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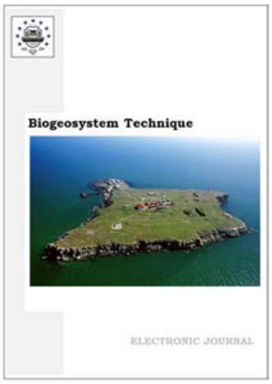

Articles

Forecasting the Spatiotemporal Dynamics of Trace-Element Concentrations in Soil Based on Multi-Year Monitoring

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Abstract

Mathematical forecasting methods were developed to evaluate the spatiotemporal dynamics of trace elements, including Fe, Zn, Cu, Mn, Cr, and V, in soils at the study sites. To detect trends and generate predictions, various models were employed, including linear and smoothing techniques. The trace-element composition in the studied soils shows moderate variability, mostly smooth and gradual, indicating the influence of long-term geochemical processes. Regional differences also emerged, highlighting the unequal impact of natural conditions and human activities on the trace-element background. These characteristics are crucial diagnostic tools for analyzing forecast results.

Keyword: trace metals, machine learning, spatiotemporal dynamics, linear regression, LOESS regression.

1. Introduction

Protecting the environment from pollution is critical to ensuring public safety and sustainable development. Natural environmental changes, alternating with anthropogenic impacts, alter natural geochemical cycles. A combination of the climatic factors, territory's lithological and geochemical features, soil formation conditions, and the intensity of economic activity determines the formation of spatial anomalies and temporal trends in chemical element content, especially heavy metals (HMs) (Sukiasyan et al., 2025). The situation is complicated by the fact that in the natural biogeochemical processes the HMs can accumulate and migrate within the soil, creating a long-term environmental hazard (Gall et al., 2015). Chemicals contaminating soil with HMs, mainly due to erosion and organic matter loss, are the primary results of declining soil fertility (Smith et al., 2024). The dynamics of HMs accumulation and migration in soils are determined by multiple physical, chemical, biological, and climatic factors (Zaky, Elwa, 2020; Kicińska et al., 2022).

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However, the key determinants are the area's natural features such as relief, water permeability, and soil horizon's structure (de Matos et al., 2001). It has been established that small particles of HMs are washed from the upper slopes, leading to the formation of accumulation zones in the lower parts of the terrain (Ding et al., 2017). It is clear that achieving the Sustainable Development Goals requires moving towards integrated monitoring systems that account not only for the total content of elements but also for their chemical distribution in the soil environment, mobility, and availability to living organisms (Tóth et al., 2016).

In recent years, ecological research has increasingly shifted from basic measurements of metal content to detailed evaluations of their environmental risks. The use of multivariate statistical methods, geoinformation technologies, and ecological risk indices enables researchers to identify sources, spatial distributions, and potential threats. This progression lays the groundwork for scientifically grounded pollution control and impact mitigation strategies (Gong et al., 2024).

Spatiotemporal changes in the chemical composition of soils are a key focus in environmental research, as soils act as accumulators and converters of elemental constituents, reflecting both natural and anthropogenic processes (Shi et al., 2023). The development of spatial anomalies and temporal trends in soil element content results from a combination of climate factors, lithological and geochemical terrains, soil formation conditions, and moderate economic activity (Zhuo et al., 2019). Analysing these changes helps evaluate the current condition of ecosystems and guides their future development. Among HMs, trace elements (TEs) are particularly prominent; they occur at much lower concentrations but play a crucial role in the functioning of biological and geochemical systems (Sukiasyan, Kirakosyan, 2024).

TEs are involved in oxidation-reduction processes. They regulate other chemical elements migration. TEs respond to environmental changes, and indicate the soils mineralogical features and the soils long-term chemical variations (Zhang et al., 2022; Xu et al., 2023; Islam et al., 2023). A typical feature of the content of TEs in the soil cover is its spatial and temporal variability (Wang et al., 2020; Taghizadeh-Mehrjardi et al., 2021). This is why modern research is increasingly aimed not only at describing soils' current conditions but also at creating predictive models for their spatiotemporal changes (Córdoba et al., 2025).

The aim of this study is to analyze the spatiotemporal dynamics of selected TEs in soil samples from different regions of Armenia, drawing on multi-year monitoring data, with a focus on predicting changes in their concentrations using mathematical models.

2. Materials and methods

The study is based on monitoring data on the content of TEs Fe, Zn) Cu, Mn, Cr and V) in the soils of the regions Gegharkunik (Gavar and Martuni sites) and Kotayk (Hrazdan sites) is situated in the eastern part of Armenia (Figure. 1). At least five soil samples from the same site at the control points, obtained using the envelope method to a depth of up to 20 cm, were mixed. The samples were subsequently placed in dark glass containers and transported at +4°C for 24 hours for instrumental measurements in the laboratory. Direct X-ray exposure was used for elemental analysis of all soil samples using a portable XRF analyser (Thermo Scientific™ Niton™) (Sukiasyan et al., 2022).

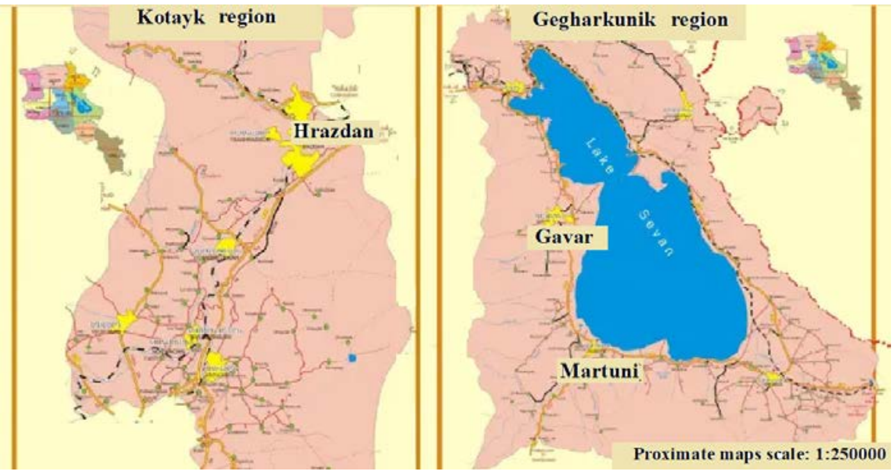

Fig. 1. Soil sampling region of Armenia

The initial time series spans from 2021 to 2023 and shows the average regional element concentrations. For analysis, averaged indicators across regions were utilised to focus on common spatiotemporal patterns. To create and forecast the temporal behaviour of TEs, various mathematical models were employed, including linear regression (LR), exponential smoothing (ETS), and locally estimated scatterplot smoothing (LOESS) regression (Hyndman, Koehler, 2002; Koyande, 2024). LOESS is a non-parametric regression method that performs local polynomial fits. It applies a low-degree polynomial to data subsets using weighted least squares, where the weights depend on the distance to the target point. This approach is particularly effective at identifying non-linear patterns, such as sudden rises or falls in metal levels. For each metal, a second-degree polynomial was fitted using LOESS, producing a locally adaptive model that predicts smooth, flexible future trends (Cleveland, Devlin, 1988).

The fitted polynomial takes the general form:

$$\hat{z}_{t+k} = \sum_{i=1}^{n} \omega_i(t+k)P_i(t+k) \quad (1)$$

where: $\hat{z}_{t+k}$ - is the future values of concentration in log-space at year x_{t+k}; $P_i(t+k)$ is a local polynomial (degree 2); $w_i(t+k)$ are weights based on proximity to t, controlled by a span parameter.

Coefficients of the fitted curve:

$$\hat{y}_t = a \cdot t^2 + b \cdot t + cy \quad (2)$$

where $a, b,$ and c are coefficients determined through local fitting.

The final predicted concentration can be calculated by:

$$\hat{y}_{t+k} = \exp(\hat{z}_{t+k}) \quad (3)$$

Model parameters were estimated individually for each TE and site. A comparative analysis of these results helped evaluate the consistency of the forecasts and the robustness of the identified trends. Forecasts were made for 2024-2026 to analyse changes in soil TE composition.

Data processing and model development employed standard statistical methods. Results were interpreted considering established geochemical mechanisms that control the migration and accumulation of TEs in soils.

3. Results and discussion

The selection of Zn, Cu, Fe, Mn, Cr, and V for regional analysis is due to their physicochemical characteristics, marked by high chemical reactivity in soil and strong responsiveness to local geochemical conditions. Based on the concentration data, a forecast of the temporal behaviour of TEs was created using mathematical models, including LR, ETS, and LOESS (Tables 1-3).

Table 1. Parameters of the linear regression model for soil sampling sites

Trace Element / Parameters	Zn	Cu	Fe	Mn	Cr	V
Hrazdan sites						
Intercept $\beta 0$	-251.02	171.45	-342.42	-52.56	735.68	-557.29
Slope β_1	0.13	-0.08	0.17	0.03	-0.37	0.28
Gavar sites						
Intercept $\beta 0$	-46.17	-153.11	-165.31	-151.53	557.94	-453.42
Slope β_1	0.02	-0.07	0.09	0.08	-0.28	0.23
Martuni sites						
Intercept $\beta 0$	186.70	299.65	-141.66	126.75	-350.33	-380.33
Slope β_1	-0.09	-0.15	0.8	-0.06	0.18	0.19

Table 2. Parameters of the exponential smoothing model for soil sampling sites

Parameters \ Trace Element	Zn	Cu	Fe	Mn	Cr	V
Hrazdan sites						
Level	4.56	4.41	10.23	6.72	4.45	4.72
Trend	0.13	-0.12	0.17	0.03	0.37	0.28
Damping	0.995	0.800	0.995	0.995	0.995	0.995
Initial Level	99.27	85.10	29633.10	849.07	97.73	124.87
Initial Trend	0.03	-16.53	-1772.30	-26.23	-3.03	-2.77
Gavar sites						
Level	4.50	4.41	10.48	6.66	4.62	4.78
Trend	0.04	-0.11	0.090	0.08	0.28	0.23
Damping	0.80	0.80	0.995	0.995	0.995	0.995
Initial Level	84.40	38515.00	819.65	113.30	113.50	130.55
Initial Trend	-13.27	-5694.33	-63.95	-5.80	-5.80	-4.38
Martuni sites						
Level	4.47	4.26	10.33	6.63	4.85	4.67
Trend	-0.09	-0.21	0.08	-0.06	0.17	0.19
Damping	0.995	0.800	0.995	0.995	0.995	0.995
Initial Level	71.80	31548.45	737.40	135.30	135.30	116.55
Initial Trend	-14.35	-700.75	4.10	-3.35	-3.35	-7.85

Table 3. Parameters of the locally weighted scatterplot smoothing model for soil sampling sites

Parameters \ Trace Element	Zn	Cu	Fe	Mn	Cr	V
Hrazdan sites						
a	0.13	0.13	0.24	0.06	0.40	0.30
b	-509.92	-539.41	-954.84	-245.51	-1608.13	-1214.92
c	5.15e+05	5.45e+05	9.65e+05	2.48e+05	1.63e+06	1.23e+06

Gavar sites						
a	-0.11	0.10	0.247	0.16	0.33	0.26
b	430.53	-394.08	-988.66	-644.96	-1337.90	-1054.75
c	-4.35e+05	3.99e+05	1.01e+06	6.52e+05	1.35e+06	1.07e+06
Martuni sites						
a	-0.06	0.08	0.10	0.26	0.20	0.26
b	256.64	-310.73	-394.90	-1053.07	-811.55	-1052.18
c	-2.59e+05	3.14e+05	3.99e+05	-2.66e+05	8.20e+05	1.06e+06

Using the specified parameters, predicted changes in TE concentrations in soil samples across all research sites through 2026 were modelled using LR, ETS, and LOESS (Figure 2).

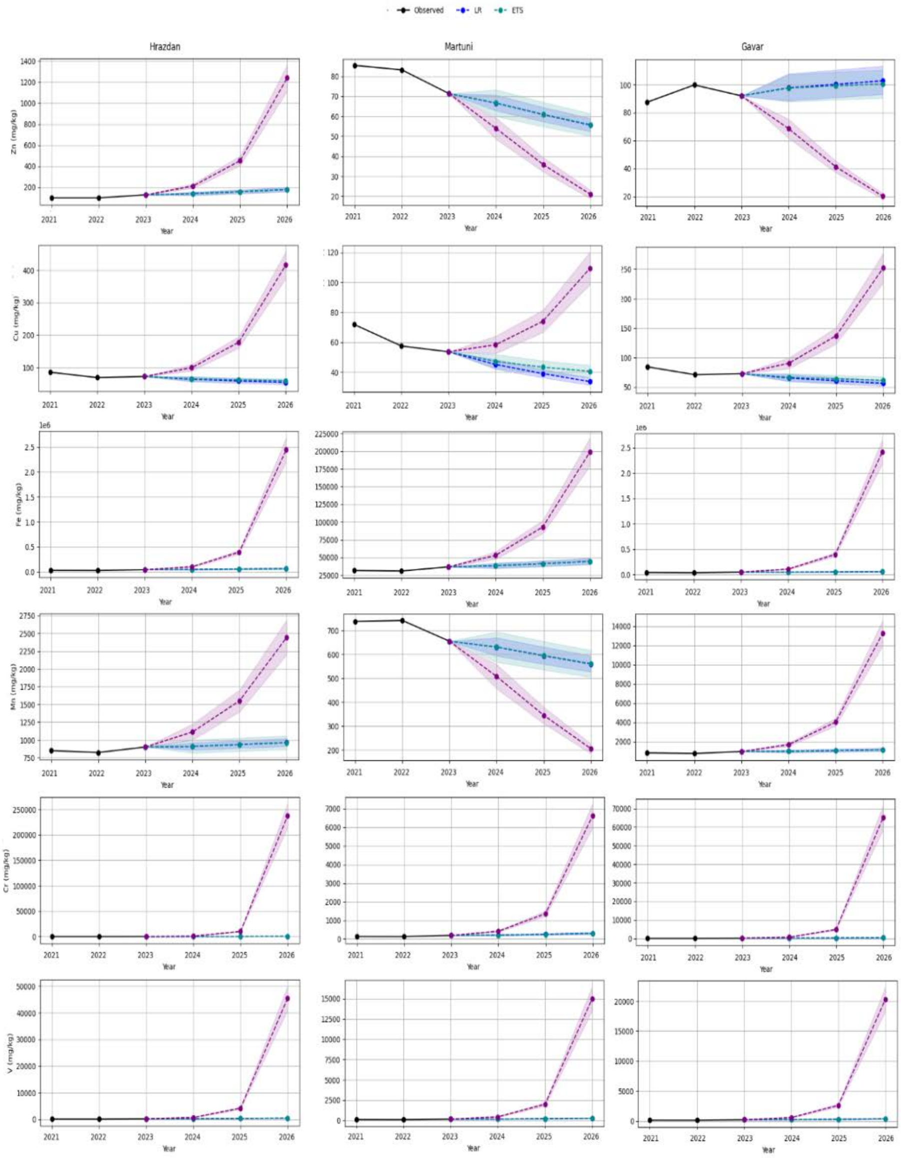

Fig. 2. Predicted trajectories of change in TE concentrations (Zn, Cu, Fe, Mn, Cr, and V) in the soils at the Hrazdan, Martuni, and Gavar sites up to 2026

For Zn, regional differences are particularly notable. At the Hrazdan sites, LR captures the ongoing directional trends over the forecast period, whereas ETS smooths fluctuations to produce a more stable trajectory. LOESS highlights local nonlinear patterns, influenced by regional factors. At Gavar and Martuni, forecast curves are more stable with minimal differences between LR and ETS, while LOESS shows slight deviations. Confidence intervals for Zn expand over time, especially for LR and LOESS, but remain within the observed range, supporting forecast interpretation. This pattern aligns with Zn's chemistry as a moderately mobile element influenced by pH and organic matter.

Cu concentration in all three regions is highly consistent across models. The predicted LR trajectories are smooth; ETS further diminishes fluctuations, and LOESS uncovers only minor nonlinear effects. Regional variations are moderate and do not cause significant differences in forecast estimates. Confidence intervals are relatively narrow and gradually widen without sudden jumps. This forecast stability is consistent with copper's chemical behaviour in soil, where it tends to bind strongly to organic matter and mineral components, restricting its movement and stabilising its temporal dynamics, even in the presence of anthropogenic activities.

Cu concentration in all three regions is highly consistent across models. The predicted LR trajectories are smooth; ETS further diminishes fluctuations, and LOESS uncovers only minor nonlinear effects. Regional variations are moderate and do not cause significant differences in forecast estimates. Confidence intervals are relatively narrow and gradually widen without sudden jumps. This forecast stability is consistent with copper's chemical behaviour in soil, where it tends to bind strongly to organic matter and mineral components, restricting its movement and stabilising its temporal dynamics, even in the presence of anthropogenic activities.

A notably different perspective emerges when examining Fe. Even after considering regional differences, all models show marked forecast volatility. LR predicts sharply rising trends in all regions, ETS enhances this trend, and LOESS highlights the nonlinear complexity of the time series. Confidence intervals widen quickly and considerably, especially in 2025-2026, signalling high uncertainty in future estimates. This model volatility underscores iron's fundamental role as a redox-sensitive element and a key geochemical regulator: transitions between Fe^{2+} and Fe^{3+} are linked to oxide phase formation, causing sudden and hard-to-predict shifts in concentrations.

Similar patterns have been observed for Mn. At the Hrazdan sites, the LR and ETS forecast curves show growth, while LOESS produces trajectories with sharp bends, highlighting the nonlinear nature of the dynamics. At the Gavar sites, the forecasts are somewhat smoother, but the overall trend of high variability remains. Confidence intervals quickly widen and become disproportionately large, signaling low forecast stability. This behaviour aligns with the chemical properties of Mn, which, like Fe, participates actively in redox reactions and can significantly change its soil speciation (Mn^{2+}/Mn^{4+}) with minor pH shifts.

Regarding Cr, regional analysis also fails to produce stable forecast estimates. In all regions, LR shows sharp upward trends, ETS amplifies the growth trend, and LOESS highlights the strong nonlinearity of the time series. Predicted values quickly surpass observed levels, and confidence intervals expand substantially. This indicates Cr's valence instability and significant differences in the mobility and toxicity of its various forms, meaning even minor environmental changes can cause disproportionate concentration shifts.

Finally, V behaves similarly to Cr and Mn. Overall, the LR and ETS projections show a clear upward trend across all sites, with LOESS capturing sharp local variations. Confidence intervals widen quickly and peak at the end of the forecast, suggesting vanadium's dynamics are highly unpredictable. This pattern is consistent with its chemistry, which features a complex valence system and high redox sensitivity.

4. Conclusion

A comparison of forecasting methods revealed notable differences. LR was sensitive to directional shifts and best captured overall trends in regions with stable dynamics. However, under high variability, it often overestimated predictions. ETS proved effective at smoothing short-term fluctuations and providing more stable forecasts for elements with moderate reactivity, such as Zn and Cu. Yet this method does not accurately model systems with strong redox-dependent dynamics.

Using LOESS allowed the detection of local nonlinear features in the time series that parametric models miss. This method was especially useful for analyzing spatial differences, but its predictive stability diminishes with shorter time series, restricting its effectiveness for long-term forecasts.

The results indicated that regional forecasting provides clear and consistent estimates for chemically stable and complexing elements like Zn and Cu. However, for redox-sensitive elements such as Fe, Mn, Cr, and V, significant uncertainty persists even when using a spatial approach. This highlights the inherent limitations of time-based models in accurately representing elements whose concentrations are more influenced by changes in soil physicochemical conditions than by temporal variations.

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