

**COMBINATION OF MACHINE LEARNING AND
MULTIVARIATE GEOSTATISTICAL FRAMEWORKS FOR
MODELING ACID MINE DRAINAGE DRIVERS: HAVERI
AU-CU TAILINGS DEPOSIT**

By

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ORIGINALITY STATEMENT

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ABSTRACT

This thesis proposes a quantitative framework that combines multivariate geostatistics and machine learning to improve spatial prediction of acid mine drainage (AMD) drivers in a legacy tailings storage facility. The study focuses on the abandoned Haveri Au-Cu mine in southwest Finland, where historical drilling has produced a heterotopic dataset of borehole samples for ten elements, from which iron (Fe) and sulfur (S) are selected as primary AMD indicators because of their central role in sulfide oxidation and acid generation. The research design begins with exploratory data analysis, including construction of a correlation matrix to confirm the strong linear association between Fe and S and to assess their relationships with other elements. Ordinary co-kriging with related means (OCK-RM) is then adopted as the core multivariate framework, allowing explicit incorporation of a data-driven mean relationship between Fe and S into the co-kriging system. This relationship is inferred from collocated Fe-S pairs using a suite of linear machine-learning regressions—Linear Regression, Support Vector Regression, Ridge, Lasso, Elastic Net and Stochastic Gradient Regression—calibrated and compared under k-fold cross-validation. The selected regression model provides the coefficients that define the related-mean constraint in OCK-RM, which is implemented on a three-dimensional block model of the tailings using a linear model of coregionalization. The performance of the ML-enhanced OCK-RM variant will be benchmarked against conventional simple co-kriging and ordinary co-kriging using cross-validation statistics, reproduction of histograms and Fe-S correlations, QQ-plots, kriging variance maps and grade-tonnage curves for Fe and S. It is expected that integrating regression-based related means into OCK-RM will provide more stable estimates under heterotopic sampling, better preserve the Fe-S relationship at block support and yield more coherent spatial patterns of AMD risk than traditional co-kriging approaches, thereby offering a transferable methodology for environmental assessment in other tailings deposits.

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NOMENCLATURE

Acronym / Abbreviation	Full term / meaning
2D	Two-dimensional
3D	Three-dimensional
Ag	Silver
AMD	Acid Mine Drainage
As	Arsenic
Au	Gold
Au-Cu	Gold-copper
CNN-RNN	Convolutional Neural Network-Recurrent Neural Network
Co	Cobalt
COV	Coefficient of Variation
CRM	Critical Raw Material
Cu	Copper
CV	Cross-validation
ENR	Elastic Net Regression
Eq.	Equation
Fe	Iron
Fe²⁺	Ferrous iron
Fe³⁺	Ferric iron
Fig.	Figure
GC-RM	Gaussian Co-simulation with Related Mean
ilr	Isometric log-ratio
LC	Linear Correlation
LMC	Linear Model of Coregionalization
LOOCV	Leave-One-Out Cross-Validation
LR	Linear Regression
MAF	Minimum/Maximum Autocorrelation Factor
ML	Machine Learning
ML-OCK-RM	Machine Learning Ordinary Co-kriging with Related Mean
Ni	Nickel
NU	Nazarbayev University
OCK	Ordinary Co-kriging
OCK-RM	Ordinary Co-kriging with Related Mean
OCK-RM-ENR	Ordinary Co-kriging with Related Mean using Elastic Net Regression
OCK-RM-Lasso	Ordinary Co-kriging with Related Mean using Lasso Regression
OCK-RM-LR	Ordinary Co-kriging with Related Mean using Linear Regression
OCK-RM-Ridge	Ordinary Co-kriging with Related Mean using Ridge Regression
OCK-RM-SGR	Ordinary Co-kriging with Related Mean using Stochastic Gradient Regression

OCK-RM-SVR	Ordinary Co-kriging with Related Mean using Support Vector Regression
Pb	Lead
pH	Potential of hydrogen
Q-Q	Quantile-Quantile
R&D	Research and Development
RMSE	Root Mean Square Error
S	Sulfur
SCK	Simple Co-kriging
SGC-RM	Sequential Gaussian Co-simulation with Related Mean
SGD	Stochastic Gradient Descent
SGR	Stochastic Gradient Regression
SO₄²⁻	Sulfate ion
SVR	Support Vector Regression
TSF	Tailings Storage Facility
USGSIM	Universal Sequential Gaussian Simulation
Zn	Zinc

1. INTRODUCTION

1.1 Background/Problem Definition

Mine tailings represent one of the largest and most persistent waste streams generated by the mining industry, consisting of finely ground rock residues stored in tailings storage facilities (TSFs). These facilities collectively contain billions of tonnes of material that may still host economically interesting metal grades while simultaneously posing substantial environmental risks. Among these risks, acid mine drainage (AMD) is widely recognized as one of the most severe and long-lasting challenges. It arises primarily from the oxidation of sulfide minerals, especially pyrite (FeS_2), when exposed to oxygen and water. This process releases iron (Fe) and sulfur (S), generates sulfuric acid, and promotes the mobilization of potentially toxic elements into surrounding soils and water bodies. As a result, Fe and S are key geochemical indicators for assessing AMD potential and designing monitoring and remediation programs in legacy TSFs.

Robust spatial modeling of Fe and S in tailings is therefore essential for predicting AMD occurrence and delineating zones of elevated environmental risk. Geostatistical methods, particularly kriging and co-kriging, provide a principled framework for incorporating spatial autocorrelation and multivariate relationships when interpolating between sample locations. In multivariate settings, co-kriging enables joint modeling of several correlated variables, which is especially useful in heterotopic sampling scenarios where primary and secondary variables are not measured at identical locations—a common situation in historical or legacy tailings datasets. However, conventional co-kriging approaches such as simple co-kriging (SCK) and ordinary co-kriging (OCK) face limitations when data are sparse, heterotopic, or preferentially sampled. SCK is sensitive to assumptions about the global mean, whereas OCK can become numerically unstable or biased in the absence of sufficient primary data near the estimation location.

Ordinary co-kriging with related mean (OCK-RM) has been proposed as a more robust alternative that explicitly models the mean relationship between variables rather than assuming known mean values. In OCK-RM, the unknown means of the primary and secondary variables are linked through a regression model, which is then embedded into the co-kriging system. This approach has shown promise in various mining and environmental applications, particularly where secondary variables are more densely sampled or where physically meaningful relationships between variables exist. Nonetheless, most existing implementations of OCK-RM

rely on simple linear regression to describe the related means. While convenient, this choice can be restrictive in geoscientific datasets, which often exhibit nonlinearity, heteroscedasticity, multicollinearity, and outliers.

Machine learning (ML) regression methods offer a flexible alternative for modeling such relationships. Techniques such as Support Vector Regression, Elastic Net, Lasso, Ridge, Stochastic Gradient Descent, and classical Linear Regression provide different forms of regularization and robustness that can improve generalization, especially when data are noisy or unevenly distributed. Integrating these ML approaches into an OCK-RM framework has the potential to yield more accurate mean estimates, enhance multivariate consistency, and improve the spatial prediction of AMD-related variables.

The Haveri Au-Cu tailings in Finland provide a suitable case study for investigating this integration. The dataset exhibits a strong correlation between Fe and S, along with partial sampling overlap and heterotopic patterns typical of legacy TSFs. This context is ideal for testing whether a machine learning-enhanced OCK-RM framework can outperform standard geostatistical approaches in modeling AMD drivers and supporting environmental risk mapping.

Although geostatistical co-kriging frameworks are widely used for multivariate modeling in mining and environmental applications, their performance is often constrained by the quality of the assumed mean structure and the nature of the sampling design. Simple co-kriging assumes a known, constant mean, which is rarely realistic in complex tailings deposits and can introduce bias when the mean is misspecified. Ordinary co-kriging relaxes this assumption but might produce unstable weights and unreliable estimates under heterotopic and preferential sampling, conditions that are common in legacy TSFs where sampling campaigns were not originally designed for environmental modeling.

In order to solve the problem of failing OCK in some neighborhoods, OCK-RM addresses these challenges by explicitly incorporating a related mean relationship between the variables, typically using simple linear regression. However, in datasets characterized by nonlinearity, heteroscedasticity, and noises such as Fe and S in AMD-prone tailings-the linear regression assumption may be inadequate to capture the true mean dependency. This can result in suboptimal integration of secondary information, reduced predictive accuracy, and limited improvement over conventional OCK or SCK.

At present, practitioners lack a systematic, case-study-based framework that combines multivariate geostatistics with a suite of machine learning regression techniques to model the related means within OCK-RM. In particular, there is limited evidence on how different ML regression models perform when embedded in OCK-RM, how they affect spatial predictions and uncertainty quantification for AMD drivers, and whether the resulting models offer tangible advantages for environmental risk mapping in tailings facilities.

In the context of the Haveri Au-Cu tailings, where Fe and S are critical AMD indicators and exhibit strong yet potentially complex relationships, it remains unclear which regression strategy should be adopted to infer the related means and how this choice influences the performance of co-kriging-based spatial models. Consequently, there is a clear need for a systematic evaluation of ML-enhanced OCK-RM against conventional approaches, with a focus on both predictive accuracy and practical usefulness for AMD-oriented decision-making.

1.2 Objectives of the Thesis

1.2.1 Main Objectives

The primary aim of this thesis is to develop and evaluate a framework that combines machine learning regression with multivariate geostatistical modeling—specifically, ordinary co-kriging with related mean-for spatial prediction of acid mine drainage drivers in the Haveri Au-Cu tailings. The work focuses on Fe and S as key AMD-related variables and seeks to determine whether ML-assisted OCK-RM can improve spatial prediction and uncertainty characterization relative to conventional co-kriging approaches.

1.2.2 Specific Objectives

The successful completion of the following sub-objectives is fundamental within the scope of this thesis:

- To conduct a comprehensive literature review on acid mine drainage in tailings, multivariate geostatistics (with emphasis on co-kriging and OCK-RM), and machine learning regression methods relevant to geoscientific applications.
- To perform exploratory data analysis of the Haveri Au-Cu tailings dataset, characterize the spatial distribution and correlation structure of Fe and S, and assess heterotopic and preferential sampling patterns.

- To construct appropriate variogram and cross-variogram models for Fe and S and establish a multivariate geostatistical framework suitable for AMD-focused spatial modeling in the Haveri TSF.
- To implement and compare six regression techniques-Support Vector Regression, Elastic Net, Lasso, Ridge, Stochastic Gradient Descent, and Linear Regression-for inferring the mean relationship between Fe and S, using performance metrics such as root mean square error (RMSE) and linear correlation (LC) under cross-validation.
- To integrate the best-performing regression model(s) into the OCK-RM framework and generate spatial predictions for Fe and S, producing block-model outputs suitable for AMD risk assessment.
- To compare the performance of machine learning-enhanced OCK-RM against conventional co-kriging approaches (e.g., SCK and classical OCK, and where appropriate OCK-RM with simple linear regression) in terms of histogram reproduction, spatial continuity, cross-correlation, prediction accuracy, and uncertainty patterns.

1.3 Hypotheses

It is hypothesized that replacing simple linear regression with machine learning regression methods within the OCK-RM framework will lead to a more accurate and robust characterization of the mean relationship between Fe and S in the Haveri Au-Cu tailings. Specifically, it is expected that one or more ML regression models will exhibit lower RMSE and higher linear correlation in cross-validation compared to simple linear regression, thereby providing a more reliable basis for the related mean constraint.

Furthermore, it is anticipated that integrating the best-performing machine learning regression model into OCK-RM will improve the spatial prediction of Fe and S relative to conventional co-kriging approaches. The ML-enhanced OCK-RM is expected to better reproduce key statistical properties (such as histograms, variances, and cross-correlations) and spatial continuity, while also yielding more coherent uncertainty patterns and more informative AMD risk maps. Consequently, the combined ML-geostatistical framework is hypothesized to offer a practical and methodologically sound improvement for multivariate AMD modeling in legacy tailings facilities.

1.4 Justification of the R&D

Kazakhstan, as one of the world's leading mining nations, hosts numerous legacy and active tailings storage facilities that pose potential environmental risks, including acid mine drainage (AMD). Ensuring the safe management and rehabilitation of these sites is a strategic priority for sustainable resource development and environmental protection in the country. Consequently, advanced and reliable methods for assessing AMD potential are essential for supporting responsible mining practices and aligning with national and international environmental standards.

Accurate spatial modeling of AMD drivers in tailings deposits is crucial for modern mining practice and environmental management. Reliable predictions of Fe and S distributions underpin the assessment of AMD potential, the design of monitoring networks, the prioritization of remediation efforts, and the evaluation of reprocessing opportunities in legacy TSFs. As regulatory requirements tighten and societal expectations regarding environmental stewardship increase, mining companies and authorities require modeling approaches that are both scientifically rigorous and operationally efficient.

The integration of machine learning regression into an OCK-RM framework directly addresses several practical challenges encountered in tailings modeling. By providing a more flexible and robust means of capturing relationships between Fe and S under heterotopic and preferential sampling, the proposed framework has the potential to improve the quality of spatial predictions and associated uncertainty estimates. This, in turn, can lead to more accurate delineation of high-risk AMD zones, better targeting of field investigations, and more informed decisions about mitigation strategies and long-term closure planning.

From an industry perspective, the methodology developed in this thesis offers a generalizable template for combining multivariate geostatistics and machine learning in other tailings facilities or waste storage contexts. Beyond AMD, similar approaches could be used to model multi-element contamination plumes, reprocessing targets, or geometallurgical indicators. Thus, the outcomes of this work provide both site-specific insights for the Haveri Au–Cu tailings and broader methodological contributions that can enhance environmental risk management across a range of mining operations, including those in Kazakhstan.

1.5 Scope of Work

This thesis focuses on the development and application of a machine learning-integrated OCK-RM framework for modeling AMD-related variables in the Haveri Au-Cu tailings. The study is restricted to two key variables, Fe and S, which are directly linked to pyrite oxidation and AMD generation. The analysis is based on the available Haveri tailings dataset, characterized by spatially distributed borehole samples with partial overlap and heterotopic sampling patterns.

The work begins with data preparation and exploratory analysis, including the examination of univariate statistics, spatial trends, and Fe-S correlations. Variogram and cross-variogram models are then constructed to describe the spatial continuity and multivariate structure of Fe and S.

Subsequently, six machine learning regression methods-Support Vector Regression, Elastic Net, Lasso, Ridge, Stochastic Gradient Descent, and Linear Regression-are implemented to infer the mean relationship between Fe and S. Their performance is evaluated through cross-validation using metrics such as RMSE and linear correlation, and the most suitable model(s) are selected for integration into the OCK-RM framework.

The chosen ML-based related mean model is then embedded within OCK-RM to produce spatial predictions and block-model outputs for Fe and S in the Haveri TSF. For comparison, conventional co-kriging approaches (SCK, OCK, and where feasible OCK-RM with simple linear regression) are also implemented using consistent variogram models, search parameters, and block configurations. The resulting models are assessed in terms of statistical reproduction, spatial continuity, cross-correlations, prediction accuracy, and uncertainty patterns, with particular emphasis on their implications for AMD risk mapping.

The scope of the thesis is limited to the available drilling data, two AMD-related variables, and a single tailings facility. Hydrogeological processes, reactive transport modeling, and detailed geochemical speciation are beyond the scope of this work and are not explicitly modeled. Instead, the emphasis is placed on improving the geostatistical representation of Fe and S as primary AMD indicators through the combined use of multivariate geostatistics and machine learning regression.

2. LITERATURE REVIEW

2.1 Acid mine drainage in sulfidic mine tailings

Acid mine drainage (AMD) arises primarily from the oxidative weathering of sulfide minerals, most notably pyrite (FeS_2), when mine wastes are exposed to oxygen and water. Pyrite oxidation releases Fe and sulfate, generates acidity, and promotes the dissolution and mobilization of trace metals and metalloids into surrounding soils and waters (Blowes et al., 2014; Nordstrom, 2011; Rimstidt et al., 2003). Comprehensive reviews of sulfide mine tailings emphasize that Fe- and S-bearing minerals control both acidity generation and secondary mineral formation, which in turn govern the speciation, sorption, and long-term mobility of contaminants.

Case studies from Nordic sulfidic tailings show that AMD development is strongly site-specific, depending on mineralogy, neutralizing capacity, hydrological setting, and tailings deposition history. Heikkinen et al. (2009) contrasted neutral mine drainage at low-sulfide, carbonate-bearing tailings with classic AMD at high-sulfide, multi-metal tailings, highlighting the role of pyrite abundance, grain size, and oxidation fronts in producing low-pH, Fe- and SO_4 -rich seepage with elevated Cu, Zn, Ni, and other metals. Global reviews of acid rock and mine drainage prediction synthesize a range of static and kinetic tests but stress that accurate long-term prediction remains difficult, especially where heterogeneous tailings stratigraphy and changing hydrological conditions alter reaction pathways over time.

At the abandoned Haveri Au-Cu mine in southwest Finland, Parviainen (2009) documented tailings mineralogy, geochemistry, and drainage water composition, showing that oxidation of Fe-sulfides in the upper tailings layers produces acidic, metal-bearing waters while deeper, less oxidized zones retain reactive sulfide and secondary Fe phases. The study demonstrated that Fe and S distributions within the tailings are tightly linked to sulfide oxidation fronts, secondary Fe(oxyhydr)oxide formation, and the spatial pattern of dissolved metals in seepage. This supports the view that Fe and S can be treated as first-order geochemical indicators of AMD risk, and that their spatial variability must be quantified to assess current and future contamination loads.

Recent reviews of AMD characterization and remediation reinforce this conclusion: Fe and sulfate concentrations, together with pH, are widely used as operational indicators of AMD severity and for monitoring treatment performance.

2.2 Geostatistical modeling of tailings deposits and AMD-related indicators

Geostatistical modelling has become central to evaluating both resource potential and environmental risk in TSFs. Early work on legacy tailings focused on reconstructing remaining metal inventories and assessing reprocessing potential. For the Haveri tailings, Parviainen et al (2020) combined historical drilling data with three-dimensional block modelling to estimate Au, Cu, and Co resources, highlighting the strong vertical and lateral heterogeneity created by decades of slurry deposition and processing changes. This work already underlined that tailings should be treated as complex, stratified deposits rather than homogeneous waste volumes.

Subsequent studies have extended geostatistical methods to capture both economic and environmental aspects of tailings. Blannin et al. (2023) modelled the Davidschacht tailings in Germany using universal sequential Gaussian simulation (USGSIM) to account for strong spatial trends and anisotropy in Zn, Pb, Cu, In and associated elements. Their results showed that robust three-dimensional models of grades, porosity, and bulk density can support simultaneous assessment of remaining metal resources and zones of elevated environmental risk. A follow-up study proposed a sampling protocol for CRMs in TSFs, demonstrating that geostatistical simulations can guide efficient sampling strategies and resource classification in highly heterogeneous tailings bodies.

Karacan et al. (2023) developed a compositional geostatistical framework for the Katherine Mine tailings in Arizona, combining compositional data analysis, isometric log-ratio transformation, and minimum/maximum autocorrelation factor (MAF) transformation with sequential Gaussian simulation. This approach allowed the joint modelling of valuable and hazardous elements and yielded probabilistic tonnage and grade distributions, emphasizing that multielement and compositional nature of tailings must be taken into account when assessing both resource potential and environmental hazards.

Beyond individual case studies, recent systematic reviews synthesize the role of geostatistical models in tailings revalorization and risk assessment. Cotrina-Teatino et al. (2025) reviewed geostatistical models, recovery strategies, and economic evaluations in mine tailings, identifying three main themes: resource estimation, reprocessing and recovery, and integrated techno-economic assessment. Their review stresses that spatial variability and uncertainty are critical drivers of both technical feasibility and economic outcomes, and that geostatistical models are increasingly used as the backbone for scenario analysis.

However, most tailings-focused geostatistical studies concentrate on resource variables (e.g., Au, Cu, Co, Zn) and only indirectly address AMD-related indicators. While some include Fe or S among modelled elements, they rarely treat them as primary geochemical drivers for spatial AMD risk mapping, and uncertainty analysis is typically framed in terms of metal grades rather than acid-generation potential. Moreover, geostatistical workflows often remain univariate or compositional rather than fully multivariate in the sense of explicitly preserving cross-covariance structures between AMD drivers and associated elements at block support.

2.3 Multivariate geostatistics and co-kriging in environmental and geometallurgical applications

Multivariate geostatistics extends univariate modelling by explicitly representing spatial cross-dependence between two or more variables. The key construct is the linear model of coregionalization (LMC), which expresses all direct and cross-variograms as linear combinations of common basic structures with positive semi-definite sill matrices. This framework underpins classical co-kriging and Gaussian co-simulation algorithms, allowing the joint interpolation or simulation of several variables while preserving their covariance structure at the scale of interest (e.g., block support).

In environmental and geometallurgical contexts, multivariate geostatistics is often combined with transformation strategies tailored to geochemical data. For multi-element compositions subject to constant-sum constraints, log-ratio transformations and MAF decomposition have been used to decorrelate variables prior to Gaussian simulation, with inverse transforms applied afterward to recover original units. The workflow implemented at the Katherine Mine tailings by Karacan et al. (2023) is a prominent example: compositional clustering, *ilr* transformation, MAF rotation, and sequential Gaussian simulation were used to model both valuable metals and hazardous elements jointly, yielding realistic realizations of multi-element distributions and their uncertainty.

Recent multivariate developments also focus on domain transitions and soft geological boundaries. Ekolle-Essoh et al. (2022) proposed a multivariate Matérn correlation model for resource estimation in a multi-unit iron ore deposit, fitting direct and cross-variograms of several elements simultaneously and enforcing smooth transitions across domain boundaries. Their work shows that a properly specified multivariate covariance model can handle structural

complexity more naturally than separate univariate models joined by hard boundaries. In geometallurgical applications, Maleki, Madani, and Emery (2014) studied capping and kriging strategies for long-tailed grade distributions, highlighting how multivariate settings aggravate robustness issues and require careful treatment of outliers and extreme values.

Despite these advances, multivariate geostatistics has been applied only sparingly to AMD-specific variables. Most multivariate case studies either target economic metals (e.g., Cu-Mo systems, multi-element iron ore) or combine metals and environmental indicators without explicitly focusing on acid-generation processes. While covariance-preserving co-kriging and co-simulation frameworks are available in theory, in practice AMD-related studies often revert to univariate kriging of Fe, SO₄ or pH, or interpret AMD controls qualitatively from geochemical trends rather than from fully multivariate spatial models.

2.4 Ordinary co-kriging with related means (OCK-RM)

Ordinary co-kriging (OCK) is widely used for modelling coregionalized variables because it does not require prior knowledge of the global mean. However, under heterotopic sampling—where primary and secondary variables are not collocated—the OCK system can become unstable or even unsolvable when local data configurations provide insufficient primary information. This issue is exacerbated by preferential sampling designs that cluster data in zones of interest and leave large regions poorly informed about the primary variable.

Emery (2012) introduced a variant known as co-kriging with related means, in which the unknown mean values of each variable are constrained to satisfy a set of linear relationships with known coefficients. In the OCK-RM formulation, the mean of the primary variable is expressed as a linear function of the secondary means, reflecting prior knowledge or empirically fitted relationships between variables. This additional structure stabilizes the co-kriging system in heterotopic settings and ensures that the mean behaviour of the variables remains consistent with their known or inferred relationships, especially where secondary variables are more densely sampled.

OCK-RM has been applied in several geoscientific contexts. Emery (2012) illustrated its use in systems where soluble and total copper grades are related through known linear coefficients, showing that OCK-RM yields less biased and more geologically consistent estimates than

conventional OCK. Adeli et al. (2021) extended the concept to metallurgical recovery, a non-additive response defined as the ratio of metal mass in concentrate to metal mass in feed. Their methodology cokriges additive metal masses while constraining the means via a related-mean structure, thereby accounting simultaneously for non-additivity and preferential sampling in recovery prediction. Ekolle-Essoh et al. (2022) embedded an OCK-RM-type relationship within a multivariate Matérn model for iron ore grades in Nkout, Cameroon, using related means to ensure continuity of mean grade across soft boundaries between geological units.

Across these applications, the mean relationships have typically been inferred using simple linear regression or specified a priori from geological or process knowledge. While this is sufficient when relationships are approximately linear and data are abundant, it may be suboptimal in complex geochemical systems with nonlinearity, heteroscedasticity, or outliers. In such cases, mis-specified mean relationships can propagate bias throughout the OCK-RM system and reduce the benefit of using secondary variables.

2.5 Machine learning regression in geochemistry, tailings and environmental modelling

Machine learning (ML) has rapidly gained prominence in geosciences for tasks ranging from lithological classification to geochemical mapping, water-quality prediction, and mineral prospectivity analysis. A comprehensive review by He et al. (2022) shows that supervised ML methods-including support vector machines, random forests, gradient boosting, and neural networks-are now widely used to model complex, nonlinear relationships in geochemical datasets, often outperforming classical linear regression in predictive accuracy and robustness to multicollinearity.

In regional geochemical mapping, Kirkwood et al. (2016) applied quantile regression forests to predict soil element concentrations, loss on ignition, and pH from high-resolution geophysical and remote-sensing data, finding that ML-based predictions generally improved on ordinary kriging, particularly for immobile elements with strong relationships to auxiliary variables. Zhang et al. (2021) used multiple ML algorithms to predict trace element concentrations from major and minor element data in the Karoo large igneous province, demonstrating that ML can accurately capture complex geochemical relationships without strict distributional assumptions and can use residuals to delineate geochemical anomalies for prospectivity mapping.

In tailings and resource estimation, ML has only recently begun to complement or compete with geostatistical approaches. Cotrina-Teatino et al. (2025) developed a data-driven ML framework to estimate silver resources in the Quiulacocha tailings deposit in Peru, comparing random forest and extreme gradient boosting models with ordinary kriging. Their results showed that ML can better identify high-grade zones and balance tonnage and metal content in low-continuity settings, although they relied on ML as a direct surrogate for spatial interpolation rather than as a component of a co-kriging system. Anvari et al. (2025) proposed a hybrid geostatistical-deep learning framework for modelling the geochemical composition of historical mine tailings, where kriging-derived covariance information is fed into a CNN-RNN architecture to learn nonlinear dependencies, illustrating how ML can be coupled with geostatistics at the level of spatial features.

Beyond solid tailings, ML regression has been used to predict water chemistry, including major and trace elements and water contents, from geochemical or spectral predictors, further demonstrating the flexibility of methods such as random forests, support vector regression, and gradient-based ensembles in environmental applications. Nevertheless, most of these applications treat ML as an alternative to kriging—either mapping target variables directly or providing auxiliary predictions that are then mapped using geostatistics. Only a few recent studies explicitly integrate ML outputs with geostatistical models in a tightly coupled way, for example by using kriging to augment sparse data before ML-based clustering.

2.6 Research gaps and positioning of the present study

The literature reviewed above suggests a progressive convergence of three strands: (i) detailed AMD geochemistry and tailings characterization, (ii) multivariate and block-support geostatistical modelling, and (iii) flexible machine learning regression. Yet these strands have rarely been fully integrated in a single framework focused on AMD drivers in legacy tailings. AMD studies emphasise Fe and S as key geochemical indicators but typically rely on point-scale monitoring and univariate analysis. Tailings geostatistics increasingly capture multielement variability and uncertainty but seldom elevate AMD drivers to primary modelling targets, and are often formulated as univariate or compositional simulations rather than as coregionalized systems at block support.

Within multivariate geostatistics, OCK-RM offers a principled way to stabilize co-kriging in heterotopic or preferential sampling settings by imposing related-mean constraints, but existing applications rely almost exclusively on simple linear regression or fixed linear relationships to specify those means. At the same time, ML regression has proven its value in capturing complex geochemical relationships and improving prediction accuracy in both regional mapping and tailings resource estimation, yet it is usually deployed as a stand-alone predictor or as an input to post-hoc spatial modelling, rather than as an internal component of the co-kriging system.

This thesis is positioned at the intersection of these gaps. By focusing on Fe and S as AMD drivers in the Haveri Au-Cu tailings, it deploys a multivariate OCK-RM framework specifically tailored to AMD-relevant variables under heterotopic sampling.

3. METHODOLOGY

3.1 Overall research design

This thesis adopts a quantitative, case-study-based research design that integrates multivariate geostatistics and supervised machine learning to model acid mine drainage (AMD) drivers in the Haveri Au-Cu tailings. The main objective is to develop and apply a workflow in which ordinary co-kriging with related means (OCK-RM) is coupled with regression models to define the mean relationship between iron (Fe) and sulfur (S), and to use this framework to obtain spatial predictions of these AMD-related variables under heterotopic sampling conditions. The methodology follows the same conceptual basis as the article on which this work is built, but it is extended and formalized for thesis-level application.

- 1) The Haveri tailings dataset is compiled, cleaned and prepared for analysis, with Fe and S selected as the primary modelling variables.
- 2) Exploratory data analysis is carried out, including the construction of a correlation matrix to verify the strength of the Fe-S relationship and to examine correlations with other available variables.
- 3) The OCK-RM framework is specified at the theoretical level, including the way linear mean constraints are incorporated in the cokriging system.
- 4) Several regression models are tuned and compared to infer the mean relationship between Fe and S from the data.
- 5) The regression results are embedded in the OCK-RM system, which is then used to perform spatial estimation of Fe and S over a three-dimensional block model of the tailings deposit.
- 6) Cross-validation and error analysis are used to evaluate the predictive performance of the combined ML-OCK-RM workflow.

3.2 Data, variables and exploratory analysis

The empirical basis of the research is a drillhole dataset from the former Haveri Au-Cu mine tailings in southwest Finland. The tailings are a legacy deposit formed by historical processing of Au-Cu ores and now consist of a stratified and partially oxidised mass in which pyrite and other sulfide minerals have undergone varying degrees of weathering. Sampling campaigns have produced downhole geochemical data at numerous locations within the TSF.

Exploratory data analysis is carried out on the cleaned database. For Fe and S, basic descriptive statistics are calculated, including means, variances, quantiles and measures of skewness and kurtosis, in order to characterize the marginal distributions. Spatial plots in plan view and in vertical sections are used to obtain a qualitative impression of grade patterns, possible trends and any obvious zonation within the tailings deposit.

An important methodological step in this exploratory phase is the construction of a correlation matrix. Using only the subset of data where Fe and S (and other elements, where available) are measured at the same locations, a standard Pearson correlation matrix is computed. This matrix quantifies the linear correlation between Fe and S and between each of these variables and other elements. The matrix is used to confirm, in a reproducible way, that the Fe-S correlation is sufficiently strong to justify joint multivariate modelling and the imposition of a related-mean structure in OCK-RM. It is also used to screen other variables for possible future inclusion as auxiliary variables, although the core methodology in this thesis remains focused on Fe and S.

3.3 Theoretical framework of OCK-RM

Following Emery (2012), the starting point is a second-order stationary multivariate random field with $\mathbf{N}$ real-valued components defined on $\mathbb{R}^d$. This field is written as $\mathbf{Z} = (\mathbf{Z}_1, \mathbf{Z}_2, \dots, \mathbf{Z}_N)^T$, with a constant mean vector $\mathbf{m} = (\mathbf{m}_1, \mathbf{m}_2, \dots, \mathbf{m}_N)^T$ and a matrix-valued covariance function $\mathbf{C}(\mathbf{h}) = (\mathbf{C}_{ij}(\mathbf{h}))$, where each $\mathbf{C}_{ij}(\mathbf{h})$ denotes the covariance between components $\mathbf{Z}_i$ and $\mathbf{Z}_j$ separated by lag $\mathbf{h} \in \mathbb{R}^d$.

The components of the mean vector are assumed to satisfy a system of $\mathbf{K}$ linear constraints of the form:

$$\sum_{i=1}^N \mathbf{a}_{k,i} \mathbf{m}_i = \mathbf{b}_k, \text{ for } k = 1, \dots, K \quad (1)$$

where $\mathbf{b} = (\mathbf{b}_1, \dots, \mathbf{b}_K)^T \in \mathbb{R}^d$ is a known vector in $\mathbb{R}^K$ and $\mathbf{A} = (\mathbf{a}_{k,i})$ is a $K \times N$ matrix of rank $\mathbf{K}$. Because the rows of $\mathbf{A}$ are linearly independent, the constraint system is consistent and non-redundant.

After a possible reordering of the variables, these constraints can be written compactly as:

$$\mathbf{A}\mathbf{m} = \mathbf{b} \quad (2)$$

The matrix $\mathbf{A}$ is then partitioned into two submatrices: $\mathbf{A}_1 \in \mathbb{R}^{K \times (N-K)}$ and $\mathbf{A}_2 \in \mathbb{R}^{K \times K}$, so that $\mathbf{A} = [\mathbf{A}_1, \mathbf{A}_2]$. Without loss of generality, the right-hand side can be shifted to zero by redefining the random field with a vector $\boldsymbol{\delta}$ that satisfies $\mathbf{A}\boldsymbol{\delta} = \mathbf{B}$. Under this zero-mean constraint, the last K components of the mean vector, $\mathbf{m}_2$, can be written as a linear function of the first $N - K$ components, $\mathbf{m}_1$:

$$\mathbf{m}_2 = \boldsymbol{\Omega} \mathbf{m}_1 \quad (3)$$

where the transformation matrix is $\boldsymbol{\Omega} = -\mathbf{A}_2^{-1} \mathbf{A}_1$. The full mean vector can therefore be expressed as:

$$\mathbf{m} = \mathbf{F} \mathbf{m}_1, \text{ with } \mathbf{F} = \begin{pmatrix} \mathbf{I}_{N-K} \\ \boldsymbol{\Omega} \end{pmatrix} \quad (4)$$

and, $\mathbf{I}_{N-K}$ the $(N - K) \times (N - K)$ identity matrix. This representation shows that the number of independent mean components is reduced from N to $N - K$, in agreement with the number of independent constraints.

The goal is to estimate the value of the multivariate field $\mathbf{Z}$ at some unsampled location $\mathbf{x}_0 \in \mathbb{R}^d$, using measurements of its components at locations $\mathbf{x}_a$. Consider, in particular, a partially heterotopic sampling configuration with two variables ($N = 2$), where $\mathbf{Z}_1$ and $\mathbf{Z}_2$ are observed at partially overlapping sets of points, with some positions common to both. In this configuration, the cokriging estimator of the i -th component at $\mathbf{x}_0$ ($i = 1, 2$) is written as a linear combination of all available observations of both variables,

$$\mathbf{Z}_i^*(\mathbf{x}_0) = \sum_{a_1=1}^{n_1} \lambda_{a_1}^{(i,1)}(\mathbf{x}_0) \mathbf{Z}_1(\mathbf{x}_{a_1}) + \sum_{a_2=1}^{n_2} \lambda_{a_2}^{(i,2)}(\mathbf{x}_0) \mathbf{Z}_2(\mathbf{x}_{a_2}) \quad (5)$$

Where $\lambda_{a_j}^{(i,j)}(\mathbf{x}_0)$ are scalar weights associated with the contribution of variable j to the estimation of component i at location $\mathbf{x}_0$. These weights are obtained by solving the cokriging system.

The expected value of the estimation error can be written as

$$\mathbf{E}\{\mathbf{Z}^*(\mathbf{x}_0) - \mathbf{Z}(\mathbf{x}_0)\} = (\sum_{a=1}^n \boldsymbol{\Lambda}_a^T - \mathbf{I}_N) \mathbf{m} = (\sum_{a=1}^n \boldsymbol{\Lambda}_a^T - \mathbf{I}_N) \mathbf{F} \mathbf{m}_1 \quad (6)$$

with $\mathbf{I}_N$ the $N \times N$ identity matrix and Λ_a the weight matrices. Because the vector $\mathbf{m}_1$ contains free mean components that can take any real value, the only way to guarantee an unbiased estimator (zero expected error for any admissible $\mathbf{m}_1$) is to impose

$$(\sum_{a=1}^n \lambda_a^T - \mathbf{I}_N) \mathbf{F} = \mathbf{0} \quad (7)$$

The estimates are obtained by minimizing the prediction error variances for each component of $\mathbf{Z}$, subject to this unbiasedness condition. After the usual derivations, this leads to a linear system of the form

$$\begin{pmatrix} \mathbf{C}(\mathbf{x}_1 - \mathbf{x}_1) & \dots & \mathbf{C}(\mathbf{x}_1 - \mathbf{x}_n) & \mathbf{F} \\ \vdots & \ddots & \vdots & \vdots \\ \mathbf{C}(\mathbf{x}_n - \mathbf{x}_1) & \dots & \mathbf{C}(\mathbf{x}_n - \mathbf{x}_n) & \mathbf{F} \\ \mathbf{F}^T & \dots & \mathbf{F}^T & 0 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_n \\ \mathbf{M} \end{pmatrix} = \begin{pmatrix} \mathbf{C}(\mathbf{x}_1 - \mathbf{x}_0) \\ \vdots \\ \mathbf{C}(\mathbf{x}_n - \mathbf{x}_0) \\ \mathbf{F}^T \end{pmatrix} \quad (8)$$

where the λ_a are vectors of cokriging weights and $\mathbf{M}$ gathers the Lagrange multipliers associated with the related-mean constraints.

The variance-covariance matrix of the prediction error, Σ , is defined as the expectation of the outer product of the estimation error and is given by

$$\Sigma = \mathbf{C}(\mathbf{x}_0 - \mathbf{x}_0) - \sum_{a=1}^n \Lambda_a^T [\mathbf{C}(\mathbf{x}_a - \mathbf{x}_0) + \mathbf{F} \mathbf{M}] \quad (9)$$

Within this framework, the central aim of the study is to establish the relationship between the unknown mean values of the variables so that the matrix F in equation (8) can be specified and used to implement OCK-RM. For the case of two variables Z_1 and Z_2 , the link between m_1 and m_2 can be inferred via a regression model in which, for example, Z_2 is expressed as a function of Z_1 , or vice versa. Earlier applications have typically relied on a simple linear regression model for this purpose, as in Emery (2012) and Adeli et al. (2021).

3.4 Machine learning regression for related means

To infer the related-mean relationship between Fe and S, several regression techniques are applied to the collocated subset of the dataset. The goal is to estimate a linear mapping from one variable to the other at the mean level, in a way that is robust to noise, heterotopy and potential outliers. The generic formulation assumes that one variable, say S, can be expressed as a function of Fe through a linear model plus residual noise. This does not imply that the pointwise relationship between Fe and S is perfectly linear, but it provides a pragmatic representation of the relationship between their mean values as required by OCK-RM.

The collocated data are first standardized or scaled if needed by the algorithms, while preserving interpretability of the regression coefficients. The dataset is then partitioned using a k-fold cross-validation scheme. For each fold, a subset of the data is held out for validation, and the regression models are trained on the remaining observations. The thesis considers a set of models that includes ordinary Linear Regression, Support Vector Regression, Elastic Net Regression, Lasso Regression, Ridge Regression and Stochastic Gradient Regression. Each model is configured so that the mapping is linear in the input features; what distinguishes them is how they regularize coefficients, handle noisy data and scale computationally.

Hyperparameters for each model are tuned within the cross-validation framework using simple search strategies. For each fold and model, predictions are generated for the validation subset, and performance is quantified by the root mean square error and the linear correlation between observed and predicted values. These metrics provide a consistent basis for comparing models. The model that provides the best compromise between low error, high correlation and stable, interpretable coefficients is selected as the preferred estimator of the mean relationship between Fe and S. Its fitted coefficients (intercept and slope) are then used to define the elements of the transformation matrix F in the OCK-RM system.

3.5 Geostatistical implementation

Once the OCK-RM framework and the regression-based mean relationship are specified, the geostatistical implementation proceeds through a series of steps. The first is variogram analysis. Experimental direct variograms are computed for Fe and S using the legacy dataset, and an experimental cross-variogram is computed for the Fe-S pair. On the basis of these experimental structures, a linear model of coregionalization is fitted that reproduces the main features of the direct and cross-variograms while remaining positive semi-definite.

In parallel, a three-dimensional block model is defined to cover the entire tailings volume. The horizontal and vertical block dimensions are chosen according to drilling density, tailings geometry and the spatial resolution required for AMD-related interpretations. Each block centroid is taken as an estimation location. For each centroid, a search neighborhood is defined as an anisotropic ellipsoid aligned with the principal continuity directions inferred from variography. The search radii, maximum number of samples per variable and any constraints on the number of drillholes are specified as a priori and may be adjusted iteratively based on

cross-validation performance and computational considerations. Minimum data requirements are set so that estimates are produced only where sufficient data support exists.

The OCK-RM estimation procedure is then applied at each block centroid. For a given location, all Fe and S data within the neighborhood are extracted. The regression coefficients derived in the previous stage are used to construct the transformation matrix F that links the mean of S to the mean of Fe (or vice versa, depending on the chosen parametrisation). Using the LMC, the covariance terms between all pairs of data and between data and the estimation location are computed. These covariance values, together with the matrix $\mathbf{F}$, are assembled into the OCK-RM system of equations. The system is solved to obtain the co-kriging weights and the associated Lagrange multipliers, and the estimated Fe and S grades at the block centroid are computed as weighted sums of the nearby sample values. At the same time, the prediction error covariance matrix is calculated, providing local measures of uncertainty for Fe and S.

This procedure is repeated for all blocks in the model grid. The result is a coherent set of block estimates and associated uncertainties for Fe and S that jointly honor the observed data, the fitted covariance structure and the regression-based related-mean constraint.

3.6 Validation and methodological assessment

The methodology is evaluated at two levels: the regression component used to define related means and the OCK-RM spatial predictions. For the regression models, validation is inherently built into the k-fold cross-validation procedure described earlier. The distribution of errors across folds and the consistency of performance metrics guide the selection of the final model.

For the OCK-RM model, cross-validation is conducted at the sample locations. In a leave-one-out or k-fold scheme, individual samples or groups of samples are temporarily removed, Fe and S are re-estimated at those locations using the remaining data, and the differences between estimated and observed values are recorded. From these differences, mean errors, root mean square errors and standardised errors are computed for both Fe and S. These statistics are used to assess bias, overall accuracy and the coherence between prediction errors and the kriging variances.

From a methodological point of view, the proposed workflow has clear advantages. It explicitly exploits the strong correlation between Fe and S revealed by the correlation matrix, it embeds

a data-driven mean relationship into the co-kriging system rather than assuming one, and it maintains the multivariate spatial structure through a valid LMC. At the same time, it relies on assumptions of second-order stationarity and linear related means, and its success depends on the availability of sufficient data to fit variograms and train regression models.

4. RESULTS

4.1 Exploratory data analysis

The dataset used in this study originates from the Haveri Au–Cu tailings storage facility (TSF) located in southwestern Finland (Figure 1) and comprises borehole samples for ten elements: Zn (ppm), S (%), Pb (ppm), Ni (ppm), Fe (%), Cu (ppm), Co (ppm), Au (ppm), As (ppm), and Ag (ppm). Among these variables, iron (Fe) and sulfur (S) were selected as the principal focus of the investigation.

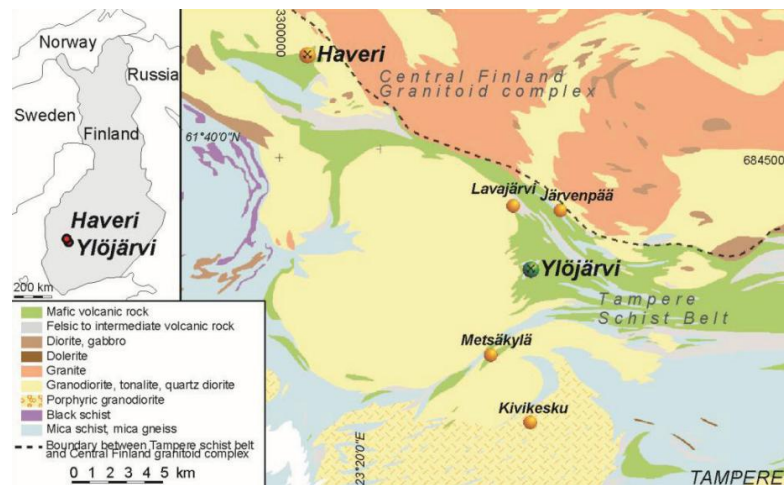


Figure 1. The location of the Haveri TSF (Eilu, 2012). Coordinate system is in local grid

The emphasis on Fe and S is justified by their fundamental role in the formation of acid mine drainage (AMD), as they are directly involved in sulfide mineral oxidation. When sulfide minerals, particularly pyrite, are exposed to oxygen and water, they undergo oxidative weathering, producing sulfuric acid and sulfate ions (SO_4^{2-}) and thereby contributing to acid generation in mine waste environments. During this process, ferrous iron (Fe^{2+}) is released and subsequently oxidized to ferric iron (Fe^{3+}), which generates additional acidity and acts as a powerful oxidizing agent capable of sustaining sulfide degradation even under acidic and oxygen-deficient conditions. The hydrolysis and precipitation of Fe^{3+} into secondary minerals such as ferrihydrite and schwertmannite further intensify acidity through proton release. These interconnected iron and sulfur oxidation reactions establish a self-perpetuating geochemical feedback mechanism that enhances the persistence and severity of AMD. Consequently, the concentrations and spatial distributions of Fe and S in tailings serve as critical indicators for AMD prediction and must be incorporated into geostatistical and remediation-oriented modeling frameworks (Blowes et al., 2003).

Two-dimensional borehole location maps of Fe (%) and S (%) are presented in Figure 2. The boreholes are predominantly concentrated in the central portion of the TSF. The spatial distributions of Fe and S reveal distinct geochemical zoning within the deposit. As shown in Figure 2a, Fe concentrations are elevated in the central area, forming a densely clustered zone. This enrichment may reflect the deposition of iron-rich processing residues or post-depositional redistribution processes such as oxidation-driven migration and reprecipitation of Fe-bearing minerals. In contrast, S concentrations (Figure 2b) exhibit a more dispersed pattern with a wider spatial extent, particularly toward the southwestern quadrant of the TSF. This distribution may indicate localized sulfide accumulation during deposition or hydrological controls influencing sulfur retention. The partial spatial decoupling of Fe and S suggests differences in source processes or mobility, which have important implications for AMD prediction and remediation planning.

Beyond qualitative observations, potential departures from stationarity were assessed as part of the exploratory data analysis. Although the sample maps in Figure 2 display geochemical zonation—with elevated Fe in the central region and higher S concentrations extending southwest—no clear large-scale deterministic trends were identified across the modeling domain. Directional and omnidirectional experimental variograms for Fe and S (Figure 5) were modeled using a linear model of coregionalization (Eq. 10), incorporating a nugget effect and two nested spherical structures with horizontal ranges of 25 m and 185 m and a vertical range of 10 m. The total model sills are 5.048 (%²) for Fe and 1.452 (%²) for S, closely matching the global sample variances of 4.664 and 1.270 %², respectively. Both variograms reach a practical sill at approximately 185 m, indicating bounded spatial variability. This behavior supports the assumption that Fe and S can be treated as second-order stationary random fields within the ordinary co-kriging framework adopted in this study. For spatially non-stationary or sparsely sampled datasets, alternative approaches such as kriging with sparse covariance representations and enhanced measurement error treatment (Miao & Wang, 2024, 2025), comparative interpolation methods for sparse data (Wang et al., 2017), and value-of-information analyses accounting for model and measurement uncertainties (Khan et al., 2020) may also be considered.

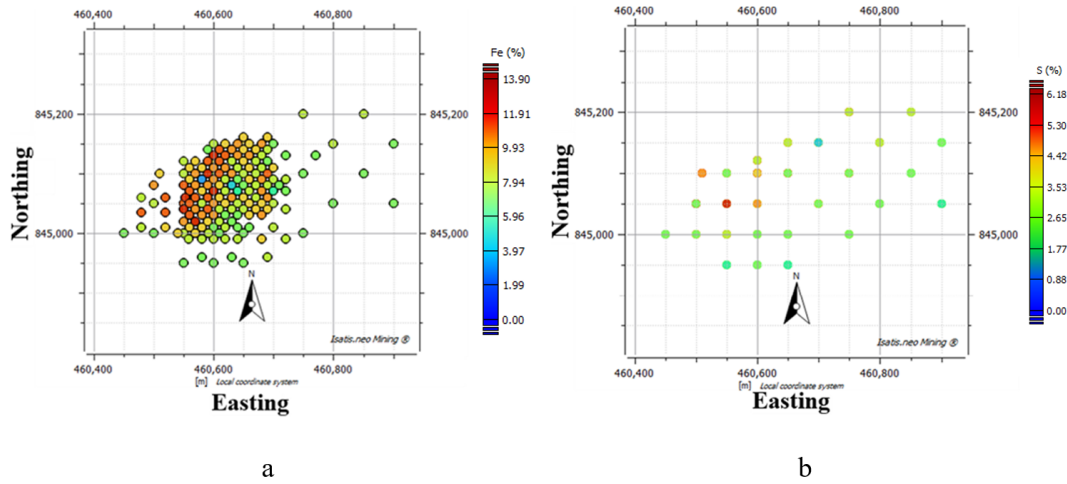


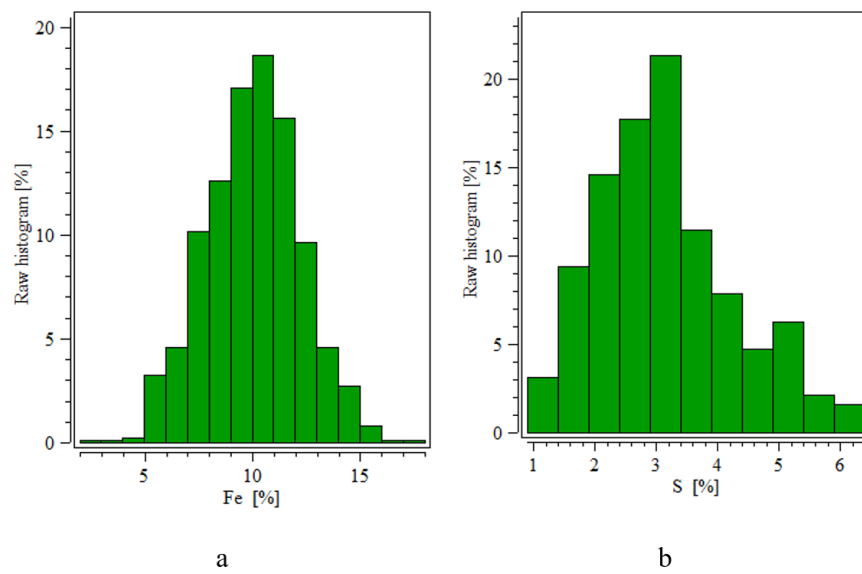
Figure 2. Spatial distribution maps of borehole samples from the Haveri TSF: (a) – Fe (%); (b) – S (%). Coordinate system is in meters (local grid)

The thickness of the tailings deposit ranges from 2 to 9 m, with an average of 6.5 m. The only stratigraphic feature characterized in detail is an oxidized surface layer, ranging from 0.5 to 1.4 m in thickness (Parviainen, 2009; Parviainen et al., 2012). Owing to the limited availability of data within this zone, Fe and S were modeled within a single geostatistical domain. Consequently, the vertical range of 10 m in the fitted variograms is interpreted as representing variability across the entire tailings thickness, including the oxidized cap. In deposits where distinct stratigraphic layers with contrasting properties can be identified, layer-specific covariance models or Bayesian stratigraphic identification methods based on the soil behavior type index (Miao et al., 2025) may be integrated with the OCK-RM framework.

Table 1 presents descriptive statistical parameters, while Figure 3 illustrates the histograms of Fe (%) and S (%) concentrations measured in the Haveri TSF. The Fe dataset, comprising 1,114 samples, exhibits an approximately symmetrical bell-shaped distribution (Figure 3a), indicating a near-normal distribution across the study area. The mean Fe concentration is 10.02%, with a variance of 4.664 ($\%^2$) and a coefficient of variation (COV) of 0.216, suggesting low relative variability. Fe concentrations range from 2.79% to 17.01%, reflecting occasional localized anomalies but overall stable distribution characteristics.

Table 1. Descriptive statistics of Fe and S concentrations in the Haveri TSF

Variable	Number of samples	Mean	Variance	COV	Minimum	Maximum
Fe (%)	1,114	10.02	4.664	0.216	2.79	17.01
S (%)	192	3.14	1.27	0.359	0.93	6.13

**Figure 3.** Histograms of Fe (%) (a) and S (%) (b) concentrations in the Haveri TSF dataset

In contrast, the S dataset consists of 192 samples and displays a positively skewed distribution (Figure 3b), characterized by a predominance of low concentrations and fewer high-value occurrences. The mean S concentration is 3.14%, with a variance of 1.270 ($\%^2$) and a COV of 0.359, indicating comparatively higher variability. Sulfur concentrations range from 0.93% to 6.13%, highlighting localized heterogeneity and non-uniform spatial distribution.

The substantial disparity in sample sizes between the Fe and S datasets reflects differences in assaying strategies across exploration campaigns. Both elements were analyzed during the 1980 drilling program, which included 192 samples. However, in the subsequent 1983 campaign—during which 922 additional samples were collected—only Fe and selected other elements were assayed, while S was excluded from the analytical suite. As a result, Fe was systematically and

comprehensively sampled across the study area, producing a robust dataset for statistical analysis. Conversely, the limited number of S samples and their skewed distribution suggest preferential sampling in the central portion of the deposit. Consequently, the TSF exhibits a partially heterotopic sampling pattern, with sulfur undersampled relative to iron. This disparity highlights the importance of multivariate geostatistical modeling for improving the spatial prediction of S.

The Pearson correlation coefficient between Fe (%) and S (%) is 0.85, indicating a strong positive relationship. This correlation is closely linked to the potential for AMD formation, as pyrite and pyrrhotite are the principal iron-bearing sulfide minerals present in the tailings. AMD generation reduces pore-water pH, increasing acidity and enhancing the dissolution and mobility of potentially toxic elements. Because Fe and S are both associated with sulfide minerals, their strong correlation reflects their shared role in AMD processes. The relationship between these elements is illustrated in Figure 4.

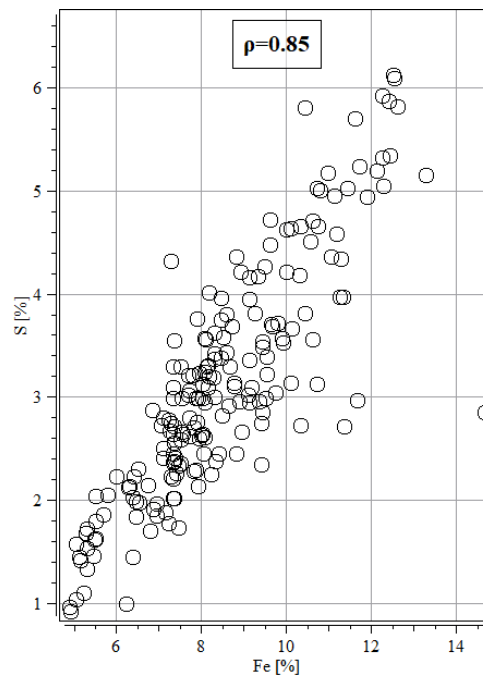


Figure 4. Scatter plot of the relationship between sulfur (S) and iron (Fe) concentrations

4.2 Geostatistical modeling

To implement co-kriging algorithms, it is necessary to first model the direct and cross-variograms. To evaluate potential anisotropy, experimental direct and cross-variograms of Fe

and S were computed in both horizontal and vertical directions. The results indicate isotropic behavior within the horizontal plane, whereas the vertical direction exhibits pronounced anisotropy characterized by shorter ranges and reduced spatial continuity. This pattern is typical of tailings deposits, where horizontal layering during slurry deposition promotes lateral uniformity in geochemical and mineralogical properties, while vertical variability increases due to stratification, compaction, and temporal changes in depositional conditions (Madani et al., 2025). The variograms were subsequently fitted using a linear model of coregionalization that incorporates a nugget effect and two nested spherical structures. This modeling approach ensures that the variograms share common ranges while permitting distinct, valid sill matrices. The resulting cross-variogram is presented in Equation 10 and illustrated in Figure 5.

$$\begin{pmatrix} \gamma_{Fe} & \gamma_{Fe/S} \\ \gamma_{Fe/S} & \gamma_S \end{pmatrix} = \begin{pmatrix} 2.137 & 0.406 \\ 0.406 & 0.44 \end{pmatrix} \text{nugget} + \begin{pmatrix} 1.225 & 0.302 \\ 0.302 & 0.075 \end{pmatrix} \text{Sph}(25\text{m}, 25\text{m}, 10\text{m}) + \begin{pmatrix} 1.686 & 1.256 \\ 1.256 & 0.937 \end{pmatrix} \text{Sph}(185\text{m}, 185\text{m}, 10\text{m}) \quad (10)$$

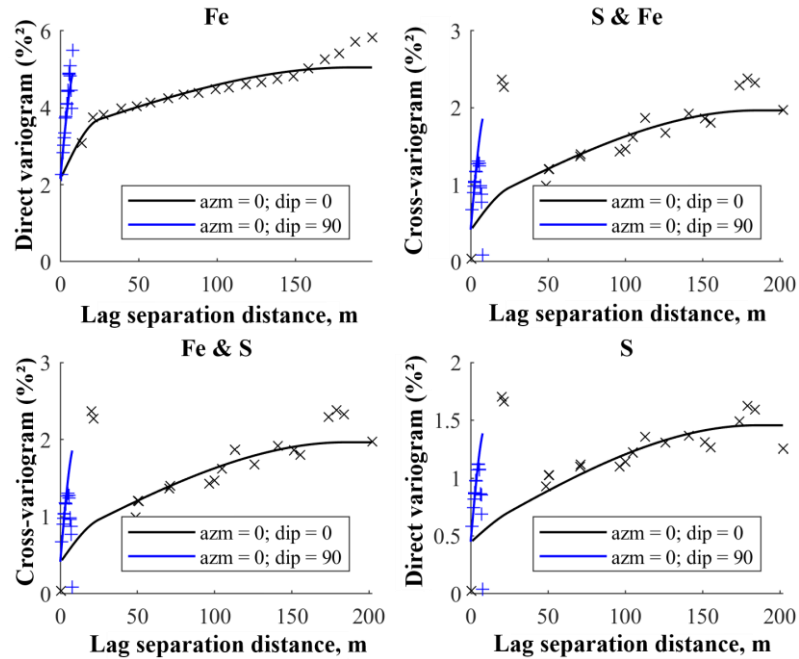


Figure 5. Direct and cross-variograms of Fe and S concentrations in the Haveri TSF

After establishing the variogram structure, a five-fold cross-validation procedure was conducted to determine the relationship between the mean values of sulfur and iron, expressed as $S = f(\text{Fe})$, where the mean Fe served as the predictor and the mean S as the response

variable. The dataset was divided into five subsets; during each iteration, four subsets were used to train the regression model and derive the predictive equation, while the remaining subset was reserved for validation. This process was repeated five times to ensure that each subset was used once as the test set. The regression-based techniques outlined in the methodology section were applied within each fold. The coefficients of the resulting regression equations (summarized in Table 2) were obtained by averaging the parameters across all folds, thereby producing robust estimates and reducing the risk of overfitting. For regularized models—namely Ridge, Lasso, and Elastic Net—the optimal regularization strength was determined within each training fold through internal cross-validation based on RMSE minimization. Although the regression employed a single predictor (Fe), appropriate preprocessing was applied according to the requirements of each estimator: no scaling was required for linear regularized models, whereas algorithms sensitive to feature scaling, such as support vector regression (SVR) and stochastic gradient descent (SGD) solvers, were standardized within each training fold only to prevent information leakage.

Table 2. Inferred equations of regression models in the form of $S = f(Fe)$

Regression model	Equation
Linear Regression	$S = -1.069 + 0.497Fe$
SVR	$S = -1.356 + 0.536Fe$
ENR	$S = -0.631 + 0.446Fe$
Lasso	$S = -0.571 + 0.438Fe$
Ridge	$S = -1.047 + 0.495Fe$
SGR	$S = -1.113 + 0.503Fe$

To facilitate a meaningful comparison of OCK-RM results obtained using the different regression functions listed in Table 3, a conventional leave-one-out cross-validation (LOOCV) procedure—widely employed in geostatistical applications (Emery & Séguret, 2020)—was performed alongside the traditional OCK and SCK methods (Table 3). In this approach, each sample is sequentially removed from the dataset and its value is estimated using the remaining observations, enabling a comprehensive evaluation of model performance based on prediction accuracy. All models were implemented using an identical neighborhood configuration, with maximum search radii of (250 m, 250 m, 10 m) in the rotated coordinate system, and the same linear model of coregionalization defined in Equation 10 for the co-kriging computations.

Table 3. Leave-one-out cross-validation performance (LC, RMSE) for Fe and S across OCK-RM regression options; OCK and SCK are shown for reference

Co-kriging variant	Fe: LC	Fe: RMSE	S: LC	S: RMSE
OCK-RM-SVR	0.799	1.214	0.712	0.817
OCK-RM-ENR	0.800	1.225	0.724	0.787
OCK-RM-Lasso	0.800	1.226	0.724	0.785
OCK-RM-Ridge	0.766	1.263	0.602	1.245
OCK-RM-SGR	0.764	1.278	0.593	1.300
OCK-RM-LR	0.766	1.402	0.718	0.800
SCK	0.764	1.434	0.695	0.819
OCK	0.772	1.389	0.714	0.791

Because the best-performing regression models produce nearly identical linear correlation (LC) values—differing only at the third decimal place—point estimates alone are insufficient to establish a reliable ranking. Therefore, model selection is primarily based on downstream block-model performance under heterotopic sampling conditions, including completeness, stability of the related-mean constraint, and the ability to reproduce spatially varying Fe–S coupling, rather than on marginal differences in cross-validated LC.

As shown in Figures 6a and 6b, the OCK-RM method applied to Fe, using Elastic Net and Lasso regression to define the mean relationship between Fe and S, achieves the highest LC values of 0.800, with relatively low RMSE values of 1.225 and 1.226, respectively. The OCK-RM approach incorporating support vector regression (SVR) performs comparably, yielding an LC of 0.799 and the lowest RMSE of 1.214, thereby demonstrating superior accuracy in terms of error minimization. In contrast, OCK-RM implementations using Ridge Regression and stochastic gradient regression (SGR) exhibit reduced predictive capability, with lower LC values of 0.766 and 0.764, respectively, accompanied by higher RMSE values. The weakest performance is observed for OCK-RM with Linear Regression, which produces the highest RMSE of 1.402, indicating that simpler linear models are less effective at capturing Fe variability.

A similar pattern is observed for sulfur predictions. OCK-RM with Elastic Net and Lasso achieves the highest LC values of 0.724 and 0.725, respectively, together with relatively low RMSE values of 0.787 and 0.786. The SVR-based OCK-RM model also demonstrates competitive performance, yielding an LC of 0.712 and an RMSE of 0.818. Conversely, the Ridge and SGR models perform less effectively for S, with LC values decreasing to 0.602 and 0.593, respectively, and corresponding increases in RMSE. OCK-RM with Linear Regression exhibits moderate predictive capability, achieving an LC of 0.719 and an RMSE of 0.800.

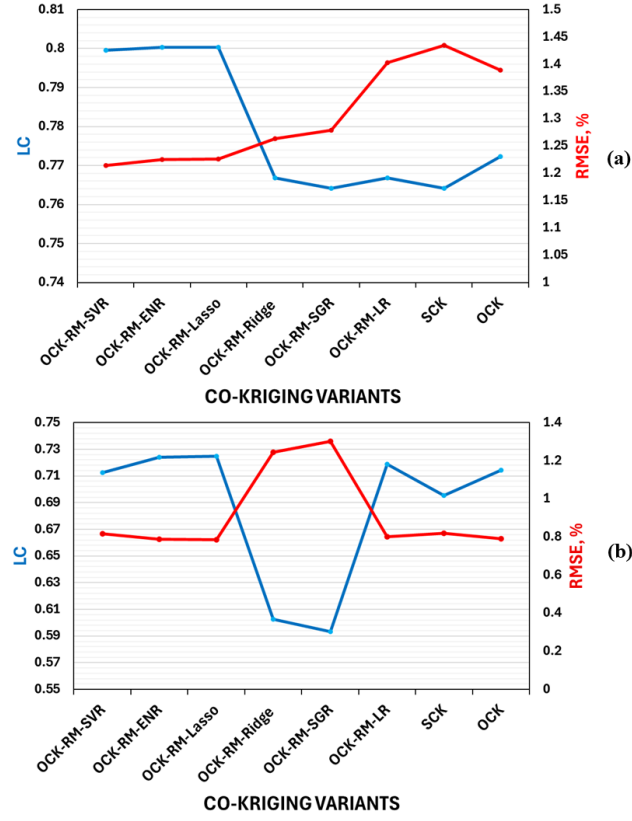


Figure 6. Cross-validation performance (LC and RMSE) of OCK, SCK, and OCK-RM with different regression functions for Fe (a) and S (b)

When comparing the three co-kriging variants, OCK-RM-Lasso consistently demonstrated superior performance relative to conventional OCK, SCK, and other OCK-RM alternatives employing different regression functions for both Fe and S. For iron, OCK-RM-Lasso achieved the lowest RMSE (1.226) and the highest linear correlation ($LC = 0.800$), whereas OCK and SCK yielded inferior results, with RMSE values of 1.389 and 1.434 and LC values of 0.772 and 0.764, respectively. A similar trend was observed for sulfur, where OCK-RM-Lasso attained the best predictive performance ($RMSE = 0.786$, $LC = 0.725$), surpassing OCK ($RMSE = 0.791$, $LC = 0.714$) and SCK ($RMSE = 0.820$, $LC = 0.695$). These improvements underscore the effectiveness of incorporating Lasso-derived related means into the co-kriging with related mean framework.

Following the identification of Lasso as the most effective regression approach, OCK-RM-Lasso, together with conventional OCK and SCK, was applied to estimate Fe and S concentrations across all 90,000 grid nodes defined by a resolution of $5 \text{ m} \times 5 \text{ m} \times 0.5 \text{ m}$. The

same search neighborhood employed during the leave-one-out cross-validation was maintained for these estimations to ensure methodological consistency.

Before presenting the visual comparison maps of SCK, OCK, and OCK-RM-Lasso, a quantitative evaluation was conducted to assess how effectively each co-kriging method reproduces the Fe–S relationships derived from the Lasso regression analysis (Table 4). To this end, linear regression analyses were performed on the estimated block models generated by each method. For instance, in the 90,000 blocks estimated using OCK-RM-Lasso, a simple linear regression of the form $S = f(\text{Fe})$ was fitted to the predicted S and Fe values. The same procedure was subsequently applied to the results obtained from OCK and SCK. The resulting regression equations are summarized in Table 4 and graphically compared in Figure 7.

Table 4. Linear relations $S = f(\text{Fe})$ fitted to the estimated block models from SCK, OCK, and OCK-RM-Lasso, compared with the original Lasso relation used to define the OCK-RM constraint.

Co-kriging variant	Regression equation
SCK	$S = 0.678 * \text{Fe} - 3.605$
OCK	$S = 0.455 * \text{Fe} - 0.998$
OCK-RM	$S = 0.476 * \text{Fe} - 1.076$
Original Lasso Regression	$S = 0.438 * \text{Fe} - 0.571$

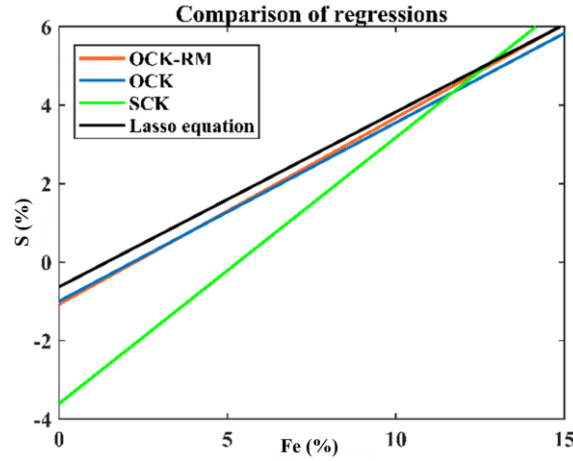


Figure 7. Comparison of S–Fe relations derived from the estimated block models (SCK, OCK, and OCK-RM-Lasso) against the original Lasso reference relation

As observed, both variants of ordinary co-kriging—conventional OCK and OCK-RM—demonstrated improved predictive accuracy by adjusting the intercept and more effectively accounting for the underrepresented nature of sulfur in the dataset. Among these approaches, OCK-RM combined with Lasso regression exhibited the best performance in reproducing the original mean relationship, particularly within the upper quintiles of Fe and S. In contrast, simple co-kriging (SCK) deviates notably from the original trend, overestimating the slope and underestimating the intercept, thereby reflecting its limited ability to preserve the underlying mean relationship between the two variables.

The statistical characteristics of Fe and S grades were evaluated using the predicted block models generated by OCK, SCK, and OCK-RM-Lasso and subsequently compared with those of the original dataset. The assessed parameters include the mean, variance, minimum, and maximum values for both elements, as summarized in Table 5. In the original dataset, Fe exhibits a mean of 10.018% and a variance of 4.664 (%²). In the block models, the mean values are slightly lower, with SCK (9.815%), OCK (8.941%), and OCK-RM-Lasso (8.981%) yielding comparable results. A reduction in variance is observed across all block models, with SCK producing the lowest variance (1.064 %²), followed by OCK (2.381 %²) and OCK-RM-Lasso (2.462 %²).

For sulfur, the original dataset shows a mean of 3.105% and a variance of 1.270 (%²). In the block estimates, OCK-RM-Lasso yields the highest mean value (3.228%), followed by OCK (3.071%) and SCK (3.052%). As with iron, the variance of sulfur is reduced in all block models

relative to the original data. The lowest variance is obtained using SCK (0.512 %²), followed by OCK-RM-Lasso (0.611 %²) and OCK (0.653 %²). These results reflect the smoothing effect inherent in kriging-based estimators while highlighting the capability of OCK-RM-Lasso to better preserve the statistical characteristics of the original dataset.

Table 5. Summary statistics (mean, variance, minimum, maximum) of Fe and S for the original samples and the estimated block models produced by SCK, OCK, and OCK-RM-Lasso

Variable	Statistical Parameter	Original Dataset	SCK	OCK	OCK-RM-Lasso
Fe (%)	Mean	10.018	9.815	8.941	8.981
	Variance	4.664	1.064	2.381	2.462
	Minimum	2.79	3.63	3.63	3.63
	Maximum	17.01	13.93	13.9	13.83
S (%)	Mean	3.105	3.052	3.071	3.191
	Variance	1.27	0.512	0.653	0.611
	Minimum	0.93	0.597	0.626	1.252
	Maximum	6.13	5.457	6.183	5.79

The comparison between the statistical parameters of the block models and those of the original dataset indicates that all co-kriging variants yield slightly lower mean values and variances for both Fe and S. This reduction reflects the smoothing effect, a well-known characteristic of kriging and co-kriging algorithms. Among the evaluated methods, SCK exhibits the most pronounced smoothing, as evidenced by the lowest spatial variance. This behavior arises from the assumption of a known and constant mean, which restricts the method's ability to accommodate local variability. Consequently, the interpolated values tend to be overly

smoothed, suppressing local fluctuations and reducing overall variability compared with OCK and OCK-RM-Lasso.

The observed reduction in Fe variance—from 4.664 to 2.462 ($\%^2$), corresponding to approximately 47%—is consistent with the inherent smoothing effect of kriging and co-kriging estimators, which are formulated as minimum-variance linear unbiased predictors. Such attenuation of variance is therefore an intrinsic property of estimation and should be interpreted in relation to the intended application rather than viewed as an implementation artifact. In this study, the block model primarily serves as a conservative screening tool for comparing spatial patterns, recovery functions, and methodological behavior under heterotopic sampling, rather than for reproducing local extremes or the full high-tail variability at point support. From this perspective, a certain degree of smoothing is acceptable, as it provides stable block-scale estimates and reduces the risk of overinterpreting isolated high values.

However, when the primary objective is the identification of AMD hotspots—namely, the delineation of localized high-risk zones where preserving variance and extreme values is essential—conditional simulation approaches are generally more suitable. Gaussian co-simulation frameworks are capable of preserving spatial variability, including high-value tails, and of generating multiple equiprobable realizations for uncertainty quantification, thereby supporting more informed decision-making in hotspot mapping. Accordingly, simulation-based modeling is recommended as a complementary extension when variance preservation and the representation of extremes are critical. In line with this perspective, extending the related-mean concept to a co-simulation framework (e.g., a GC-RM analogue) would require reformulating the regression-based related-mean component within an ordinary co-kriging related-mean setting; this represents a promising direction for future research.

Final two-dimensional estimation maps, generated at a depth of 4.5 m below the surface using the three co-kriging variants, are presented in Figure 8 for both Fe and S. In the OCK results, 417 blocks could not be estimated and are depicted as void (white) areas in Figure 8. This outcome highlights a key limitation of the OCK method when applied to heterotopic sampling scenarios, where primary and secondary variables are not co-located. Because OCK relies on the presence of nearby primary data to solve its system of equations, the absence of such data renders the system underdetermined, leading to numerical instability or an inability to generate estimates. In such cases, the method cannot assign valid kriging weights that satisfy the unbiasedness constraint. By contrast, both SCK and OCK-RM-Lasso successfully estimated all

90,000 blocks. Nevertheless, SCK tends to predict mean values in locations lacking available data for both Fe and S, reflecting its tendency toward excessive smoothing.

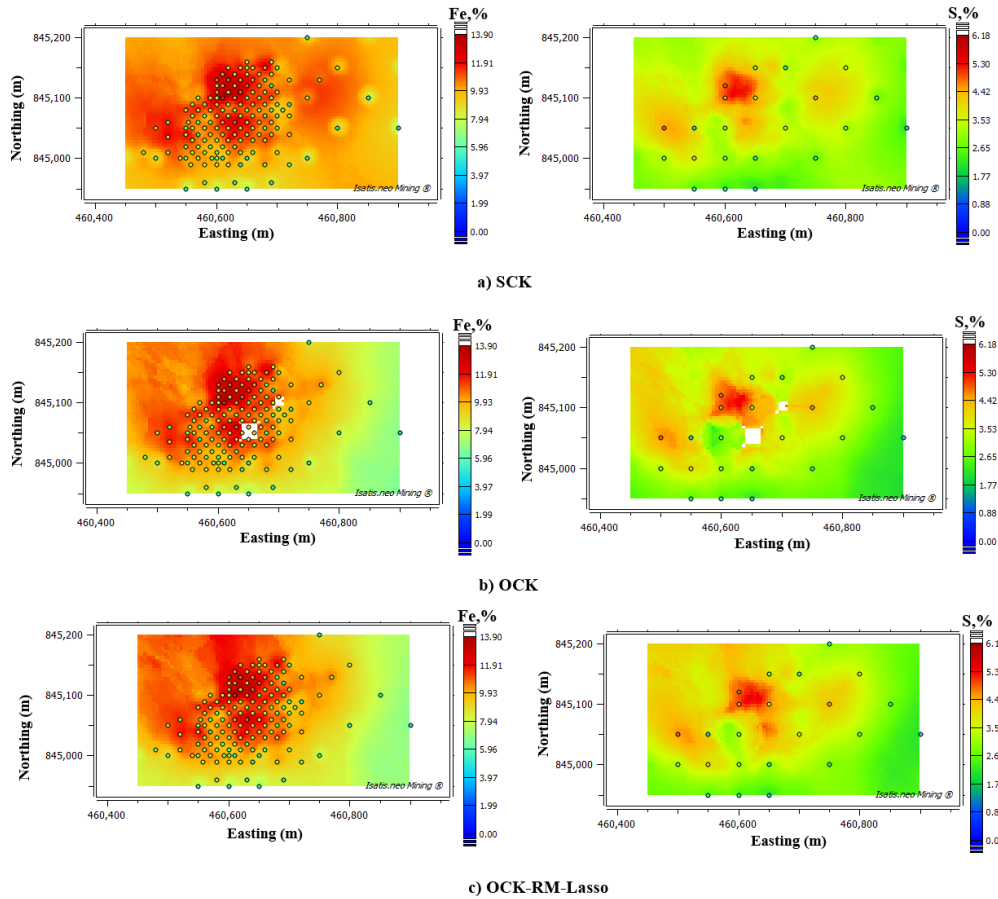


Figure 8. Final 2D estimation maps ($Z = -4.5\text{m}$) obtained by SCK (a), OCK (b), and OCK-RM-Lasso (c) of Fe (left) and S (right); void/white regions are the blocks that failed to be estimated in OCK; points are assayed drillholes. Map coordinates are in the local coordinates

The blocks identified as non-estimable are predominantly located in the central portions of the deposit, where the primary variable (Fe) is well represented but the secondary variable (S) is locally sparse within the defined search neighborhood. These areas should not be interpreted as “S-only regions”; rather, they correspond to locations where the co-kriging system cannot be reliably constructed because the neighborhood lacks enough nearby S samples to support the required cross-covariance terms and ensure numerical stability.

This behavior does not indicate a flaw in the implementation of the OCK algorithm. Instead, it arises from the minimum neighborhood and conditioning criteria imposed to prevent ill-posed

or poorly conditioned co-kriging systems, such as those associated with near-singular covariance matrices or unstable kriging weights. In such circumstances, the estimator is intentionally prevented from producing results, and the corresponding blocks are flagged as non-estimable to avoid introducing unreliable values driven by extrapolation or numerical instability.

Expanding the search neighborhood would reduce the number of non-estimable blocks by incorporating more distant S samples and enabling the co-kriging system to be solved at a greater number of locations. However, this adjustment introduces an inherent trade-off: larger neighborhoods diminish the locality of estimates and typically increase smoothing, particularly in environments characterized by pronounced short-range variability. For this reason, the neighborhood size was deliberately constrained to preserve local representativeness and to ensure that the estimates rely on adequate nearby secondary support rather than distant information.

The final two-dimensional variance maps, generated at a depth of 4.5 m below the surface using the three co-kriging methods, are presented in Figure 9 for both Fe and S. These maps depict the kriging estimation variance, which quantifies the uncertainty associated with predicted values based on their proximity to available drillhole data. In general, areas located near drillholes—where data density is high—exhibit lower variance, indicating greater confidence in the estimates, whereas regions farther from sampling locations display higher variance, reflecting increased uncertainty. In the case of OCK, variance could not be computed for 417 blocks due to insufficient nearby S data, and these are represented as blank (white) areas in the figure. This outcome underscores a fundamental limitation of the OCK method under heterotopic sampling conditions, where the lack of spatial overlap between primary and secondary datasets disrupts the kriging system. In contrast, both SCK and OCK-RM-Lasso successfully generated variance estimates for all 90,000 blocks. Nevertheless, in data-sparse areas—particularly where neither Fe nor S samples are available—SCK tends to underestimate uncertainty by producing artificially low variance values due to its reliance on global means, thereby misrepresenting the true level of estimation confidence.

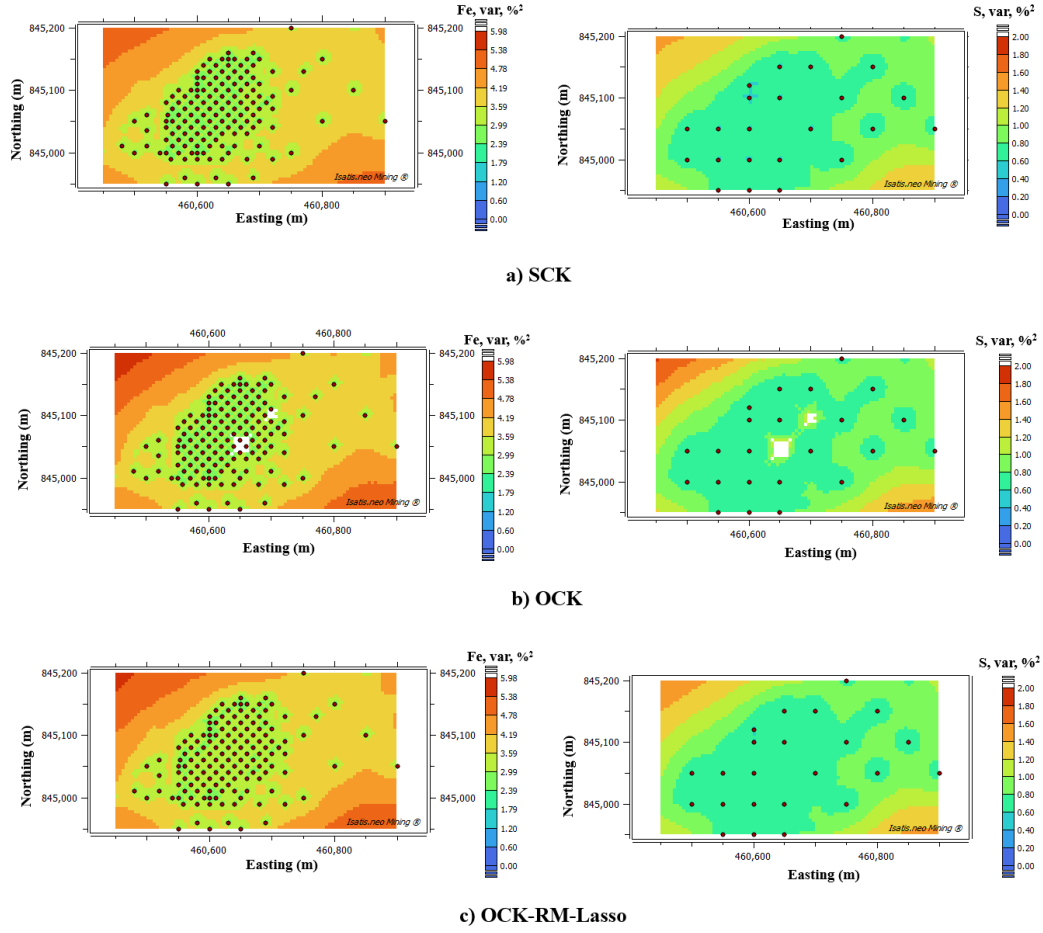


Figure 9. Final 2D variance maps ($Z = -4.5\text{m}$) obtained by SCK (a), OCK (b), and OCK-RM-Lasso (c) of Fe (left) and S (right); empty regions are the blocks that failed to be estimated; points are assayed drillholes. Map coordinates are in meters in the local coordinates

Another approach for comparing the co-kriging variants involves evaluating how closely the distributions of the estimated Fe and S values match the original data using quantile–quantile (Q–Q) plots. Figure 10 presents the Q–Q plots for SCK, OCK, and OCK-RM-Lasso relative to the original distributions of Fe and S. When the plotted points align with the 45-degree diagonal line, the predicted values closely follow the actual distribution; deviations from this line indicate discrepancies in model performance.

The Q–Q plot for Fe reveals that SCK (green circles) exhibits the most pronounced deviation from the 1:1 line, particularly at the lower and upper quantiles. This suggests that SCK tends to underestimate low Fe concentrations and overestimate high ones, indicating limitations in accurately reproducing extreme values. In contrast, OCK (red crosses) and OCK-RM-Lasso (blue crosses) align more closely with the diagonal, especially within the central quantile range, demonstrating better agreement with the observed Fe distribution. Notably, OCK-RM-Lasso

provides a slightly improved fit at the distribution tails compared with conventional OCK, indicating that the incorporation of Lasso-derived related means helps mitigate bias at the extremes.

A similar comparison for sulfur shows that SCK provides a better fit in the lower quantiles, effectively capturing low S concentrations. However, it deviates from the 1:1 line at higher quantiles, indicating a tendency to overestimate elevated S values. Conversely, OCK and OCK-RM-Lasso exhibit closer agreement with the theoretical quantiles in the upper tail, demonstrating superior performance in modeling high S concentrations. Among the three methods, OCK-RM-Lasso achieves the most balanced overall performance, closely following the 1:1 line across the mid-to-upper quantiles. This behavior indicates an enhanced capability to reproduce both moderate and high sulfur values, although it shows slightly weaker performance in the lower tail compared with SCK.

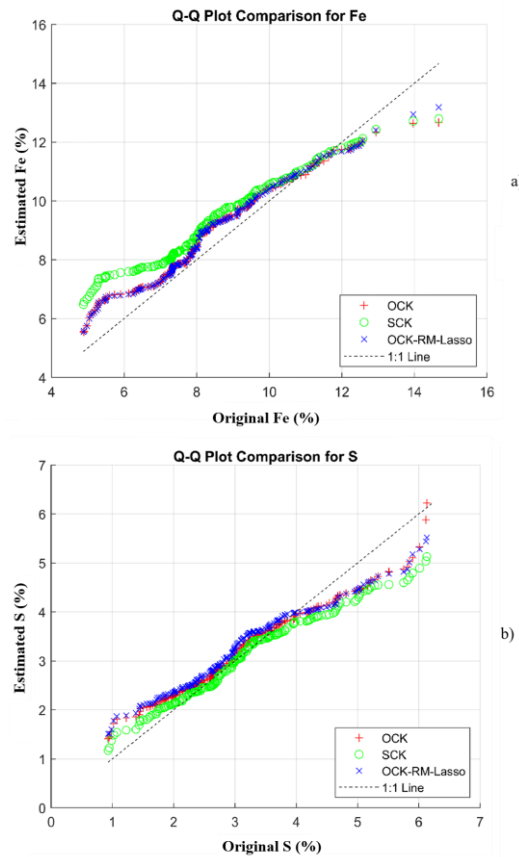


Figure 10. Q–Q plots comparing the distributions of estimated block values to the original data for Fe (a) and S (b) using SCK, OCK, and OCK-RM-Lasso

4.3 Recovery functions

An important component of tailings management—particularly in the context of acid mine drainage (AMD) mitigation—is the evaluation of Fe and S distributions through recovery function analysis. Figure 11 presents the grade–tonnage curves derived at varying cut-off grades using OCK, SCK, and several OCK-based machine-learning variants, including Lasso, Ridge, SVR, Random Forest, and Linear Regression. In all cases, increasing the cut-off grade results in a monotonic decrease in tonnage accompanied by an increase in average grade, reflecting the progressive exclusion of lower-grade material.

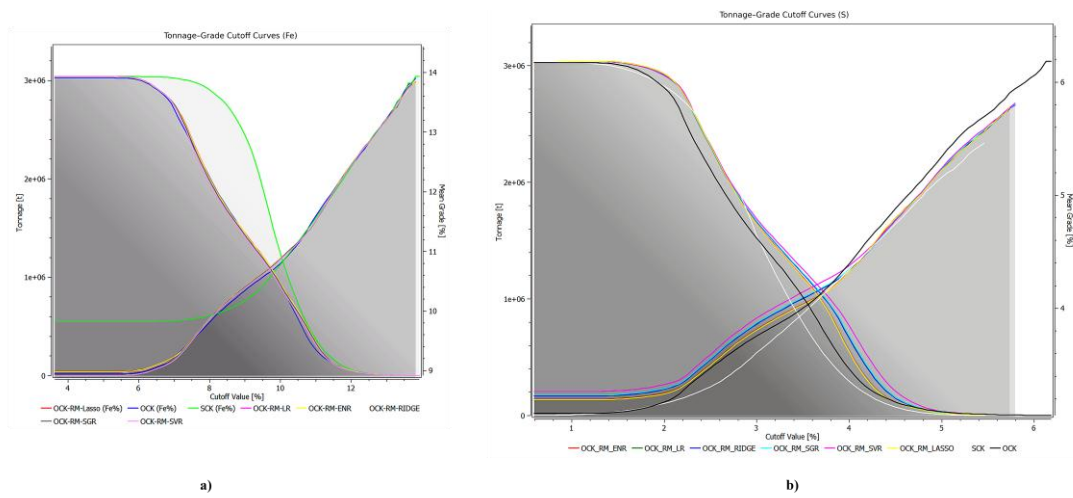


Figure 11. Grade–tonnage curves for (a) Fe and (b) S under varying cut-off values using OCK, SCK, and OCK-based machine-learning variants

For Fe, all OCK-based variants produce nearly identical grade–tonnage curves. This consistency is expected because Fe is well represented in the dataset and supported by sufficient primary data. As a result, the incorporation of secondary modeling strategies has minimal influence on the global grade–tonnage response. In contrast, SCK exhibits slightly different behavior within the intermediate cut-off range, likely due to its assumption of known global means and its reliance on a purely covariance-driven weighting scheme. In heterogeneous tailings environments, dependence on a stationary global mean can introduce additional smoothing and shift the grade distribution relative to OCK-based approaches that implicitly estimate local means.

More pronounced differences are observed for sulfur (S), the undersampled variable. Owing to the limited availability of primary S data, its estimation depends more heavily on cross-correlation with Fe and on the specific cokriging formulation. Consequently, discrepancies among OCK, SCK, and the OCK-based variants become more evident, particularly within the mid-range of cut-off grades. The wider dispersion among the S curves reflects higher estimation uncertainty and greater sensitivity to the adopted multivariate modeling strategy.

Importantly, although cross-validation metrics reveal only modest numerical differences between the methods—with OCK-Lasso demonstrating slight improvements—the grade-tonnage curves indicate that these variations translate into materially distinct estimates of recoverable resources at operational cut-offs. In this context, OCK-Lasso delivers a more stable and consistent economic response, suggesting that even minor enhancements in predictive accuracy can have significant implications at the resource scale. Therefore, among the evaluated approaches, OCK-Lasso provides the most reliable balance between predictive performance and economically meaningful resource delineation.

5. DISCUSSION

For the Haveri dataset, the strong linear correlation between Fe and S leads all six regression models to converge toward nearly identical linear Fe–S relationships, yielding very similar RMSE and LC values. Consequently, the purpose of the regression step is not to alter the functional form of the relationship but rather to estimate it using regularization and cross-validation, while assessing how this choice influences OCK-RM performance under heterotopic sampling conditions.

Although the differences in cross-validated RMSE and LC between OCK-RM-Lasso and conventional OCK are modest, they are systematic and correspond to improvements that are significant at the block scale. First, OCK-RM-Lasso produces a complete block model, whereas conventional OCK fails to generate estimates in 417 blocks under heterotopic sampling (Figures 8 and 9), resulting in gaps in AMD risk mapping. Second, OCK-RM-Lasso preserves block-scale variances closer to those of the original dataset than SCK, while avoiding both the excessive smoothing characteristic of SCK and the missing estimates observed in OCK (Table 5). Although cross-validation indicates only marginal improvements in pointwise RMSE, grade–tonnage analysis demonstrates that small predictive differences can translate into materially distinct recoverable resource estimates.

From a practical perspective, the applicability of the machine learning–assisted OCK-RM framework depends on the quantity and quality of available data. In the Haveri TSF case, the Fe and S datasets, although limited, are sufficient to support stable variogram modeling and cross-validated regression. However, when sampling density is lower or measurement error is substantial, the stability of both the regression step and the inferred spatial variability becomes increasingly sensitive to the choice of regularization, model complexity, and cross-validation strategy.

Despite its advantages in predictive accuracy and robustness under heterotopic sampling, the OCK-RM-Lasso method is not without limitations. A key drawback, consistent with previous studies, is the pronounced smoothing effect inherent to kriging-based estimators. This effect tends to attenuate local variability and extreme values, particularly in areas of high spatial heterogeneity. As a result, fine-scale geochemical features or localized anomalies may be diluted, potentially affecting decision-making in AMD mitigation and resource recovery planning.

It is also important to note that ordinary (co-)kriging formulations, including OCK-RM, are inherently designed for estimation and cannot be directly incorporated into sequential Gaussian (co-)simulation workflows. Sequential Gaussian co-simulation requires an explicitly defined local conditional distribution at each simulation step, typically obtained using simple (co-)kriging with a fully specified mean function, often standardized to zero following normal-score transformation. In contrast, ordinary (co-)kriging and its related-mean or regression-mean variants treat the mean as unknown and enforce unbiasedness through kriging constraints. Consequently, they do not provide an explicit mean function that can be iteratively updated within a sequential simulation algorithm. For this reason, the direct implementation of a “SGC-RM” analogue is not straightforward. Integrating a regression-based mean relationship into a sequential Gaussian co-simulation framework would require reformulating the related-mean concept within a simple co-kriging setting—such as by defining a deterministic drift or mean model and simulating residuals—followed by rigorous verification that both variance and cross-covariance structures are preserved. As the present study focuses on block-scale estimation, including recovery functions, smoothing behavior, and method comparison, the OCK-RM framework provides an appropriate and internally consistent approach. Extending the proposed regression-based mean modeling strategy to sequential Gaussian co-simulation represents a promising direction for future research and will be pursued in subsequent studies.

6. CONCLUSIONS AND RECOMMENDATIONS

This study successfully integrates advanced geostatistical methods with machine learning techniques to enhance the spatial prediction of Fe and S concentrations in the Haveri Au–Cu mine tailings, thereby supporting both Acid Mine Drainage (AMD) mitigation and tailings reprocessing initiatives. The implementation of ordinary co-kriging with a related mean (OCK-RM) combined with Lasso regression improves estimation accuracy, particularly in addressing challenges associated with undersampled and heterotopic datasets. Cross-validation results indicate that, among the evaluated regression models, Lasso regression achieved the highest linear correlation (0.800 for Fe and 0.725 for S) alongside competitive RMSE values (1.226 for Fe and 0.786 for S), making it the most suitable approach for integration within the OCK-RM framework.

Comparisons of statistical parameters across the co-kriging methods reveal the characteristic smoothing effect of kriging-based estimators. For Fe, the variance decreased from 4.664 in the original dataset to 1.064 using SCK, 2.381 using OCK, and 2.462 using OCK-RM-Lasso. Similarly, for S, the variance declined from 1.270 to 0.512, 0.653, and 0.611, respectively. These reductions confirm that all co-kriging techniques attenuate local variability, with SCK exhibiting the strongest smoothing effect. In contrast, OCK-RM-Lasso preserves relatively higher variance and retains greater spatial heterogeneity.

Furthermore, Q–Q plot analyses demonstrate that OCK-RM-Lasso provides the closest alignment with the 1:1 diagonal, indicating minimal bias and superior predictive performance compared with SCK and conventional OCK. Overall, this research advances geostatistical methodologies for sustainable mine waste management by refining spatial estimation techniques and improving the reliability of AMD risk assessments. Future studies should focus on further developing hybrid geostatistical–machine learning frameworks to enhance predictive capabilities and support sustainable mine tailings reprocessing.

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