ABSTRACT

of the dissertation research by

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on the topic: **“ECOLOGICAL ASSESSMENT AND PREDICTION OF SOIL CONTAMINATION BY PRODUCTS OF LEAD-ZINC SLAG PROCESSING”**

submitted for the degree of Doctor of Philosophy (PhD) in the specialty

8D05210 – “Ecology”.

General Characteristics of the Research.

Based on a comparative analysis of international experience in geochemical investigations of soils contaminated with lead–zinc slag, followed by an examination of the physicochemical and biological characteristics of contaminated soils and lead–zinc slag in Shymkent, and a quantitative assessment of environmental risks to human health, the Monte Carlo method was used to model the probability of exceeding established environmental risk thresholds and to assess the sensitivity of the calculated risks to changes in the quantitative and qualitative parameters of arsenic.

The dissertation research is submitted for defense in the form of a series of scientific articles in accordance with Clause 5-1 of the Rules for Awarding Academic Degrees, approved by Order No. 127 dated March 31, 2011, taking into account the amendments and additions introduced by Order No. 422 of the Minister of Science and Higher Education of the Republic of Kazakhstan dated September 3, 2026.

The choice of this format is justified by the applicant's authorship of three (3) publications in international peer-reviewed scientific journals indexed in the Web of Science Core Collection and ranked in the first and second quartiles (Q1, Q2). The set of submitted articles constitutes a unified, completed scientific study, integrated by a common research objective, methodology, and object of research.

Compliance with National Scientific Programs.

The dissertation research was conducted in accordance with the priority area of scientific and scientific-technical development of the Republic of Kazakhstan, “Ecology, Environment, and Rational Use of Natural Resources.”

The research was carried out within the framework of scientific project AP25795537, “Ecological Assessment of Lead–Zinc Slag Disposal Sites in Environmental Components and Development of a Technology for the Reclamation of Slag Dumps,” funded under the “Zhas Galym” program for 2025–2027.

Relevance of the Dissertation Research.

The accumulation and spatial distribution of heavy metals and arsenic in soils resulting from lead–zinc slag reprocessing represent a significant environmental problem affecting ecosystem sustainability and environmental safety (Kisiňska et al., 2021; Terzič et al., 2024; Nowiňska et al., 2024; Sun et al., 2025). Existing scientific approaches to soil contamination assessment require further improvement in terms of the comprehensive integration of geochemical (Li et al., 2025), biological, and ecological risk indicators, as well as the consideration of uncertainty in risk assessment (Wang et al., 2025; Jia et al., 2025).

The high level of contamination and its spatial heterogeneity identified at the lead–zinc slag reprocessing site in Shymkent highlight the scientific significance of quantitatively assessing environmental consequences (Ramazanova et al., 2021). In this regard, comprehensive investigation of the patterns of anthropogenic soil contamination, probabilistic prediction of environmental and human health risks, and scientific justification of priority measures for the remediation of contaminated areas are of particular relevance.

Purpose of the Research.

The purpose of the dissertation research is to determine the level of soil contamination by products of lead–zinc slag reprocessing and the patterns of its spatial distribution, to conduct a comprehensive assessment of environmental and human health risks using geochemical and bioindication methods, and to provide a scientific justification for priority measures for the remediation of contaminated areas by modeling the probability of exceeding established risk thresholds.

Research Objectives:

1. To systematize international scientific experience in the ecological assessment of soils contaminated with lead-zinc slag, to identify the features of existing methodological approaches and insufficiently studied scientific issues based on a comparative analysis of methods for geochemical investigation, assessment, and prediction of environmental risks.

2. To investigate the chemical composition, mineralogical and microstructural characteristics of soils and slag in the territory of Shymkent city affected by lead-zinc slag processing, to determine the patterns of spatial distribution of heavy metals at various distances from the source of contamination, and to assess the eco-economic damage caused by soil contamination.

3. To conduct a comprehensive study of the elemental composition of soils and local vegetation in the area of lead-zinc slag processing, to perform a quantitative assessment of soil contamination levels, environmental risks, and risks to human health based on geochemical contamination indicators, to identify ecologically hazardous zones, and to scientifically substantiate priority directions for remediation of contaminated territories.

4. To simulate, using the Monte Carlo method, the probability of exceeding established threshold levels of carcinogenic and non-carcinogenic risks associated with soil contamination by heavy metals and arsenic (As) in the territory of lead-zinc slag processing, to perform probabilistic forecasting of risk levels, and to assess the sensitivity of the calculated risks to changes in the toxicological parameters of arsenic.

The object of the research is the territory of lead-zinc slag processing in the city of Shymkent and the adjacent soil cover.

Research methodology is based on a systematic and comprehensive approach to environmental assessment. The study was conducted following the principle of sequential transition from scientific and methodological analysis to experimental research, integrated evaluation of the obtained results, and probabilistic modeling.

Sampling of contaminated soil and lead-zinc slags was carried out in accordance with the requirements of GOST R 58595-2019, GOST 17.4.3.01-2017, and GOST 17.4.4.02-2017. Elemental analysis of samples was performed at the analytical laboratory of KazEcoAnalysis LLP using an inductively coupled plasma atomic emission spectrometer (ICP-OES, Shimadzu ICPE-9000) in accordance with Method M 02-902-157-10.

The literature review was conducted according to the PRISMA-ScR (2018) protocol: a total of 410 publications from 2010–2025 were identified in the Dimensions (n = 351), PubMed (n = 10), and OpenAlex (n = 49) databases (search date: 16.03.2026); publication selection was performed on the Rayyan platform, data extraction was carried out using Elicit and Microsoft Excel 2021; the quality of 56 included studies was assessed according to four criteria (number of samples ≥ 20; analytical methods ICP-MS, ICP-OES, AAS or pXRF with quality control; presence of background samples; use of a standardized evaluation system) (Article 1).

The chemical composition and morphology of slags and soils in the industrial zone of Shymkent were studied on samples collected in May–June 2024 along a transect at distances of 0, 50, 100, 200, 500, and 1000 m from the source of contamination; sample preparation was performed according to ISO 11464:2006 (drying at 105°C, grinding to 0.1 mm). The content of Pb, Zn, Cu, and Fe was determined by atomic absorption method (ContrAA 300); the morphology and phase distribution of slags were analyzed by scanning electron microscopy (JSM-6490LV, JEOL), and the mineral composition by X-ray diffraction (XRD); concentrations were compared to maximum permissible limits. The eco-economic damage was calculated according to the Rules for the Economic Assessment of Environmental Pollution Damage (Article 2).

Comprehensive assessment (Article 3) was carried out on 24 soil samples collected on April 24, 2026, from a 0–50 cm layer along four transects (north, south, east, west) at distances of 0, 1, 5, 10, 50, and 100 m from the perimeter of the dump, two comparative samples (300 m and 1.5 km), and four composite samples of

aboveground biomass of Centaurea pseudosquarrosa and Plantago lanceolata. The content of 10 elements (As, Cd, Cr, Cu, Fe, Hg, Mn, Ni, Pb, Zn) was determined by ICP-OES (soils – M 02-902-157-10, plants – PND F 16.1:2.3:3.11-98; ISO 17294-2, EPA 3050B) with quality control according to ISO/IEC 17025 (blank samples, standard samples, extraction 80–120%). Soil contamination was assessed using six geochemical indices relative to the upper continental crust Clarke values – CF, Igeo, EF, PLI, mCd, and RI (by Hakanson); metal transfer to plants was assessed by the Cplant/Csoil ratio; environmental risk was evaluated using the RCR = PEC/PNEC (REACH) coefficient; human health risk was assessed using the US EPA RAGS model (oral, inhalation, and dermal exposure routes; CDI, HQ, HI, CR); for spatial analysis, buffer zones of 200, 500, and 1000 m were defined.

Probabilistic risk assessment (Article 4) was performed on data from 24 transect samples for eight elements (Pb, Zn, Cd, Cu, As, Hg, Ni, Cr) with reference to an adult worker in an open area: concentration distributions were approximated by a log-normal law (maximum likelihood method), exposure parameters were set by stochastic distributions; Monte Carlo modeling was carried out in 100,000 iterations (PCG64 generator) for two sets of toxicological parameters for arsenic: baseline (slope factor 1.5 $(mg/kg \cdot day)^{-1}$) and updated IRIS 2025 (32 $(mg/kg \cdot day)^{-1}$; RfD 6.0×10^{-5} mg/kg·day); probabilities of exceeding threshold values for carcinogenic risk (10^{-6}, 10^{-4}, 10^{-3}) and hazard index (HI = 1 and 10) were calculated.

Statistical data processing included descriptive statistics (mean ± standard deviation), Pearson correlation analysis ($p < 0.05$) – for heavy metal concentrations (Article 2), one-way analysis of variance (one-way ANOVA) with Tukey's post hoc test (HSD, $\alpha = 0.05$) – for differences between transects (Article 3), the Shapiro–Wilk normality test and Spearman rank correlation for sensitivity analysis (Article 4). Calculations were performed in Python 3.11 (pandas, NumPy, SciPy).

All measurements were performed in at least three replicates.

Scientific novelty of the obtained results:

1. Based on the systematization of global experience in scientific and methodological approaches to the environmental assessment of soils contaminated with lead-zinc slag, a comparative analysis was carried out and it was established that systematic mapping using methods for assessing the state of slag-contaminated soils does not exist, and data for Central and Middle Asia, including Kazakhstan, are completely lacking. Critical gaps are associated with the limited capacity for predictive modeling and the absence of standardized protocols. The results are presented in a review-analytical article (*Sustainability*, 2026, 18, 3934).

2. The geochemical characteristics of lead-zinc slags and contaminated soils in Shymkent were specified, with the identification of features of the spatial distribution of heavy metals and a quantitative assessment of the eco-economic damage caused by

soil contamination. A strong positive correlation was found among the concentrations of heavy metals, indicating their common anthropogenic origin and simultaneous migration in the soil profile. The total ecological damage exceeds 750 million tenge per year, with iron and lead making the greatest contribution to the total damage. The results are published in an experimental research article (*Engineering, Technology & Applied Science Research*, 2026, 16(3), 36790–36795).

3. Based on the integration of geochemical pollution indices, data on the elemental composition of plants, and indicators of environmental risk, a comprehensive assessment of soil contamination was performed, an approach to identifying environmentally hazardous zones and determining three levels of priority for remediation of contaminated areas was substantiated. It was established that peak concentrations exceed the maximum permissible levels in Kazakhstan by several times. A three-level remediation system was developed, including stages of engineering isolation, phytostabilization, and controlled reduction of concentrations, which combines resource restoration and pollution control and can be replicated in similar areas. The results are published in the journal *Sustainability* (2026, 18, 6742).

4. Based on probabilistic modeling using the Monte Carlo method, the probability of exceeding established threshold levels of carcinogenic and non-carcinogenic risks was quantitatively determined, and the sensitivity of risk assessment results to updated toxicological parameters for arsenic was evaluated. The probability of exceeding the carcinogenicity threshold of 10^{-4} was 69.9%, and for HI = 1 it was 82.1%; the mean and worst-case values indicated on the website corresponded to the 76.9th and 97.2nd percentiles of the modeled distribution. According to 2025 data, the mean risk was 21 times higher, and the probability of exceeding was 99.3% and 97.3%, respectively. It was established that arsenic concentration ($\rho = +0.867$) is a limiting factor for accuracy under any parameterization. The results are published in the journal *Toxics* (2026, 14, 894).

Principal statements submitted for defense:

1. Soil contamination with heavy metals in the lead-zinc slag processing area is characterized by spatial heterogeneity, varying with distance from the contamination source.

2. Elevated concentrations of heavy metals and arsenic in soils show a direct correlation with increased levels of geochemical pollution and heightened risks to ecosystems and human health.

3. The prioritization of remediation activities for contaminated areas is determined by a comprehensive consideration of the degree of geochemical pollution and the levels of ecological risk.

4. The probability of exceeding established threshold levels for carcinogenic and non-carcinogenic risks to human health depends on the specified toxicological

parameters for arsenic, with changes in these parameters substantially influencing the results of risk assessment.

Practical significance of the research results.

According to the results of the conducted research, the eco-economic damage caused by soil contamination with heavy metals in the area of lead-zinc slag processing in Shymkent was estimated at over 750 million tenge per year.

Based on a comprehensive analysis of geochemical pollution indicators and environmental risk levels, a scientifically substantiated three-level system of prioritization for remediation measures of contaminated areas was developed, which can be recommended for use by environmental and nature protection organizations.

The use of probabilistic modeling with the Monte Carlo method showed that the application of updated toxicological parameters for arsenic changes the calculated probability of exceeding the established threshold level of carcinogenic risk from 70% to 99%, and for non-carcinogenic risk from 82% to 97%. The obtained results may be used by regulatory bodies in assessing risks to human health.

The results of the dissertation research can be used in educational programs for students and master's students specializing in “Ecology.”

The practical application of certain research results is confirmed by an implementation act from 2023 and an approbation act from 2024 by the “Center for Environmental Support and Expertise” LLP.

Approbation of research results: The main results of the research were presented at the VII International Scientific and Practical Conference “Quality Management: Search and Solutions” (Houston, USA, 2021), the IX International Scientific and Practical Conference “Industrial Technologies and Engineering” ICITE-2022 (Shymkent, Kazakhstan, 2022), in the peer-reviewed journal “Productive Forces and Natural Resources of Georgia” (Tbilisi, Georgia, 2022), at the International Scientific and Practical Conference “Auezov Readings-20” (Shymkent, Kazakhstan, 2022), the X International Scientific and Practical Conference “Innovation Management and Technology in the Era of Globalization” (Manchester, UK, 2023), in the scientific journal “Auezov University”, No. 2(10) (Shymkent, Kazakhstan, 2024), in the international scientific journal “Vestnik Nauki”, No. 9(78) (Tolyatti, Russia, 2024), at the International Scientific and Practical Conference “Environmental Protection and Sustainable Development” (Tbilisi, Georgia, 2024), in the peer-reviewed journal “International Journal of Innovative Research and Scientific Studies” (2025), and at the LXX International Scientific and Practical Conference “Advances in Science and Technology” (Moscow, Russia, 2025).

The dissertation includes the following publications:

1. **Pernebayev Z.,** Aitimbetova G. Scoping Review on Soil Contamination from Pb–Zn Slag and Environmental Assessment Methods // Sustainability. – 2026. – Vol. 18. – Article 3934. DOI: 10.3390/su18083934.

(Applicant's contribution: the applicant initiated the review study, prepared its main part, conducted a systematic analysis of scientific literature, performed a comparative analysis of existing methods for environmental assessment of soil contamination by lead-zinc slags, and synthesized the obtained results.)

2. **Pernebayev Z.,** Aitimbetova G., Abubakirova A. Integrated Geochemical, Vegetation, and Risk Assessment of a Pb–Zn Slag Reprocessing Site in Southern Kazakhstan: Implications for Sustainable Remediation Prioritization // Sustainability. – 2026. – Vol. 18. – Article 6742. DOI: 10.3390/su18136742.

(Applicant's contribution: the applicant made a major contribution to the analysis of geochemical pollution indicators, the assessment of environmental risks, the scientific substantiation of priority areas for remediation of contaminated territories, and also proposed environmental solutions aimed at reducing the identified risks.)

3. Pernebayev Z., Issayeva A., Baiduisenova T., Ansari M.-u.-R., Aitimbetova A., Nurseiit K. Exceedance Probability and Toxicity-Value Sensitivity in Health-Risk Assessment of a Pb–Zn Slag Reprocessing Site Under the 2025 IRIS Arsenic Values // Toxics. – 2026. – Vol. 14, No. 10. – Article 894. DOI: 10.3390/toxics14100894.

(Applicant's contribution: the applicant participated in the development of the scientific concept of the study, the development of the methodology for probabilistic risk assessment, the analysis of Monte Carlo simulation results, and the scientific substantiation of the obtained conclusions.)

The following certificates of state registration of copyright objects were obtained on the topic of the dissertation research:

1. Certificate of entry into the state register of objects protected by copyright, No. 56867 (April 15, 2025) – The influence of lead-zinc wastes on the formation of phytocenoses.

(Applicant's contribution: the applicant participated in the study of the influence of lead-zinc wastes on the formation of phytocenoses, analysis of scientific data, and synthesis of the obtained results.)

2. Certificate of entry into the state register of objects protected by copyright, No. 57022 (April 22, 2025) – "The influence of soil contamination by lead and cadmium ions on the formation of phytocenoses in contaminated areas."

(Applicant's contribution: the applicant participated in the analysis of the influence of soil contamination by lead and cadmium ions on the formation of

phytocenoses, scientific interpretation of results, formulation of conclusions, as well as in the preparation of materials for the registration of the copyright object.)

Structure of the dissertation presented as a series of articles.

The dissertation is presented as a series of four scientific articles, published by the applicant in co-authorship in journals indexed in the Web of Science (Q1, Q2), as well as protective documents for intellectual property objects. These works consistently present and substantiate the main scientific statements of the dissertation, supported by the results of experimental research, geochemical analysis, and mathematical modeling.