objective optimization problem, Harrington's desirability functions were applied. As the global optima search method, the "differential evolution" algorithm was selected. The calculated optimal point corresponds to the findings of the authors' previous studies on the influence of pH and sorbent dose on the sorption process.

Approaches presented are essential for the cost-effective adaptation of sorption technologies to local needs. The integration of statistical and AI-driven models facilitates the development of intelligent decision-support systems for water treatment, contributing to both scientific advancement and practical environmental protection.

The application of computational modeling forms a cornerstone of modern research on sorption technologies. It enhances scientific understanding, enables data-driven design, and promotes the scalable implementation of innovative, sustainable water purification solutions.

Keywords: *water treatment, defluorination, sorbents, computer modeling, neural networks, multigoal optimization, global optimum.*

In Ukraine, the problem of fluoride contamination in natural water sources has become increasingly relevant, particularly in rural areas and regions with naturally elevated fluoride levels in groundwater [1]. The lack of centralized water treatment infrastructure in many such areas exacerbates the health risks associated with excessive fluoride intake, including dental and skeletal fluorosis. These challenges highlight the need for affordable and locally adaptable solutions for decentralized water purification.

This study is devoted to the neural network approximation and optimization of sorption-based water treatment processes – primarily for natural water – aimed at the removal of fluoride compounds using iron-containing sorbents derived from water treatment waste.

Scientific research focused on the development of granulated iron-containing sorbents synthesized from industrial and agricultural waste materials is of critical importance in this context [2]. These materials offer dual environmental benefits: (1) effective adsorption of fluoride ions from contaminated water, and (2) valorization of local waste streams, such as metallurgical by-products or agricultural residues, which are abundant in many regions of Ukraine.

The use of granulated forms enhances operational feasibility in small-scale water treatment units, allowing for improved contact efficiency, ease of handling, and potential for regeneration. This is especially important for rural communities, where infrastructure investment is limited and simplicity of use is essential.

From an ecological perspective, presented research supports circular economy principles and aligns with Ukraine’s national priorities in environmental protection and sustainable development. It contributes to the reduction of hazardous pollutants, promotes waste reuse, and helps safeguard public health through low-cost, scalable water treatment technologies.

Continued investigation into such sorbents, including optimization of their physicochemical properties and production technology, as well as development of optimal technological regimes for the sorbents use, is essential for their effective implementation across fluoride-affected regions of Ukraine.

Modern environmental technologies require not only effective materials but also precise tools for modeling, prediction, and optimization of treatment processes. In the context of sorption-based water purification, including the removal of fluoride ions from natural waters, computer modeling plays a critical role in accelerating the design, evaluation, and scaling of treatment systems.

Experimentally-based statistical modeling approaches, such as response surface / design of experiments methodology, allow researchers to systematically investigate the influence of multiple process variables – such as sorbent dose, contact time, pH, and initial fluoride concentration – on sorption efficiency. These models enable the identification of optimal process conditions using a limited number of experiments, which is particularly valuable when working with novel sorbents derived from industrial or agricultural waste.

Beyond classical methods, the growing availability of computational power and data has made artificial intelligence (AI) and machine learning techniques, particularly artificial neural networks, highly effective tools for capturing the complex, nonlinear relationships governing sorption processes [3]. Neural network models offer the ability to generalize from experimental data, provide accurate predictions of sorption performance under variable conditions, and support multi-objective optimization strategies – such as maximizing fluoride removal while minimizing material consumption or environmental impact.

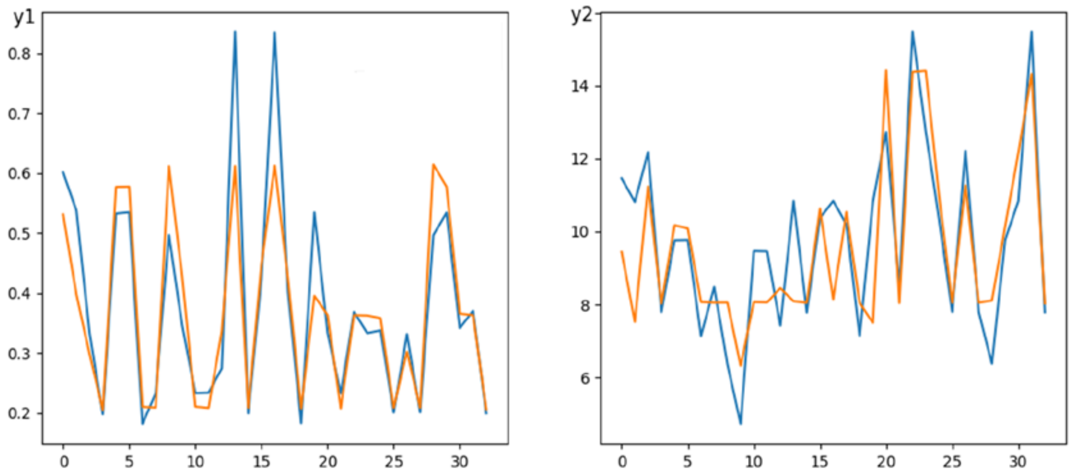
For the neural network approximation of the dependencies $y_1=f(x_1,x_2)$ – sorption capacity of the sorbent (mg/g), and $y_2=f(x_1,x_2)$ – fluoride ion removal efficiency (%), where x_1 is the sorbent dose (g), and x_2 is the pH of the medium, as well as for the subsequent search for a compromise optimum (simultaneous maximization of y_1 and y_2), a Python-based program was developed in the PyCharm environment. The components used in the implementation are described in Table 1.

Table 1. Tools used while creating the neural network modeling and optimization software

Tool	**Purpose**
pandas	Reading and processing tabular data (Excel)
scikit-learn	Scaling input data
numpy	Numerical operations
matplotlib / seaborn	Constructing graphs and visualizing results
tensorflow.keras	Building and training a neural network
scipy.optimize	Stochastic optimization (using the "differential evolution" method)

The program specifies the architecture of the neural network: two neurons for variables (x_1, x_2) in the input layer of the network, two neurons for variables (y_1, y_2) in the output layer of the network; the hidden layers (second and third) contain 16 and 32 neurons with a linear relay activation function (*relu*), respectively. Linear activation functions (linear) are used in the input and output layers.

The neural network model is trained on the provided output data using the Adam optimizer with the MSE (mean squared error) optimality criterion. The prediction accuracy of the model is quantitatively evaluated using the mean absolute error metrics. It is also possible to qualitatively assess the prediction accuracy of the neural network model by constructing graphs comparing the predicted and actual values (y_1, y_2) – Fig. 1.



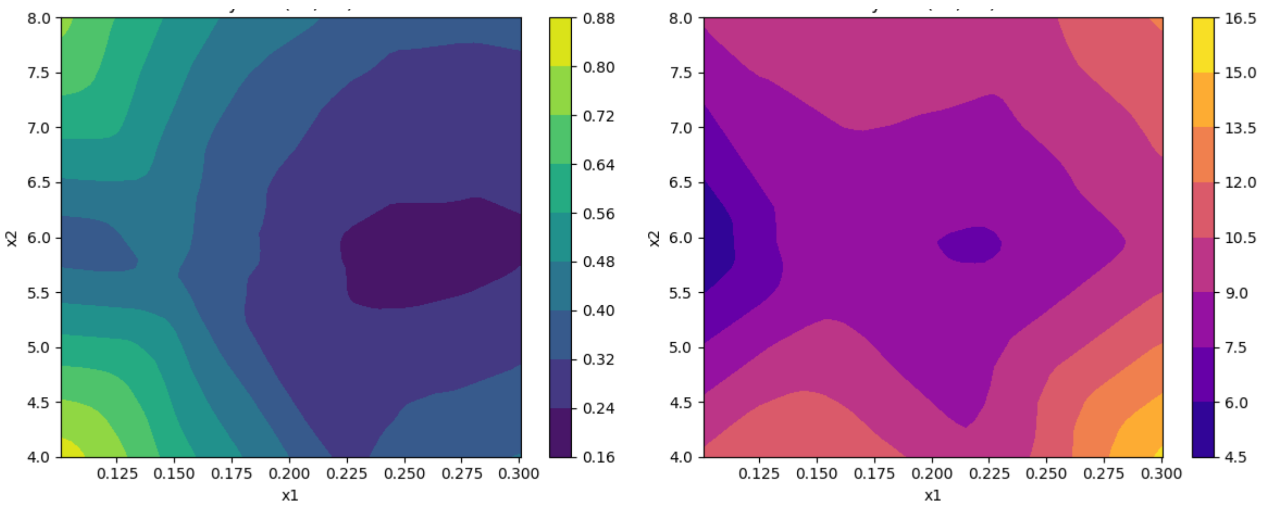
a) b)

Figure 1. *An assessment of prediction accuracy using a neural network model:*
– actual values, – predicted values; a –y_1 (sorption capacity of the sorbent) values,
b – y_2 (efficiency of fluoride ion removal) values

As a result, adequate neural network models were obtained for both investigated responses. A graphical representation of the neural network-modeled responses is presented in Figure 2.

The obtained neural network models of the sorption process were employed to support decision-making for process optimization. This task is quite complex, as it involves solving a multi-objective optimization problem [4], requiring the simultaneous consideration of two optimality criteria: the sorption capacity of the sorbent (*max* $y_1=f(x_1, x_2)$ and the fluoride ion removal efficiency (*max* $y_2=f(x_1,x_2)$).

To address the multi-objective optimization problem, Harrington's desirability functions were applied. The resulting aggregated (composite) desirability function, obtained by combining the individual desirability functions, reduces the problem to a single-objective optimization task. However, to reliably reach a global optimum of this criterion, it is necessary to apply specialized methods for solving multimodal optimization problems. As such a method, the stochastic "differential evolution" algorithm [5] available in the *optimize.differential_evolution* Python library (see Table 1) was selected.



a) b)

Figure 2. *Graphical representation of the neural network-modeled responses:*
a –y_1 (sorption capacity of the sorbent) values, b –y_2 (efficiency of fluoride ion removal) values

The calculated compromise optimal point corresponds to the values $x_1 = 0.303$ and $x_2 = 3.981$. The corresponding predicted response values (optimality criteria) are $y_1 = 0.37$ and $y_2 = 14.77$.

The reliability of the obtained results is confirmed by their correlation with the findings of the authors' previous studies on the influence of pH and sorbent dose on the sorption process.

In conclusion, it should be noted that in the Ukrainian context, where expected post-war reconstruction and regional variability in water composition present significant challenges, such modeling approaches are essential for the cost-effective adaptation of sorption technologies to local needs. The integration of AI-driven models facilitates the development of intelligent decision-support systems for water treatment, contributing to both scientific advancement and practical environmental protection.

Consequently, the application of computational modeling (especially when combined with experimental validation) forms a cornerstone of modern research on sorption technologies. It enhances scientific understanding, enables data-driven design, and promotes the scalable implementation of innovative, sustainable water purification solutions.

The presented study was conducted within the framework of the research projects "Pollutants removal of various nature from multi-component aqueous solutions by adsorption and flotation methods" (No. 0124U002058), "Industrial Wastewater Treatment Technologies Improvement Using of Artificial Neural Networks" (No. 0124U001966), "Technological principles of minimizing the content of chlorites in drinking water after disinfection with chlorine dioxide" (No. 0125U001784), and "Computer simulation and optimization of sustainable water management technological networks" (No. 0124U002127).

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ДЕЯКІ ПИТАННЯ КОМП'ЮТЕРНОГО МОДЕЛЮВАННЯ ТА ОПТИМІЗАЦІЇ ПРОЦЕСІВ СОРБЦІЙНОГО ОЧИЩЕННЯ ВОДИ ВІД СПОЛУК ФТОРУ

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Анотація: Дослідження присвячене актуальній проблемі забруднення води фтором. Відсутність (зокрема, внаслідок військових дій) в деяких районах централізованої інфраструктури очищення води посилює ризики для здоров'я, пов'язані з надмірним споживанням фтору, що вказує на необхідність доступних та локально адаптованих рішень для децентралізованого очищення води від сполук фтору. Представлено результати комп’ютерного моделювання із використанням нейронних мереж (НМ) та оптимізації сорбційних процесів очищення води задля видалення сполук фтору. Досліджувалися залізовмісні сорбенти, отримані з відходів водоочищення. Для нейромережевого наближення ключових характеристик якості сорбентів (сорбційної ємності та ефективності видалення фторид-іонів), а також для подальшого пошуку компромісного оптимуму (одночасної багатоцільової максимізації) було розроблено програму на основі Python. Для вирішення задачі багатоцільової оптимізації було застосовано підхід на основі функції бажаності Харрінгтона, для пошуку глобального оптимуму задачі оптимізації обрано алгоритм «диференціальної еволюції». Розрахована компромісна оптимальна точка відповідає результатам попередніх досліджень авторів щодо впливу умов проведення процесу на процес сорбції. Використання моделей, заснованих на штучному інтелекті, сприяє розробці інтелектуальних систем підтримки прийняття рішень щодо створення та модернізації систем водоочищення, сприяючи як науковому прогресу, так і практичному захисту навколишнього середовища. Застосування комп’ютерного моделювання є основою сучасних досліджень сорбційних технологій. Воно покращує наукове розуміння, дозволяє проводити проектування на основі даних та сприяє масштабованому впровадженню інноваційних, стійких рішень для очищення води.

Ключові слова: очищення води, дефторування, сорбенти, комп'ютерне моделювання, нейронні мережі, багатокритеріальна оптимізація, глобальний оптимум.