ANNOTATION

of the dissertation of Kunarbekova Makhabbat Seit-Zadayevna on the topic: "Preparation of modified carbon materials for the removal of radionuclides from contaminated water", submitted for the degree of Doctor of Philosophy (PhD) in the specialty 8D07109 – Innovative technologies and new inorganic materials.

The relevance of the topic under study.

One of the most pressing environmental issues globally and in Kazakhstan is the contamination of water with radionuclides such as cesium and iodine, resulting from past nuclear activities and ongoing industrial operations. The Semipalatinsk Test Site and uranium mining regions in Kazakhstan are major sources of long-term radioactive pollution. Conventional water purification methods are often inefficient or too costly for the specific challenge of removing these radionuclides. Therefore, the development of efficient, low-cost, and scalable sorbent materials is essential for mitigating radioactive contamination and protecting both ecosystems and human health. The use of modified activated carbon derived from agricultural biomass represents a sustainable and practical approach for addressing these challenges.

Research object: Radionuclides of iodine (I_3^-) and cesium (Cs^+); modified activated carbon sorbents obtained from rice husk, buckwheat husk, and walnut shell.

The purpose and objectives of the research.

The purpose of the study is to develop modified carbon sorbents capable of efficiently removing radioactive iodine and cesium from contaminated water. To achieve this, the following objectives were set:

- Synthesis of carbon materials from biomass and their modification with urea and ferrocyanide.
- Investigation of structural, morphological, and physicochemical characteristics of the sorbents.
- Study of sorption mechanisms through advanced spectroscopic, computational, and kinetic modeling methods.
- Evaluation of sorption efficiency in both model and real contaminated water systems.

Scientific novelty:

- For the first time, biomass-based carbon sorbents were modified via a hydrothermal method with urea and ferrocyanide to enhance sorption capacity.

- The modified sorbents demonstrated up to 95–97% efficiency for Cs^+ and over 40% improvement for I_3^- uptake compared to commercial activated carbons.
- Gaussian 16W simulations using DFT were employed to elucidate sorption mechanisms at the molecular level.
- The developed materials were successfully tested on industrial samples from the Degelen test site, confirming their practical applicability.

Practical significance:

- The study offers a sustainable approach to valorize agricultural waste into high-performance sorbents for environmental remediation.
- Modified sorbents have been validated under both laboratory and real-world nuclear contamination conditions.
- The technology is scalable, cost-effective, and compatible with Kazakhstan's environmental safety strategies.
- Patent for utility model for the synthesis of modified activated carbon sorbents was obtained.

The methods of the research

To produce activated carbons, a high-temperature chemical vapor deposition (CVD) furnace was utilized., which allowed for the supply of inert gases and included a steam generator. The synthesis preparation of carbons was conducted at various temperatures and involved the use of chemical activators. The impregnation of modifying agents, such as nitrogen groups and ferrocyanide, was carried out in an autoclave and a high-pressure Microreactor (PR 250) to account for the medium's inertia.

The sorption capacity of the modified sorbents for iodine was assessed using ultraviolet-visible (UV-Vis) spectroscopy, while the cesium content was measured using inductively coupled plasma-mass spectrometry (ICP MS) methods. The residual activity of the sorbents was evaluated through gamma spectrometry (2480 Automatic Gamma Counter) to determine the presence of the radioactive isotope ^{137}Cs.

The physicochemical properties of the modified carbon sorbents were analyzed using a variety of modern methods with complementary techniques, including Scanning Electron Microscopy- with Energy Dispersive X-ray Spectroscopy (SEM/EDS), BET nitrogen porosimetry, X-ray Fluorescence (XRF)F, X-ray Fluorescence(FT-IR), water angle wettability, zeta potential, surface charge and Raman spectroscopy.

The main provisions to be defended:

1. Biomass-derived activated carbons that undergone hydrothermal modification (surface area: 1600–2200 m^2/g) are enriched with nitrogen groups.

Improving sorption capacity of I3- up to 35% of urea modified compared to the best non-modified activated carbon.

2. Prussian Blue-modified activated carbons demonstrate high selectivity for Cs^{+} adsorption reducing total activity from 120 to <5 Bq/L in multi-ion systems ($^{90}Sr^{2+}$, Ca^{2+}, Na^{+}) from the real ground water contaminated by radionuclides.

3. Sorption mechanisms were formulated based on carbons of different pore stricture and functioning with the use of analytical techniques. Typical fragment structures and contribution of physisorption, chemisorption and electrostatic interaction has been discussed.

Connection with state programs:

The work was carried out as part of projects funded by the Ministry of Education and Science of the Republic of Kazakhstan. BR21881939 "Development of resource-saving energy generating technologies for the mining and metallurgical complex and creation of an innovative engineering center", AP19577049 "Synthesis, characterization and physico-chemical study of sorbents of biomass origin for industrial water purification from radionuclides".

The structure and scope of the dissertation:

The dissertation consists of 136 pages of typewritten text, contains 25 tables and 49 figures. It includes an introduction, three chapters, a conclusion, references (199 titles), and two appendices.

Publications:

The results of the work are reflected in: one review – in the Scientific Journal cited in the Scopus database, 1 book chapter, patent and 3 articles in journals recommended by the Committee for Quality Assurance in Education and Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan:

1. M. Kunarbekova, R. Busquets, Ye. S. Sailaukhanuly, S.V. Mikhalovsky, Toshtay K., K. Kudaibergenov, S. Azat. «Carbon adsorbents for the uptake of radioactive iodine from contaminated water effluents: A systematic review», Journal Of Water Process Engineering-Q1, 92% percentile

2. Kunarbekova, M., Busquets, R., Sapargali, I., Seimukhanova, L., Zhantikeyev, U., Kudaibergenov, K., & Azat, S. (2025). Innovative materials for industrial application: Book Chapter 11. Synthesis and Characterization of Activated Carbon from Biomass (1st ed.). IGI Global Scientific. https://doi.org/10.4018/979-8-3693-7505-1.ch011

3. K.K. Kudaibergenov, S. Azat, Zhantikeev U.E., M.S. Kunarbekova, I.O. Sapargali, L.N. Seymukhanova. "Method of obtaining sorption material for water purification from radionuclides". Patent for Utility model, No. 9470

Publications in journals recommended by the Committee for Quality Assurance in Education and Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan:

1. M.S. Kunarbekova, I.O. Sapargali, L.N. Seymukhanova, K.K. Kudaibergenov, S. Azat. "Synthesis of nanofiber composite doped with nitrogen groups from biomass by chemical activation". Combustion and plasmochemistry journal, 22(1), 3-11. https://doi.org/10.18321/cpc22 (1)3-11.
2. Kunarbekova, M., Seymukhanova, L., Sapargali, I., Zhantikeev, Y., Kudaibergenov, K., & Azat, S. (2024). Synthesis and characterization of activated carbon from biomass for the sorption of radioactive iodine. Combustion and plasmochemistry journal, 22(4), 331-341. https://doi.org/10.18321/cpc22 (4)331-341
3. Seimukhanova L.N., Zhantikeyev U.Ye., Bexeitova K.S., Kunarbekova M.S., Rakhimova B.U., Fazylov B.D., Zagitova A.M., Kudaibergenov K.K., Azat S. Production of Nanocellulose For Water Purification From Dyes. NNC RK Bulletin. 2024;(4):181-190. (In Russ.) https://doi.org/10.52676/1729-7885-2024-4-181-190