

**A HIERARCHICAL SEQUENTIAL GAUSSIAN CO-
SIMULATION ALGORITHM WITH ACCEPTANCE-
REJECTION SAMPLING TECHNIQUE FOR MINE
TAILINGS EVALUATION**

by

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ORIGINALITY STATEMENT

I, Alikhan Ibraimov, hereby declare that this submission is my own work and to the best of my knowledge it contains no materials previously published or written by another person, or substantial proportions of material which have been accepted for the award of any other degree or diploma at Nazarbayev University or any other educational institution, except where due acknowledgement is made in the thesis.

Any contribution made to the research by others, with whom I have worked at NU or elsewhere is explicitly acknowledged in the thesis.

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Signed on 25.04.2025

A handwritten signature in blue ink, appearing to read 'Alikhan Ibraimov', is written over a light blue horizontal line.

ABSTRACT

Despite the environmental impacts, it can be acknowledged that mine tailings may contain large amount of valuable and critical minerals for re-valorization or re-processing. However, evaluation of the same tailings poses a major challenge while dealing with multiple elements in the composition. Conventional methods may not appropriately capture the essence of the bivariate relationship between components of interest. To address this challenge, our research investigates the hierarchical sequential Gaussian co-simulation approach with acceptance-rejection sampling methods. This algorithm is designed towards the fulfillment of the linearity constraints dealing with two major elements among which are copper and gold. Both hierarchical and conventional co-simulation approaches were employed in the study, highlighting differences in data reproduction based on the obtained results. Notably, our findings showed that the effectiveness of the proposed algorithm is superior to those of conventional methods due to the more accurate reproduction of the linearity constraints. By using an acceptance-rejection sampling technique, the proposed technique guarantees the replication of values based on the identified linearity requirements. To apply this algorithm initially, regression analysis was performed to check the validity of linearity between copper and gold in the dataset and to obtain the coefficients of a formula which represents the required linearity constraint. Thereafter, the obtained formula with the linearity constraint was used to co-simulate the values of the copper and gold conditions to their bivariate linearity relations by either accepting or rejecting the simulated values based on whether they meet the predefined constraint. Thus, the proposed algorithm provides more accurate and reliable results in the bivariate relationships of copper and gold than the conventional co-simulation approach that does not take into account the linearity constraint. Nonetheless, the use of hierarchical Gaussian co-simulation is restricted to the chemical elements, which show a poor correlation between them.

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1. INTRODUCTION

In the context of resource recovery and sustainable mining, the management and assessment of mine tailings—the byproducts of mineral extraction—become more and more important. In addition to posing a threat to the environment through acid mine drainage, dust dispersal, and possible dam collapses, mine tailings offer a substantial opportunity for the extraction of secondary resources, especially critical raw materials (CRMs) like cobalt, which are crucial for green energy technologies (Nwaila et al., 2021). The promotion of utilization of mining waste is now on high priority since the advancement in the use of CRMs is becoming popular worldwide, this is due to its usage in the high-tech and renewable energy industries. This is being achieved through the systematic assessment of resource potential within tailings storage facilities in an effort to pursue sustainable supply chains and reduce the geopolitical rivalry associated with the exploitation of the primary resources (Parviainen et al., 2020).

The resources of the mine tailings have been estimated using geostatistical methods such as kriging and sequential Gaussian simulation, which are ways of understanding spatial distribution of metals and other valuable materials in the deposit (Deutsch et al., 2014). However, when dealing with variability and uncertainty of materials in the tailings these approaches tend to rely on stationarity of data and they have shortcomings (Pyrz & Deutsch, 2005). These challenges could be overcome and the generation of more realistic and accurate mine tailings resources evaluation by employing some of these unique sampling approaches such as acceptance-rejection sampling and hierarchical sequential Gaussian co-simulation. These, in turn, increase the efficiency of the resource estimation and allow to model the spatial correlations of several variables with consideration for their joint uncertainties (Rivoirard, 1994).

This study applies the proposed methodology to the Haveri mine tailings in Southwest Finland, a historical Copper-Gold mine site where 1,114 borehole assays were collected to assess reprocessing potential and environmental risks.

1.1 Problem Statement

Geostatistical assessment of mine tailings faces difficulties because of their complex natural variability as these conventional geostatistical methods prove ineffective. Ordinary kriging and traditional methods fail to maintain essential spatial correlations therefore leading to errors in estimating resource potentials (Nwaila et al., 2021; Rivoirard, 1994). The modeling methods often fail

to detect essential linear relationships and constraints between variables because it is necessary to generate geologically realistic resource models.

A key issue in modeling mine tailings is preserving the linear relationships that exist between variables, such as grade distributions of multiple metals. Therefore, a robust simulation-based approach that explicitly incorporates linear constraints is required.

A framework based on acceptance-rejection sampling enables hierarchical sequential Gaussian co-simulation to establish constraints which maximize estimation accuracy for multivariate systems. The simulation process includes linear dependencies directly which results in more reliable resource modeling and better resource recovery strategies and optimized mine waste management practices.

1.2 Thesis Objectives

I. Assess the current geostatistical methods for modelling tailings resource:

The research examines geostatistical modeling techniques that serve as complementary sources of valuable mineral extraction. Researchers commonly use sequential Gaussian simulation together with kriging and co-kriging methods to identify metal and valuable element distribution patterns in tailings according to Deutsch et al. (2014) and Pyrcz and Deutsch (2005). Although these approaches offer reliable structures for resource assessment, they have some drawbacks such as smoothing effects, stationarity assumption, and sparse data management. This study will focus on the advantages and disadvantages of each method, on how effective they are for different types of tailing deposits and how effective they are in minimizing uncertainty in resource estimation.

II. Determine Methodological Necessities for Geostatistical Modeling in Tailings Management:

The purpose is to determine what specific methodological requirements and conditions must exist for the use of specific geo-statistical modeling approaches in examining mine tailings. Some of these are the available data and the nature of the heterogeneity and spatial variability of the tailings and the physical and chemical environment of the site including the mineralogy and lithology of the deposits. For instance, locations with limited data and often very high variability of the grades could be better addressed with use of condition simulation method (Rivoirard, 1994). Through identifying these requirements, the paper will attempt to identify the best geostatistical techniques that can enhance the resource estimation in different mining scenarios like complicated multi-element resources in Chile and consolidated tailings in South Africa (Araya et al., 2020).

III. Examine Implementation Complexities in Geostatistical Modeling:

More precisely, the goal of this research is to explore the challenges and issues arising when imposing geostatistical methods to actual mining settings. It includes the need for high-quality data, the need for substantial computational resources, and the challenges posed by parameters in models like sequential Gaussian simulation and kriging (Nwaila et al., 2021). One also needs to measure the learning curve and how much experience is needed in order to properly implement these ideas. This analysis will help bring to light how much there could be a gap between how geostatistical concepts have evolved in theory, and how mining specialists apply them.

IV. Cover the Gaps Existent between Theory and Application of Geostatistical Analysis:

The main research goal is to minimize the gap between the industry-focused version of contemporary geostatistical techniques and the theoretical ideals that underpin them. Due to these problems highlighted earlier, the use of advanced techniques in practice has not been popularized. This study strives to expedite the resource estimation process by making complex models less complicated and more available for field application. It will assist in developing new resource estimation methods that better fit the users, are easy to use and efficient according to the operational environments of mining companies through the demonstration of the usefulness of improved models through application, for instance, valorization of the mine waste in the Central African Copperbelt (Nwaila et al., 2021).

1.3 Significance to the industry

The use of improved methodologies such as complicated geostatistical modeling may change the mining industry particularly in determination and management of mine tailing. Among these, one is the suggested hierarchical sequential Gaussian co-simulation method using the acceptance-rejection sampling method. The mining industry realizes increasing pressure to improve the sustainability of mining operations, recover higher grades of desired metals and reduce the impact on environment and the communities as the demand for Critical Raw Materials is set to increase due to applications of high tech and green energy technologies (Nwaila et al., 2021).

Although resource estimation and spatial modeling have enhanced substantially due to the use of the conventional geostatistical methods like kriging, co-kriging, sequential Gaussian co-simulation and other methods, these methods are often restricted by the assumptions of stationarity, data density requirement and even lead to smoothing effects thus producing errors (Deutsch & Journel, 1992; Rivoirard, 1994). These limitations make it difficult to assess mine tailings, which are increasingly desirable as secondary resources for metals such as cobalt, copper, and REEs, because of their high variability and heterogeneity (Parviainen et al., 2020). However, the suggested co-simulation

algorithm will extend this range of applicability and provide more efficient, precise, and reliable estimations of tailings deposits, which will help the mining industry make better decision on the exploitation of the resources.

Importance of this project can be summed up to the following areas that are very critical in the mining sector:

- **Improved Resource Utilization and Recovery:** Through incorporation of spatial variability factors, such as variations in density, granulometry, lithology, and mineralogy, into the modeling process, the proposed geostatistical approach overcomes the drawbacks of current techniques. Therefore, resource estimations more accurate and makes it easier to find material in tailings storage facilities (TSFs) that is economically feasible. Better planning for reprocessing operations, optimizing the extraction of important metals from mine tailings, and reducing dependence on primary mining operations can all result from enhanced resource modeling accuracy (Blannin et al., 2022).
- **Sustainability and Mitigation of Environmental Impact:** As stated by Kossoff et al. (2014), the possibility of effective measures for managing the mine tailings is critical in mitigating the negative impacts of environmental problems like the acid mine drainage, metal leaching and other catastrophic tailing dam failures. Through the accurate estimation of the location and concentration of potentially toxic constituents in TSFs, the advanced modeling methodologies introduced in this study can be helpful in designing safer and better designs of tailings disposal facilities. This serves industry goals of sustainable practices and management of resources through identifying precise areas that need rehabilitation and hence lessen effects of mining on the environment (Nwaila et al., 2021).
- **Support for Circular Economy Initiatives:** Including potential tailings as assets allows the assessment of mine waste within the framework of the circular economy concepts. Mining Companies may have to assist in recovery of CRMs and mitigate supply risks by engaging in continuous geostatistical analysis of the resource base of tailings (Araya et al., 2020). However, the shift in the management of resources from the conventional linear model to circular model enhance the need for CRMs globally, while achieving economic growth and protection of the environment.
- **Enhanced Decision-Making and Risk Management:** The hierarchical sequential Gaussian co-simulation algorithm and the acceptance-rejection sampling procedures can be more efficient in dealing with data uncertainties and, correlations between one or more variables. It may also

reduce costs associated with resource misestimation and greatly improve the resource estimates (Pyrzcz & Deutsch, 2005). This contribution has significant implications for risk management and strategic planning because accurate and efficient models are essential to support the view of mine tailings as a valuable commodity.

- **Development of Technological Capabilities in Mining:** The introduction of progressively more sophisticated geostatistical methods, including machine learning and artificial intelligence in the modeling of resources is beneficial for the industry as a whole. Indirectly, this project leads to enhancement of technological capacity of the mining tailings evaluation and productivity in the long run by creating a foundation for more data driven methods (Nwaila et al., 2021).

In conclusion, the project provides solutions to existing research problems and contributes to the development of new approaches that can greatly benefit the mining industries. The advancements in geostatistical modeling will prompt the industry to embrace enhanced and responsible mining practices as the methodologies will improve resource recovery, enhance sustainability, support the circular economy, and reduce risks.

2. LITERATURE REVIEW

2.1 Simulation in Geostatistics and Its Limitations for Multivariate Datasets

Simulation techniques are widely used in geostatistics to model spatial variability and uncertainty in resource estimation. Conventional approaches, such as Sequential Gaussian Simulation, generate multiple realizations of a spatial variable while preserving its statistical properties and spatial continuity (Goovaerts, 1997). However, when applied to multivariate datasets, these methods often fail to accurately reproduce cross-correlations between variables, leading to inconsistencies in the spatial modeling of correlated attributes (Journel & Huijbregts, 1978).

One of the primary challenges in multivariate simulation is ensuring that inter-variable relationships remain geologically realistic. Standard sequential simulation approaches either assume independence between variables or use simple correlation-based constraints, which may not be sufficient to maintain physical consistency (Deutsch & Journel, 1998). Additionally, conventional co-simulation techniques, such as co-kriging-based approaches, often suffer from computational inefficiencies and stability issues, particularly in sparse or highly variable datasets (Goulard & Voltz, 1992).

2.2 Co-Simulation Methods and the Advantages of Hierarchical Approaches

Co-simulation methods have been developed to jointly model multiple spatial variables while preserving their interdependencies. Traditional co-simulation approaches, such as co-kriging-based

co-simulation, rely on modeling cross-variograms and require direct and cross-covariance structures to be well-defined (Chiles & Delfiner, 2012). However, these methods present several challenges, including:

- Computational complexity: The need to model and invert large covariance matrices makes co-kriging computationally expensive (Goovaerts, 1997).
- Instability in weakly correlated datasets: When variables exhibit weak cross-correlation, co-kriging-based models may produce unreliable results (Goulard & Voltz, 1992).
- Difficulties in enforcing linearity constraints: Many traditional approaches do not explicitly incorporate geological or physical constraints, potentially leading to unrealistic results (Madani & Abulkhair, 2020).

Hierarchical co-simulation approaches solve this issue through sequence-based variable simulation that uses conditional dependencies. The hierarchical model structure enables improved modeling performance especially when modeling datasets characterized by complex dependencies. The hierarchical structure improves constraint management during multivariate spatial modeling and establishes this method as a strong alternative (Emery, 2005).

2.3 Hierarchical Co-Simulation with the Acceptance-Rejection Method

The acceptance-rejection sampling technique applied to hierarchical co-simulation provides enhanced reliability of simulated values by maintaining simulated values within predefined constraints. The method works best when physical or geochemical relationships limit possible simulation values.

The acceptance-rejection method generates variable values to accept only those which satisfy the necessary constraints and thus maintains spatial variability with inter-variable consistency (Madani & Abulkhair, 2020). Researchers have found substantial value in applying this method for multiple study objectives:

- Enforcing linear constraints between variables: Ensuring that simulated values maintain realistic relationships based on known physical and chemical processes (Goulard & Voltz, 1992).
- Handling linearity constraints in multivariate spatial datasets: Preventing non-physical values from being included in simulations (Madani & Abulkhair, 2020).

- Improving the accuracy and stability of resource models: Leading to more reliable resource assessments and better-informed decision-making in mine waste and resource management (Emery, 2005).

By integrating hierarchical co-simulation with acceptance-rejection sampling, the accuracy and stability of multivariate geostatistical models can be significantly improved, addressing key limitations of traditional simulation and co-simulation methods.

3. METHODOLOGY

3.1 Hierarchical Sequential Gaussian Co-simulation

The proposed methodology facilitates geostatistical modeling of mine tailings by treating correlated variables with established linear relationships using a hierarchical sequential Gaussian co-simulation algorithm. This approach maintains spatial continuity and natural dependency constraints through acceptance-rejection sampling, ensuring that the simulated data honors both geological patterns and variable relationships.

The simulation workflow (Figure 1) begins with regression analysis to define the relationship between the auxiliary and target variables. This step involves fitting a regression line to the bivariate distribution and adjusting it to enforce a linearity constraint, ensuring that all data points lie on the correct side of the constraint, depending on the direction of the inequality. These constraints are fundamental in preserving the physical and geochemical characteristics of the dataset.

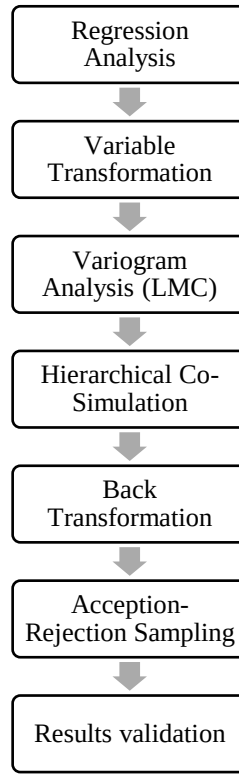


Figure 1. Hierarchical Sequential Gaussian Co-simulation Workflow Overview

To incorporate such relationships, the linearity constraint is expressed as:

$$Z_2 \leq aZ_1 + b$$

Where:

- Z_1 : Auxiliary variable grade
- Z_2 : Target variable grade
- a : Slope of a fitted regression line
- b : Intercept of a fitted regression line

This constraint may also be applied in both directions, enforcing upper and lower bounds to more fully capture the underlying geochemical relationships (Figure 2).

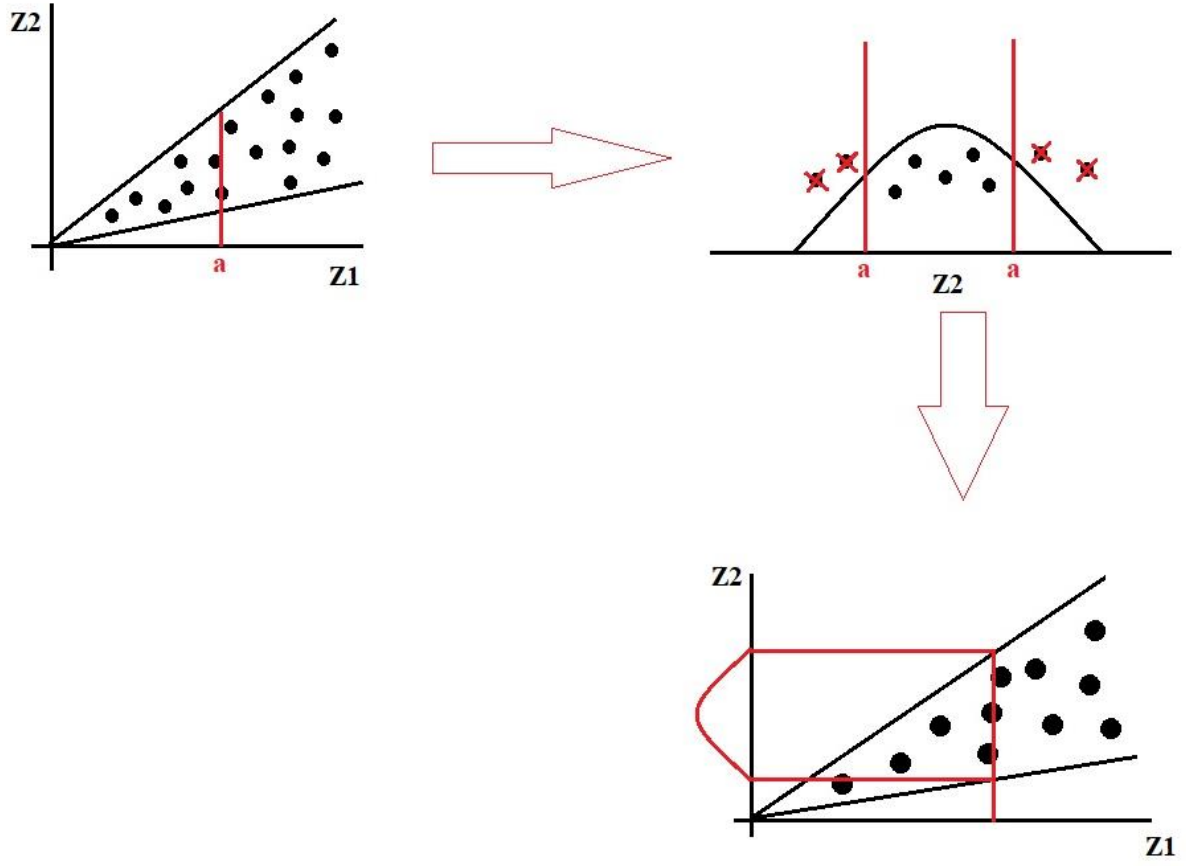


Figure 2. Visualization of the transformation process, where the red boundary defines the linearity constraint, ensuring that data points (black dots) remain within the constraint region.

The linearity constraint incorporated into the simulation process ensures that both local and global statistical properties remain consistent with observed geological patterns. In this approach, linearity can be imposed from both sides, meaning that the simulated variables must satisfy an upper and a lower bound, rather than just a single constraint.

The key innovation of this thesis lies in integrating this two-sided linearity directly into the hierarchical Gaussian co-simulation process through an acceptance-rejection sampling method. Unlike conventional approaches that either disregard such constraints or handle them separately, this method seamlessly incorporates them within the simulation framework.

Following this, the variables are transformed to a normal distribution, a prerequisite for Gaussian co-simulation. A linear coregionalized model is then applied to analyze spatial variability and inter-variable relationships. The hierarchical co-simulation process generates spatial multivariate distributions that preserve these dependencies throughout simulation.

The acceptance-rejection sampling method acts as a filter, verifying that simulated values satisfy the imposed linear constraints. After simulation, results are back-transformed to the original data scale to ensure geological interpretability. The final stage includes model validation using statistical and spatial analyses to confirm accuracy and reliability.

The key innovation of this methodology is the seamless integration of two-sided linearity constraints into the co-simulation process, ensuring that simulated outputs not only reproduce local variability but also adhere to known geochemical and mineralogical trends—something conventional methods often neglect or treat as a post-processing step.

3.1.1 Hierarchical Sequential Gaussian Co-Simulation

Hierarchical sequential Gaussian co-simulation (Goovaerts, 1997) represents a robust approach for modeling correlated variables with their defined linearity constraints. The technique takes sequential Gaussian simulation as its basis to create a hierarchy where an auxiliary variable gets simulated first before targeting the main/auxiliary variable.

The process involves the following key steps:

- i. Variables are ranked based on their spatial continuity and data availability. The choice of an auxiliary variable depends on data availability when handling heterotopic sampling data. However, both variables are available throughout all locations because this study adopts a homotopic sampling pattern. The auxiliary variable is chosen for its stronger spatial continuity relative to the target variable, enhancing the reliability of the co-simulation process.
- ii. Both variables are transformed into Gaussian-distributed normal scores using a quantile-based normal score transformation (Deutsch & Journel, 1998). This transformation ensures that the variables satisfy the multi-Gaussian assumption, which is required for co-simulation. The process involves mapping the empirical cumulative distribution function of the original variable Z_j to a standard normal cumulative distribution function G , as follows:

$$Y_j = G^{-1}\left(F(Z_j)\right), j = 1, 2$$

Where G^{-1} the inverse of the standard normal cumulative distribution function, and $F(Z_j)$ is the empirical cumulative distribution function of the original variable. This transformation

standardizes the variable, ensuring that it follows a normal distribution, which simplifies the subsequent co-simulation steps.

- iii. This step involves inferring the Linear Model of Coregionalization (LMC) by analyzing direct and cross-variograms to characterize spatial continuity and the relationships between variables.
- iv. Simulation of Auxiliary Variable (Y_1):
 - The auxiliary variable is simulated first using simple co-kriging (SCK) to obtain the conditional cumulative distribution function (CCDF). The formula for generating realizations of the auxiliary variable is:

$$Y_1^m = Y_1^{SK}(u_i) + \sqrt{\sigma^{SK}(u_i)} \cdot U_i^m$$

where:

- $Y_1^m(u_i)$: The m -th realization of the auxiliary variable at location u_i
 - $Y_1^{SK}(u_i)$: The simple co-kriged estimate of the auxiliary variable at location u_i , calculated using both auxiliary and primary data.
 - $\sigma^{SK}(u_i)$: The simple co-kriging variance, representing the uncertainty in the estimate at location u_i .
 - U_i^m : A standard Gaussian random variable ($U \sim N(0,1)$) that introduces the stochasticity required for simulation.
- The CCDF parameters (mean and variance) are used to generate realizations for Y_1 at each grid node. This ensures that Y_1 are conditioned on prior simulations, as well as both auxiliary and primary data, preserving spatial relationships and cross-dependencies.
- v. Simulation of Target Variable (Y_2):
 - The target variable simulation utilizes multi-collocated co-kriging that incorporates the Y_1 auxiliary data as well as previously generated Y_2 variables. The process to create target variable realizations follows this formula:

$$Y_2^m(u_i) = Y_2^{SMCK}(u_i) + \sqrt{\omega^{SMCK}(u_i)} \cdot U_i^m$$

- This step involves calculating CCDF parameters for Y_2 based on the spatial data and the simulated Y_1 at the same location.
- vi. After simulation completion, the normal score values (Y_1 and Y_2) need back-transformation to their original distribution.
- vii. Finally, the back-transformed value of the target variable is checked to ensure it adheres to the predefined constraints. If it falls within the upper and lower constraint boundaries, the value is accepted. Otherwise, it is rejected and re-simulated until it meets the constraints.

Unlike traditional sequential Gaussian co-simulation, which may struggle with maintaining spatial consistency and cross-correlation structure, the stepwise hierarchical method explicitly integrates these aspects. By first simulating the auxiliary variable and then using it to condition the target variable, this approach ensures that both spatial relationships and linearity constraints are upheld throughout the simulation process.

3.1.2 Acceptance-Rejection Sampling

The method proposed in this study enhances the conventional hierarchical co-simulation framework by incorporating acceptance-rejection sampling to enforce linearity constraint between simulated values at each simulation step. While it builds upon the approach introduced by Madani and Abulkhair (2020)—who applied a single linear constraint within the acceptance-rejection process—this study introduces a novel refinement by enforcing constraints between two bounding lines. This modification allows for more nuanced control, ensuring better adherence to both spatial and statistical relationships. The acceptance-rejection process involves:

- i. A value for Y_2 is simulated at a grid node using the hierarchical co-simulation algorithm.
- ii. The simulated value is checked against two linearity constraint expressed as:

$$L_1(Z_1) \leq Z_2 \leq L_2(Z_1)$$

Where $L_1(Z_1)$ and $L_2(Z_1)$ define the two bounding constraints rather than a single line, ensuring that the simulated values remain within an acceptable range.

- iii. Check the value if it meets predefined constraint:
 - If the simulated value satisfies the linearity constraint, it is accepted and added to the dataset.

- If it violates the constraints, the value is discarded, and a new value being simulated at that location until the constraint is satisfied. The procedure repeats itself until the requirement becomes valid.

This method ensures simulated realizations maintain predefined constraints together with variable spatial patterns and statistical characteristics.

3.2 Computational Environment and Software Specifications

The hierarchical sequential Gaussian co-simulation algorithm with acceptance-rejection sampling was implemented and executed using MATLAB R2022b. The selection of MATLAB was based on its robust capabilities for statistical analysis, matrix operations, and efficient handling of large datasets typically encountered in geostatistical simulations.

The simulations were carried out on a personal computer with the following specifications:

- Processor: Intel Core i7-8700H CPU 3.20 GHz
- RAM: 16 GB
- Operating System: Windows 11 Enterprise
- GPU: No dedicated GPU acceleration was utilized.

The simulation time differed significantly between the two approaches. The conventional hierarchical co-simulation required approximately 2–3 days to complete 100 realizations. In contrast, the hierarchical approach with acceptance-rejection sampling took approximately one month to generate the same number of realizations. The substantial increase in computational time for the proposed method is primarily due to the iterative nature of the acceptance-rejection process, where multiple simulated values must be discarded and re-simulated until they satisfy the linearity constraints.

4. RESULTS

4.1 Case Study

The Haveri mine ceased operations in the mid-20th century, and its tailings dam is now a closed and static facility, making it ideal for resource evaluation without the influence of ongoing deposition. This research analyzes the former Haveri mine tailings in Finland through 1,114 assay measurements of copper and gold that were obtained from drilled borehole data. These samples allow for a comparison between conventional hierarchical co-simulation and its extension incorporating acceptance-rejection approach to evaluate their effectiveness in preserving spatial relationships,

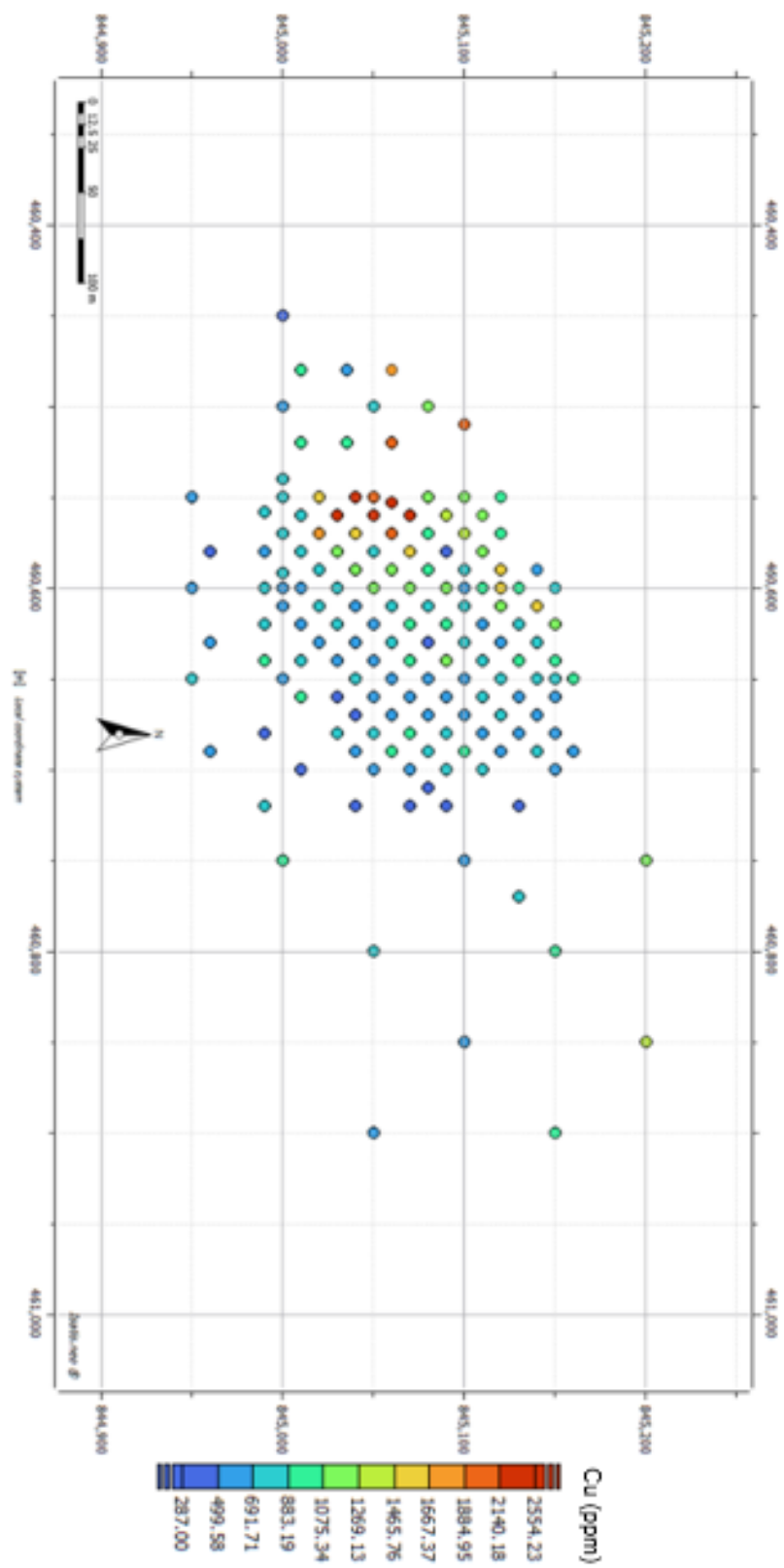
handling cross-correlation, and enforcing constraints. The hierarchical method is expected to provide improved spatial continuity and better respect the underlying linear constraints compared to conventional methods.

In the analysis, the primary focus is on Copper (Z_1), selected for its robust spatial continuity and consistent data distribution. The dataset consists of 1,114 assay measurements obtained from drilled boreholes, where samples were composited at length of 1 meter. The initial simulation employs Sequential Gaussian Simulation for Copper. Following this, Gold (Z_2) is addressed as the secondary variable, with its simulation being conditional on the simulated auxiliary Copper values. To maintain the integrity of the bivariate relationship and adhere to linearity constraints, the simulation of Gold incorporates acceptance-rejection sampling.

The Haveri mine tailing sampling distribution patterns of copper and gold can be observed through the visual 2D maps shown in Figure 4. These maps illustrate the spatial distribution of metal concentrations across the study area, highlighting variability in assay values.

The spatial variability of Copper (Cu) and Gold (Au) reveals distinct patterns. Higher Copper values are clustered in the central-western region, suggesting areas with significant residual metal content, likely due to historical processing inefficiencies. In contrast, lower Copper values are more dispersed toward the edges, indicating areas with greater dilution or natural dispersion over time. Similarly, Gold (Au) exhibits a less continuous spatial pattern, with localized high concentrations near the central regions but more scattered lower values throughout the deposit.

These spatial trends play a crucial role in guiding the simulation process, ensuring that the proposed co-simulation approach with acceptance-rejection method accurately captures the underlying spatial continuity and cross-correlation between Copper and Gold.



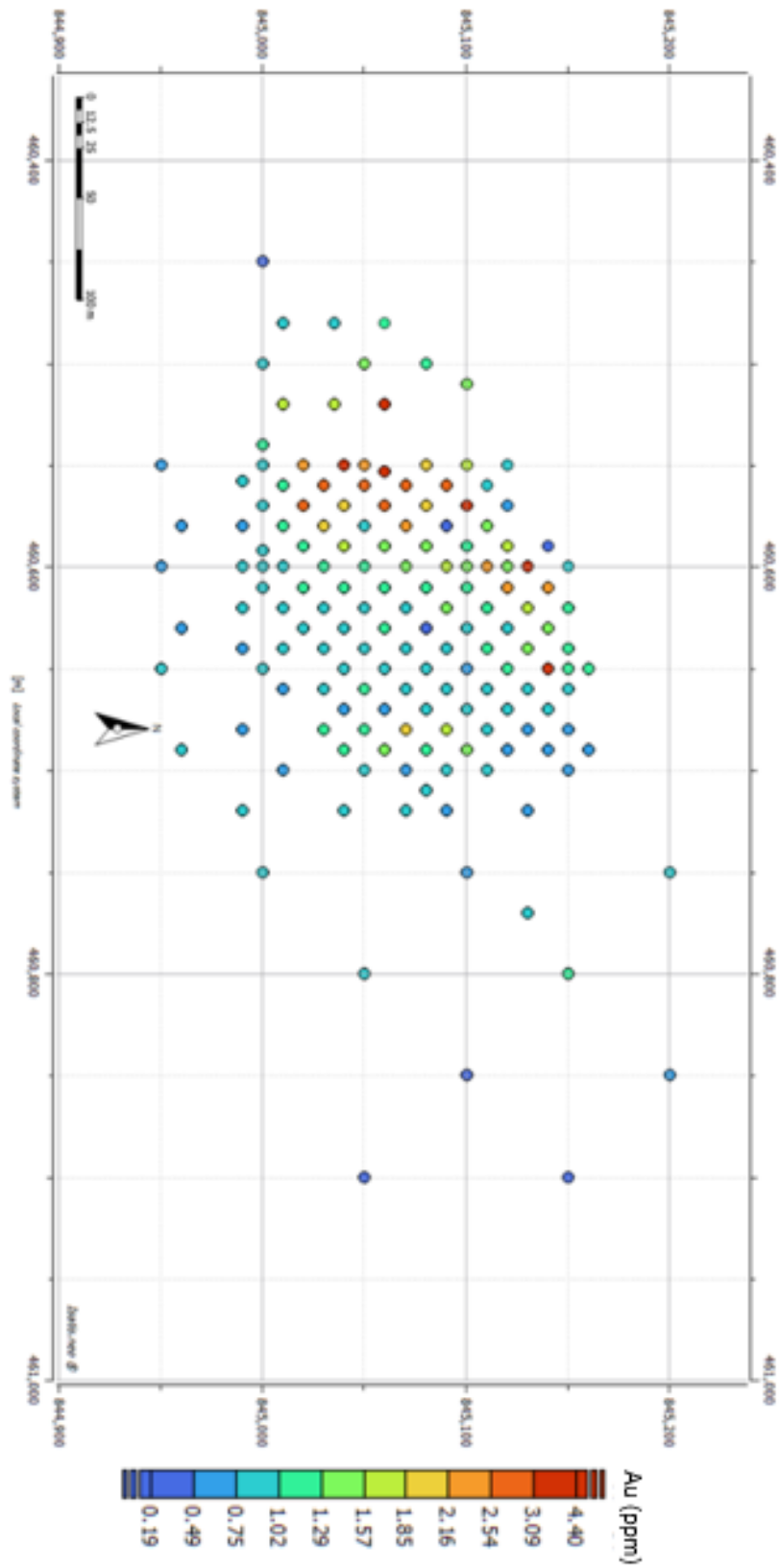


Figure 3. 2D location map of the Copper (on top) and Gold (bottom) dataset
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4.2 Exploratory Data Analysis (EDA)

An exploratory data analysis of copper and gold from the Haveri mine tailings serves to understand the global distribution of the data. The data preparation process included data cleaning along with solutions for typical problems like errors, missing data points, outliers and clustering effects.

4.2.1 Errors and Missing values

Exploratory data analysis started with checking the dataset by verifying the presence of errors that included missing values, duplicates, and negative assay values for these two variables. The dataset underwent complete analysis which revealed no errors and no missing values and no duplicated data points.

4.2.2 Outliers

After cleaning the dataset, the next step requires addressing outliers since they may impact simulation results. Histograms are effective tools for detecting outliers, providing a clear visual representation of data distribution. Outliers were treated using the capping mechanism (Genton & Hall, 2016), which involves downgrading extremely high values to a maximum acceptable threshold or upgrading extremely low values to a minimum acceptable threshold. This method helps mitigate the influence of extreme values while preserving the overall distribution of the data, ensuring that the simulation results are not overly distorted by anomalous high or low assay values.

Figure 4 below illustrate the capped histograms for copper and gold grades, respectively.

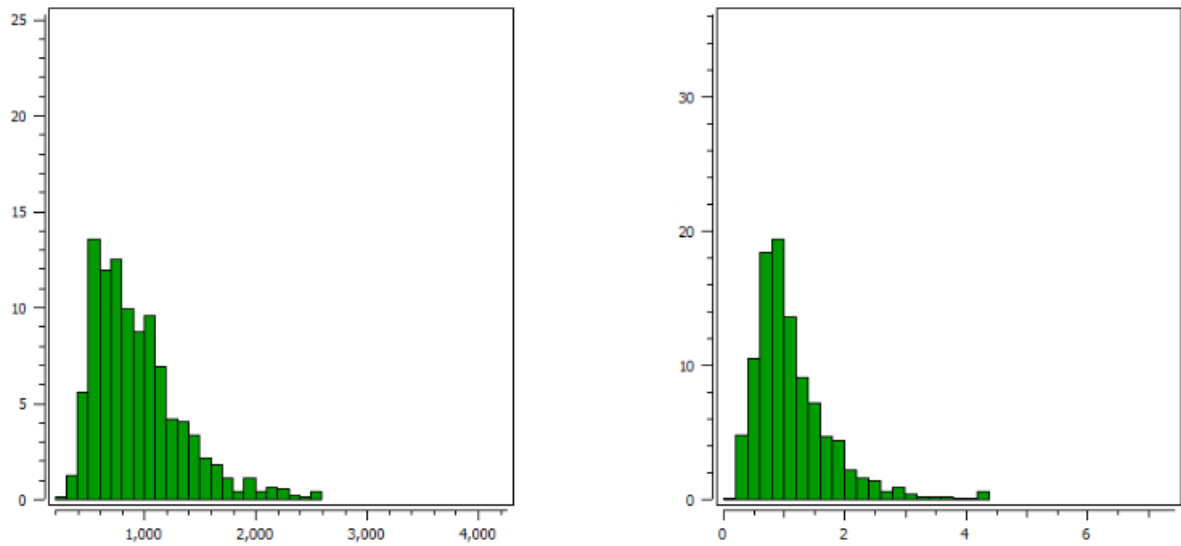


Figure 4. Histograms of copper (left) and gold (right) grades after capping.

4.2.3 Declustering

The next step in exploratory data analysis is declustering, which is essential for obtaining unbiased statistical representations of the dataset. In geostatistics, declustering adjusts for uneven spatial sampling to prevent areas with dense sampling from disproportionately influencing statistical summaries (Deutsch, 2017).

In Haveri mine tailings, cell declustering was applied in order to distribute appropriate weights to samples through spatial density methods (Deutsch & Journel, 1998). The research area was partitioned into cellular sections while denser zones possessed reduced weights when compared to areas with sparse distribution. The method provides better statistical parameter estimation particularly in calculating copper and gold grade averages.

The determination of optimal cell size involved a declustering sensitivity analysis which produced the results shown in Figure 5. Different declustering window sizes demonstrate varying weighted mean grade patterns in the graphic representation. The raw mean (933.6 ppm), represented by the dashed red line, and overestimates the actual distribution due to sampling bias. The weighted mean (837.7 ppm) stabilizes at an optimal window size of $96.8421 \times 96.8421 \times 0.0875$ m, highlighted by the red diamond in the graph. This optimal size minimizes the influence of high-density sampling regions while preserving spatial trends in lower-grade areas.

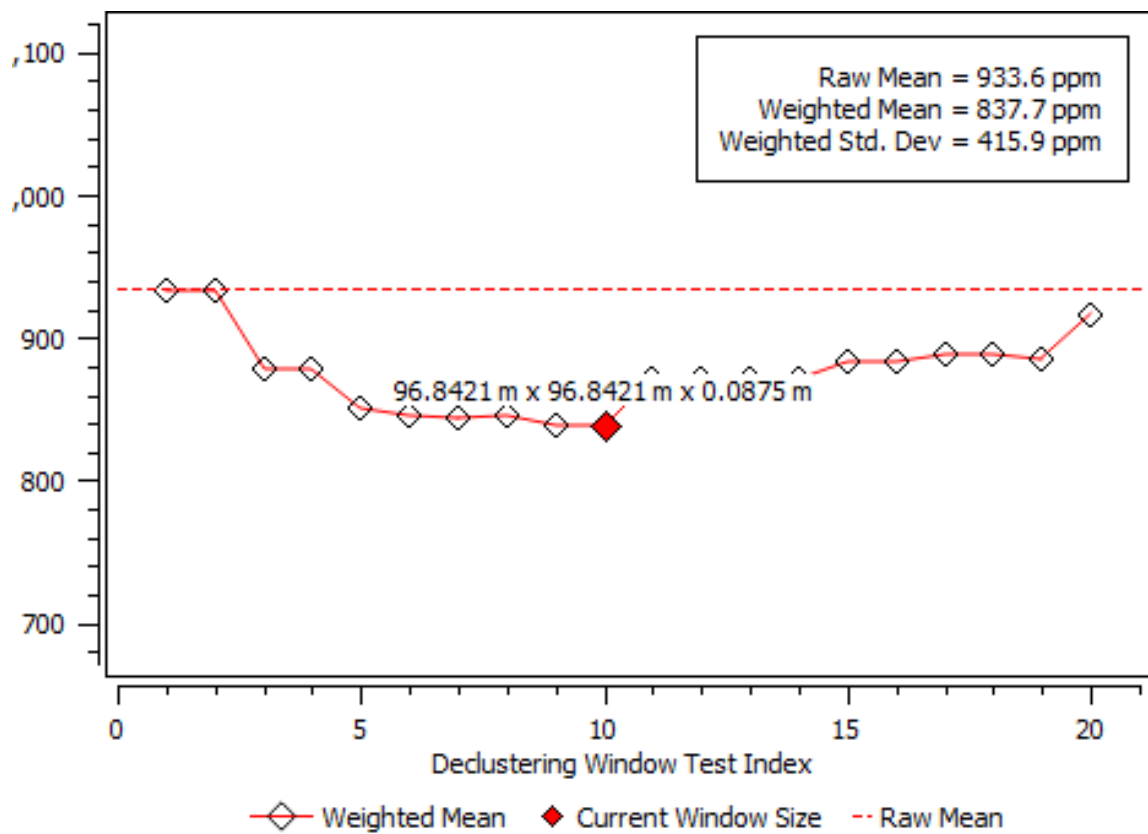


Figure 5. Declustering Sensitivity Analysis for Copper and Gold Assay Data

4.2.4 Statistical analysis

The declustering process yielded the statistical parameters presented in Table 1. For copper, the mean grade is 837.7 ppm, with a standard deviation of 415.9 ppm, resulting in a coefficient of variation (CoV) of 0.50. This indicates a moderate level of variability in copper distribution.

Similarly, gold exhibits a mean grade of 0.908 ppm and a standard deviation of 0.646 ppm, yielding a CoV of 0.71. The higher CoV for gold suggests that its relative variability is greater than that of copper. This highlights that gold concentrations are more spatially heterogeneous, while copper values are relatively more homogenous across the study area.

Table 1. Declustered statistical parameters of Copper and Gold dataset

Statistical parameter	Mean	Standard deviation	Coefficient of variation (CoV)	Correlation coefficient
Copper(ppm)	837.7	415.9	0.50	0.64
Gold(ppm)	0.908	0.646	0.71	

The linear correlation coefficient between copper and gold is 0.64 (Table 1), demonstrating a strong positive linear relationship (figure 6). This high correlation is significant, as it supports the application of co-simulation. The strong correlation ensures that the auxiliary variable (copper) can reliably guide the simulation of the target variable (gold), maintaining spatial continuity and cross-correlation between the two.

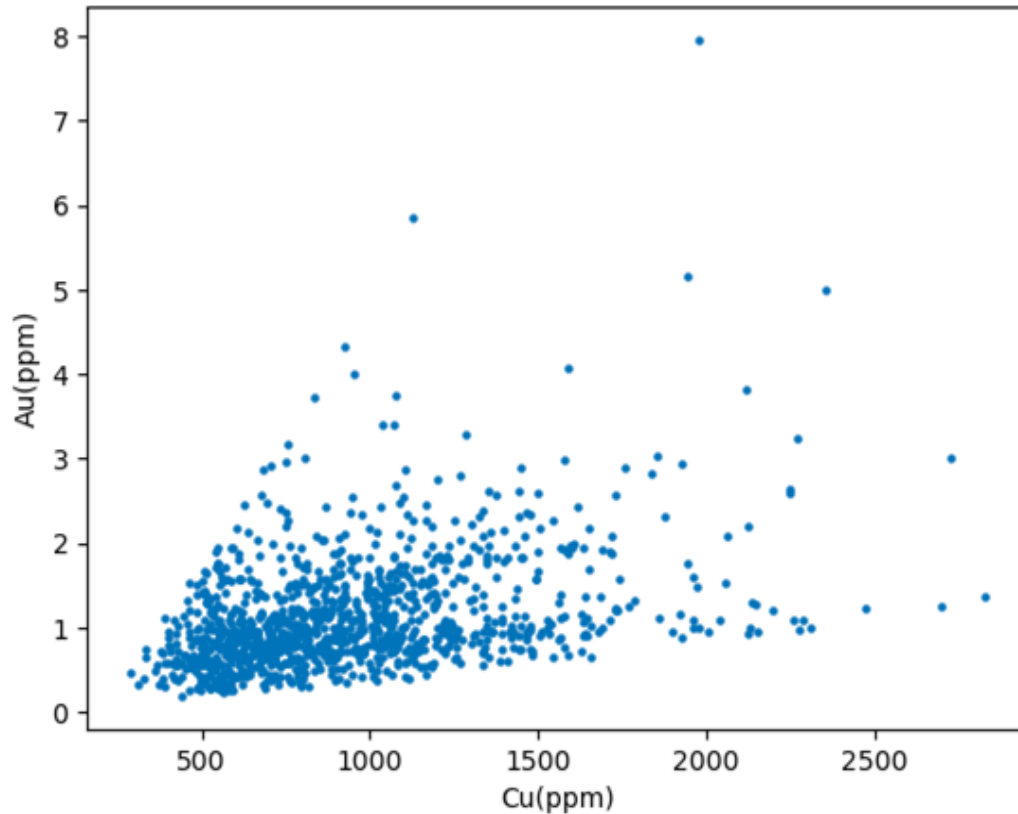


Figure 6. Scatterplot of Copper and Gold

The presence of well-defined upper and lower boundaries in the scatterplot is crucial for our simulation. These constraints will be mathematically formulated and incorporated into our hierarchical sequential Gaussian co-simulation to ensure that the simulated Gold values remain geologically realistic while preserving the observed data trends. By enforcing these constraints, the simulation will maintain spatial continuity and honor the natural relationship between Copper and Gold.

4.3 Fitting the linearity constraints

Once the constraints for the scatterplot are recognized, the upper and lower boundaries will be defined and visualized by drawing constraint regression lines, as shown in Figure 7. These boundaries will

serve as mathematical limits to guide the co-simulation. Next, the coefficients for the corresponding formulas will be derived, ensuring that the simulated values adhere to the desired linearity constraints. By incorporating these constraints into the hierarchical sequential Gaussian co-simulation, the realistic relationship between Copper and Gold will be maintained, preserving both spatial continuity and cross-correlation in the generated data.

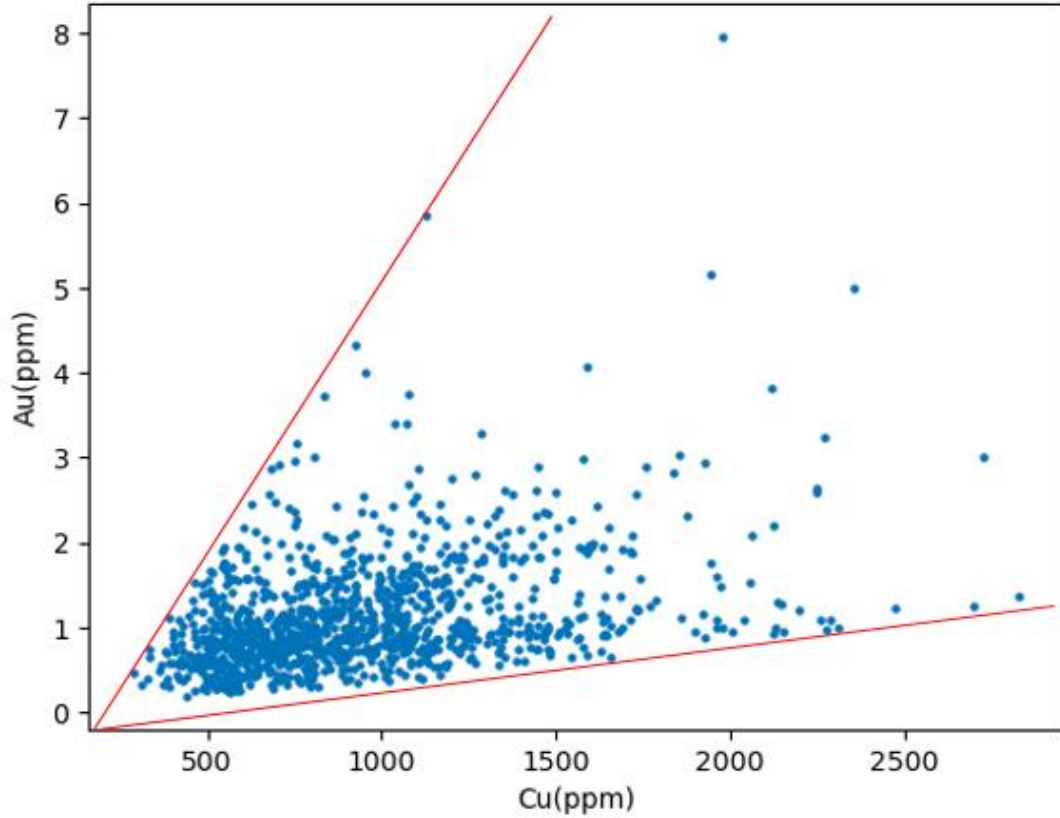


Figure 7. Upper and lower constraints of Copper and Gold dataset

The equations defining these constraints were obtained through empirical analysis of the scatterplot, assessing the general trend of data points and their natural upper and lower limits. The lower constraint is represented by the equation:

$$Au = 0.00048Cu - 0.14$$

while the upper constraint is given by:

$$Au = 0.0061Cu - 1.1667$$

These constraints were determined by examining the data distribution and defining linear approximations that capture the minimum and maximum expected values of Gold for a given Copper concentration.

The presence of these boundaries in the dataset can be attributed to natural geological and geochemical processes. The lower boundary suggests a threshold below which gold concentrations are rarely observed for a given copper content, possibly due to co-mineralization patterns or metal partitioning during ore formation. Conversely, the upper boundary may reflect a natural enrichment limit, where the deposition of gold relative to copper does not exceed a specific ratio, potentially due to metal solubility constraints or mineralogical associations in the tailings.

By integrating these constraints into the hierarchical sequential Gaussian co-simulation, the generated gold values will adhere to the observed linearity relationships while preserving both spatial continuity and cross-correlation with copper.

4.4 Variogram Analysis

4.4.1 Transformation to Gaussian distribution

To apply the Hierarchical Sequential Gaussian Co-simulation algorithm, it is essential to ensure that the variables conform to the multivariate Gaussianity assumption. To achieve this, the dataset was first transformed into normal scores, considering their respective declustering weights. This transformation ensures that each variable individually follows a standard normal distribution, a necessary condition for multi-Gaussian co-simulation.

The normal score transformation was performed using a quantile-based approach, where the empirical cumulative distribution function (CDF) of the declustered raw data was matched to the standard normal CDF (Deutsch & Journel, 1998). This method assigns each data value a normal score based on its quantile rank, effectively reshaping the distribution to follow a Gaussian form while preserving the original ranking of values.

Figures 8a and 8b illustrate that, after the transformation, both variables exhibit a Gaussian distribution, confirming univariate Gaussianity. However, verifying univariate normality alone may not be sufficient to confirm multivariate normality. Therefore, the scatterplot of the normal score variables was further examined (Figure 8c). The scatterplot reveals a characteristic elliptical shape, indicating that the relationship between the two variables is well approximated by a linear correlation structure. Additionally, the correlation coefficient of normal scores was calculated as 0.60. While this value is slightly lower than before the transformation, it still demonstrates a reasonable correlation, supporting the assumption of a joint Gaussian distribution.

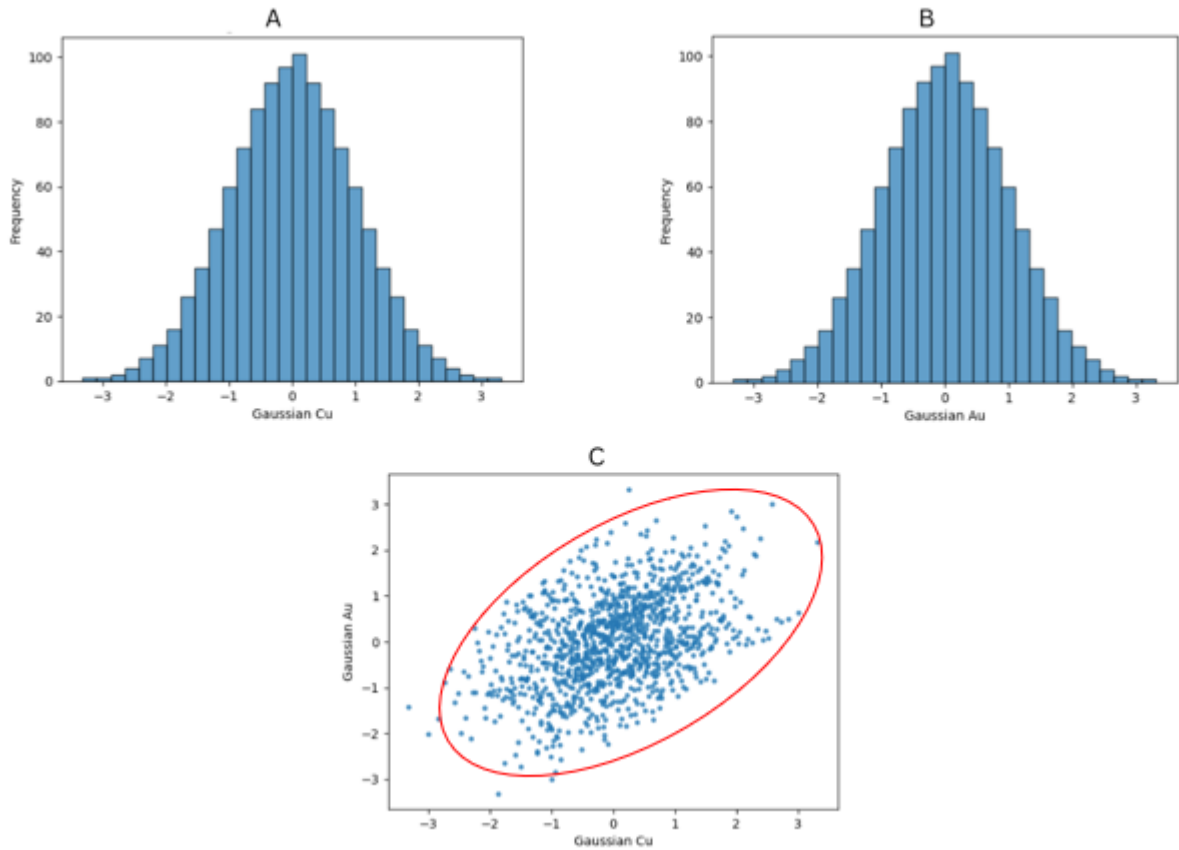


Figure 8. Histogram of normal scores of Copper (a) and Gold (b); Scatter plot between normal scores of Copper and Gold (c)

Given these observations, the dataset can reasonably be concluded to follow the multivariate Gaussian assumption, allowing for confident progression to the next steps of the Hierarchical Sequential Gaussian Co-simulation algorithm.

4.4.2 Linear Model of Coregionalization

Once the dataset was transformed to normal scores, anisotropy in the data was identified along two principal directions: horizontal and vertical. To analyze spatial continuity and variability in these directions, experimental variograms were computed and plotted along both axes. These variograms characterize the spatial correlation structure.

Next, semi-automatic fitting of theoretical variograms was performed (Emery, 2010) to ensure they accurately represent the spatial characteristics of the dataset. The fitted models, shown in Figure 9, reveal the anisotropic nature of the data and serve as the foundation for further geostatistical analysis.

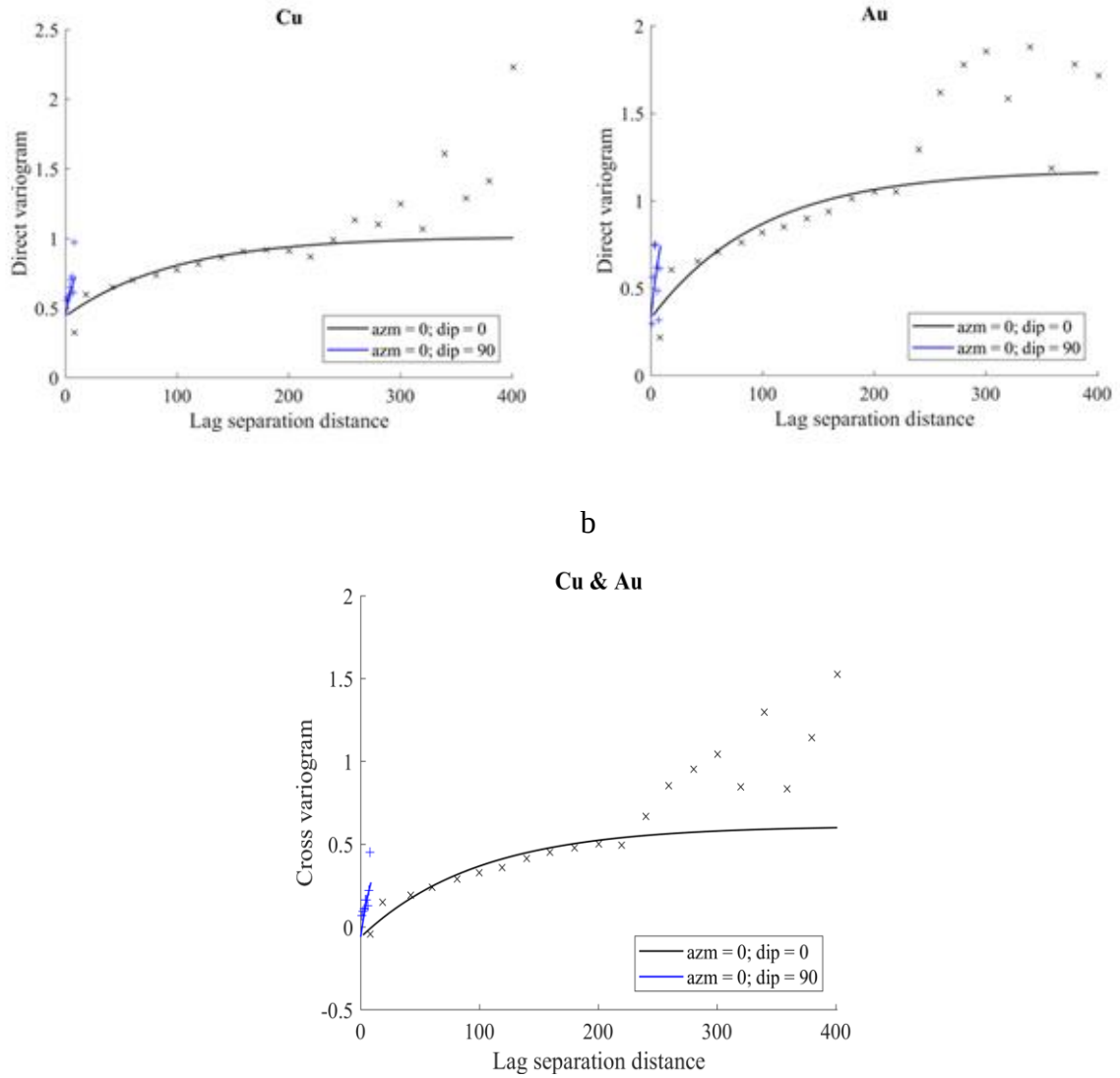


Figure 9. Direct variograms of Copper and Gold (a), and cross-variogram between Copper and Gold (b), shown along the horizontal (black) and vertical (blue) directions. Crosses represent the experimental variograms, while solid lines indicate the fitted variogram models obtained using the Linear Model of Coregionalization (LMC).

The Linear Model of Coregionalization (LMC) was used to infer spatial structure within the modeling process. LMC serves as a fundamental component that captures cross-correlations between variables without altering spatial anisotropy patterns. This step is essential for both Co-simulation methods in this study, as it relies on a well-defined coregionalization model to ensure consistency in simulated values across different variables.

The Linear Model of Coregionalization, including nugget and three structures is as follows:

$$\begin{pmatrix} y_{Cu} & y_{Cu} \\ y_{Au} & y_{Au} \end{pmatrix} = \begin{pmatrix} 0.28 & -0.02 \\ -0.02 & 0.15 \end{pmatrix} nugget + \begin{pmatrix} 0.36 & 0.00 \\ 0.00 & 0.00 \end{pmatrix} Cubic(62.9217m, 62.9217m, 5m) \\
+ \begin{pmatrix} 0.00 & 0.00 \\ 0.00 & 0.05 \end{pmatrix} Sph(107.81m, 107.81m, 785.575m) \\
+ \begin{pmatrix} 0.37 & 0.53 \\ 0.53 & 0.81 \end{pmatrix} Exp(249.77m, 249.77m, 5m)$$

By establishing an appropriate LMC, the hierarchical co-simulation process ensures spatial coherence and accurately accounts for the anisotropic behavior observed in the dataset.

4.5 Hierarchical and Conventional co-simulation

A comparative analysis is conducted between two co-simulation approaches: the conventional hierarchical and its extension using acceptance-rejection methods. This comparison aims to evaluate their effectiveness in preserving spatial relationships and statistical properties while differentiating their ability to enforce linearity constraints.

The hierarchical co-simulation with acceptance-rejection method begins with using a simple co-kriging in simulation of the auxiliary variable, Copper. The next step includes using multicollocated co-kriging for simulating the target variable, Gold, while enforcing linearity constraint in the simulation workflow.

Copper is selected as the first variable to simulate because it exhibits stronger spatial continuity, and a more stable statistical distribution compared to Gold. This stability makes copper a reliable foundation upon which the simulation of Gold can be conditioned. Additionally, Copper has a significant influence on Gold due to their geological relationship, making it a suitable auxiliary variable in the hierarchical framework.

Gold is simulated second because its pattern distribution shows irregularities along with higher variability. The hierarchical approach maintains the correlation and enforce linear constraints between Copper and Gold values by using the previously simulated Copper data as conditioning input. The systematic procedure produces geologically realistic representation of spatial relationships which improves the reliability of simulated data.

Conversely, the conventional hierarchical co-simulation approach uses search strategies that are similar to the hierarchical co-simulation with acceptance-rejection method (multi-collocated cokriging) but it does not account for linearity constraint.

The block dimensions of $10\text{m} \times 10\text{m} \times 0.5\text{m}$ are selected to balance geological accuracy and practical mining considerations. The 0.5m vertical resolution captures the thin-layered nature of tailings while aligning with the 1m composite sampling length, preventing excessive smoothing. This block size also ensures mining selectivity, allowing for precise ore-waste classification while remaining computationally efficient. Additionally, it reflects the spatial continuity of Copper and Gold within the deposit, ensuring that the simulation results are both geologically realistic and operationally viable.

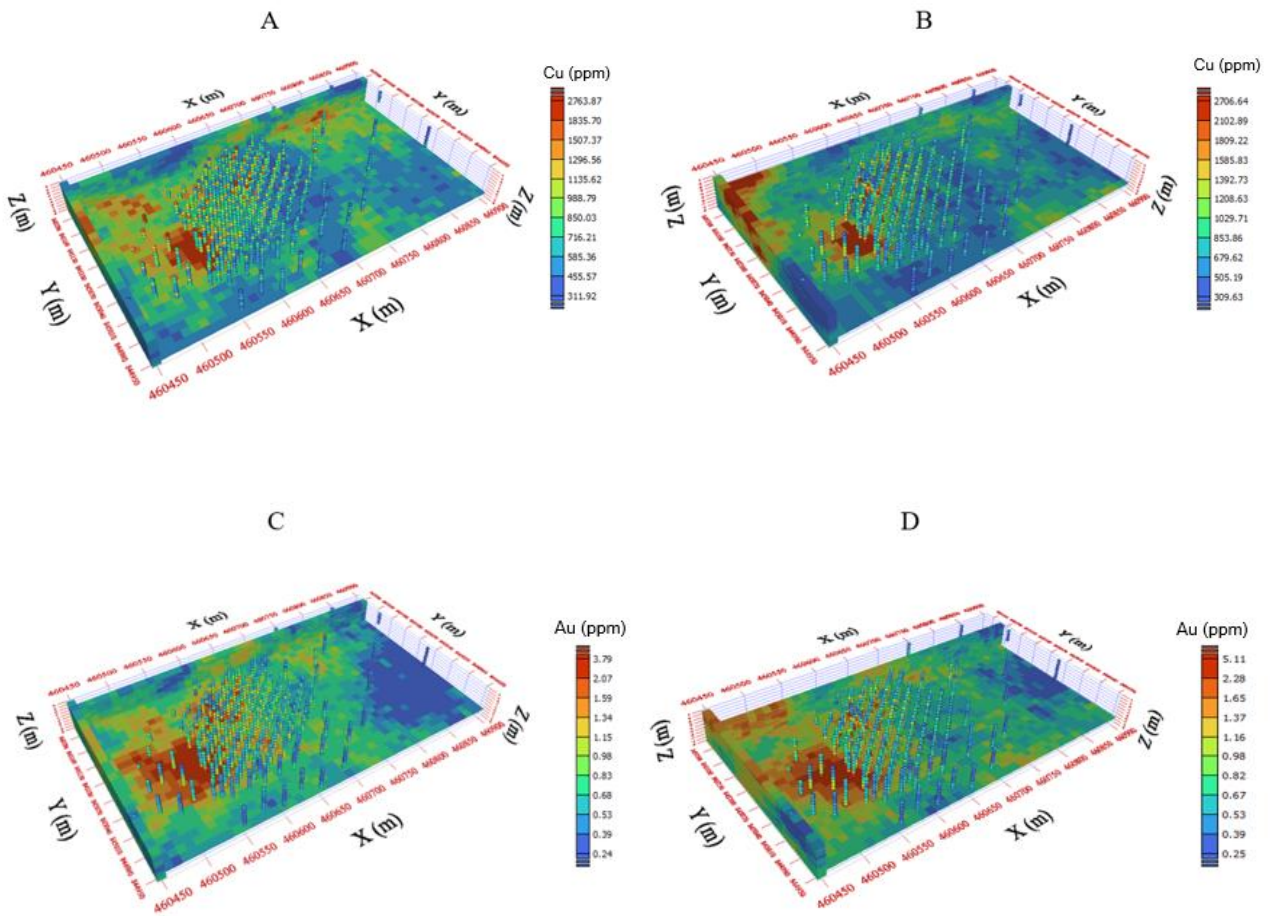


Figure 9. Realization #1 of copper and gold grades obtained from hierarchical co-simulation with acceptance-rejection method for (A) copper and (C) gold, and from conventional hierarchical co-simulation for (B) copper and (D) gold.

A visual representation of both co-simulation methods in Figure 10 displays one realization from each technique side by side. This comparison may not be enough to demonstrate how the hierarchical principles along with enforced linearity constraints differs from conventional co-simulation method. Additionally, Figure 11 presents E-type maps (average map) of Copper and Gold grades for both approaches. The hierarchical method with acceptance-rejection (A for Copper and B for Gold) exhibits slightly improved spatial continuity and better preservation of grade variations, particularly

in regions of high concentration. Conversely, the conventional hierarchical approach (C for Copper and D for Gold) produces smoother results, which may underestimate local variability. This comparison further highlights the advantages of the hierarchical framework in maintaining the correlation structure and enforcing linearity constraints, leading to a more geologically realistic representation of the deposit.

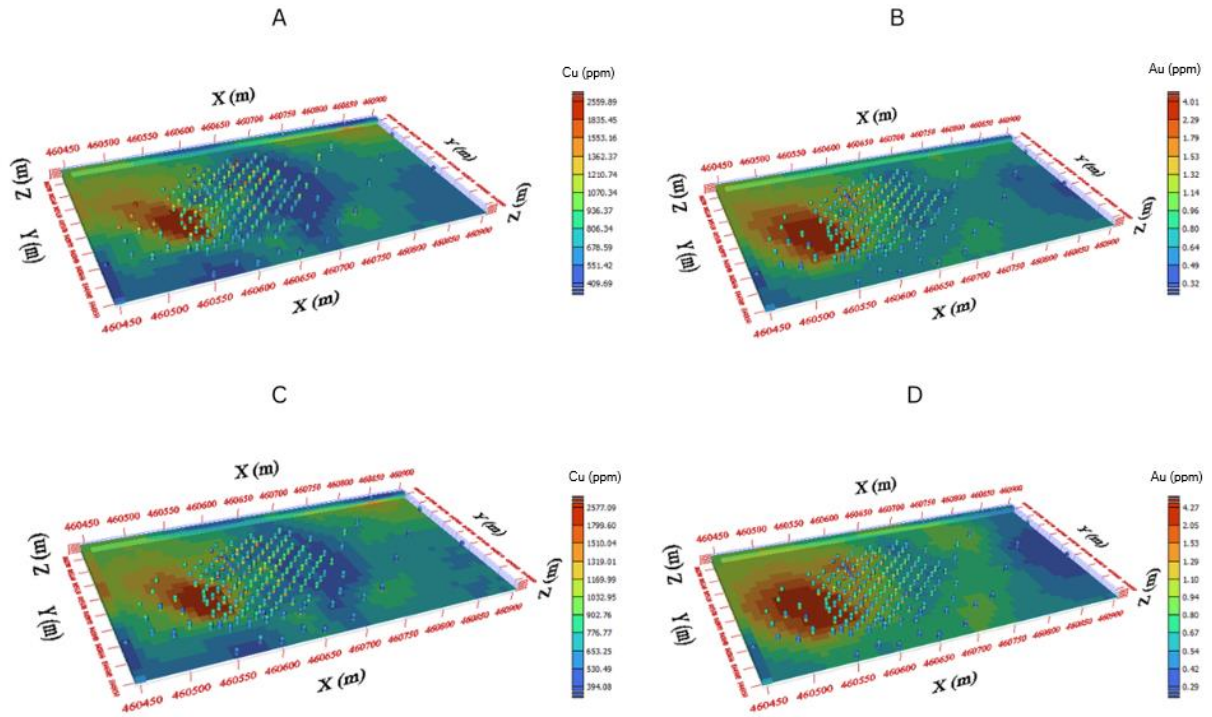


Figure 10. E-type map of copper and gold grades obtained from hierarchical co-simulation with acceptance-rejection method for (A) copper and (B) gold, and from conventional hierarchical co-simulation for (C) copper and (D) gold.

4.6 Results validation

Validation of results from both hierarchical with acceptance-rejection method and conventional hierarchical co-simulation is conducted to determine which methodology yields higher accuracy and more reliable outcomes. This study employs three validation procedures: evaluating local statistical parameters, assessing bivariate relationships, and utilizing jack-knife validation methods. By comparing metrics between hierarchical and conventional co-simulation approaches, data spatial continuity preservation and correlation maintenance can be effectively assessed.

4.6.1 Reproduction of local statistical parameters

The validation process begins by evaluating how well the generated realizations reproduce key statistical characteristics, including the mean grade, standard deviation, and correlation coefficient of the original dataset. First, each realization is individually assessed by computing these statistical parameters. Then, the values are averaged across all realizations and compared with those of the original dataset. This approach ensures that the simulation method preserves the essential statistical properties of Copper and Gold while maintaining their spatial relationships. The comparison is performed for both conventional hierarchical and hierarchical co-simulation with acceptance-rejection methods to assess their respective performance in reproducing the observed data characteristics.

As shown in Table 2, the hierarchical approach with acceptance-rejection method reproduces the mean values more closely to the declustered original dataset than the conventional hierarchical method, particularly for Copper (832.0 ppm vs. 823.8 ppm, compared to the original 837.7 ppm). A similar trend is observed in the correlation coefficient, where the hierarchical approach with acceptance-rejection method (0.59) is closer to the original dataset (0.64) than the conventional hierarchical method (0.74), which slightly overestimates the correlation. However, both methods show a notable reduction in standard deviation compared to the original dataset, with the hierarchical with acceptance-rejection method yielding slightly higher variability than the conventional one.

Table 2. Comparison of global statistical parameters

Statistical parameter	Declustered original dataset		Conventional hierarchical co-simulation		Hierarchical co-simulation with acceptance-rejection	
	Copper (ppm)	Gold (ppm)	Copper (ppm)	Gold (ppm)	Copper (ppm)	Gold (ppm)
Mean	837.7	0.9081	823.8	0.845	832.0	0.902
Standard deviation	415.9	0.6459	289.2	0.4488	296.9	0.4345
Correlation coefficient	0.64		0.74		0.59	

This difference in variability can be attributed to the way each method handles spatial correlation and data conditioning. The hierarchical approach, by simulating variables sequentially and conditioning each step on previously simulated values, tends to preserve local variability more effectively. This results in a more accurate reproduction of the original data's spatial heterogeneity, leading to higher variability measures. In contrast, conventional co-simulation methods may smooth out some of this variability due to their simultaneous simulation processes, which can average out local fluctuations. This smoothing effect often results in an underestimation of variability compared to the original dataset. For a comprehensive comparison of simulation algorithms and their impact on statistical

reproduction, refer to the study by Abulkhair and Madani (2021), which evaluates the performance of different simulation techniques in preserving statistical parameters.

The hierarchical approach with acceptance-rejection technique provides superior statistical data preservation than conventional hierarchical method while showing similar underestimation of variability between these techniques. In fact, the hierarchical approach with acceptance-rejection method provides enhanced reliability for co-simulation applications when it comes to reproduction of original global statistical parameters.

4.6.2 Jack-knife validation

Jack-knife validation operates as a statistical sampling method to assess prediction accuracy (Deutsch and Journel, 1998). To do so, the data splits into two sections where training data accounts for 70% and testing data represents 30% of the total. Co-simulations occur on test data locations using only the conditioning training data.

The simulated values at the test data locations were averaged to obtain the predicted values, which were then compared with the actual data at those locations to evaluate the accuracy of each method.

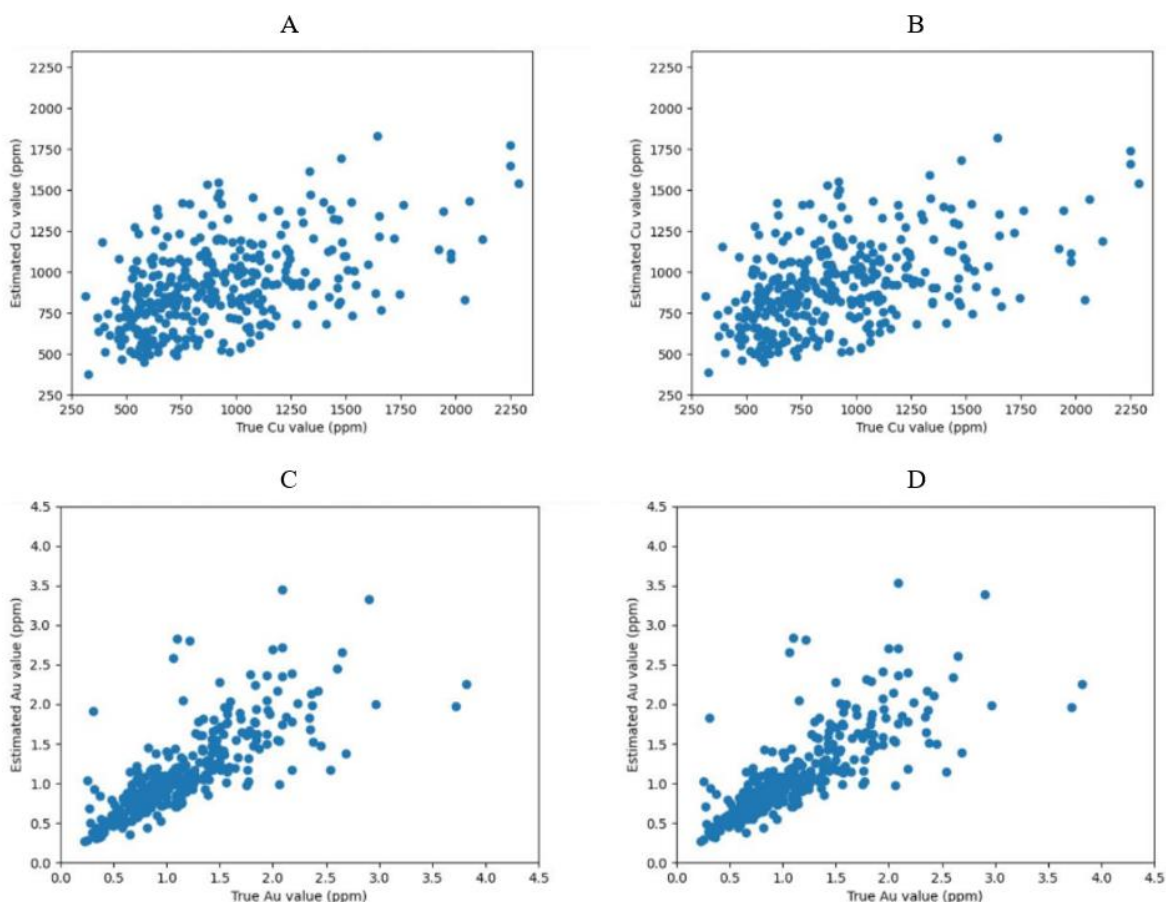


Figure 11. Scatterplots of predicted vs. true values obtained from jack-knife validation using the hierarchical (A) and conventional (B) approaches for Copper (Cu) predictions. (C) and (D) correspond to Gold (Au) predictions using the hierarchical and conventional approaches, respectively.

The comparison between simulated predicted values and observed test values is visualized through scatterplots (Figure 12), which illustrate the relationship between predicted and true values. Additionally, Table 3 presents correlation coefficients that quantify the agreement between actual and predicted Copper and Gold values, further validating the predictive performance of both co-simulation approaches.

Table 3. Correlation coefficients between true and predicted values for Copper and Gold

	Hierarchical approach with acceptance-rejection		Conventional hierarchical approach	
	Predicted Copper	Predicted Gold	Predicted Copper	Predicted Gold
True Copper	0.491652	-	0.492646	-
True Gold	-	0.73361	-	0.738411

A thorough analysis of Copper and Gold was also conducted using mean of error, error variance, standardized error mean, and standardized error variance with both co-simulation approaches (Table

4). These statistical measures provide deeper insight into the accuracy and reliability of each method by evaluating bias and variability in the predicted values.

Table 4. Error metrics for Copper (Cu) and Gold (Au) in conventional and hierarchical co-simulation.

Error Metrics	Hierarchical approach with acceptance-rejection		Conventional hierarchical approach	
	Copper	Gold	Copper	Gold
Mean of error	30.54	23.47	30.63	23.36
Error variance	733.52	1458.39	731.83	1527.97
Standardized error mean	1.13	0.62	1.13	0.60
Standardized error variance	1.00	1.00	1.00	1.00

The results of this analysis, presented in Table 4, indicate that both the hierarchical and conventional approaches yield nearly identical results across all error metrics, suggesting comparable predictive accuracy. However, since the hierarchical approach previously demonstrated superior reproduction of statistical parameters, its advantages in preserving spatial consistency and correlation structures may make it a more robust option for co-simulation.

4.6.3 Reproduction of a bivariate relationship

The final step in the validation process focuses on assessing how well each co-simulation approach reproduces the bivariate relationship between Copper and Gold. This evaluation is crucial, as maintaining both the correlation structure and the linearity constraint imposed by the two regression functions is essential for accurate modeling.

Figure 13 displays scatterplots comparing the simulated values (red points) with the original dataset (blue points) under a linearity constraint for both conventional hierarchical (A) and hierarchical with acceptance-rejection (B) co-simulation approaches. The hierarchical method with acceptance-rejection (B) demonstrates a better reproduction of the bivariate relationship, with simulated values closely following both the upper and lower constraints. In contrast, the conventional hierarchical method (A) shows greater deviations, particularly in the upper constraint region. Notably, the green-circled area in (A) highlights a clustering of underestimated values, indicating inconsistencies in the conventional co-simulation approach.

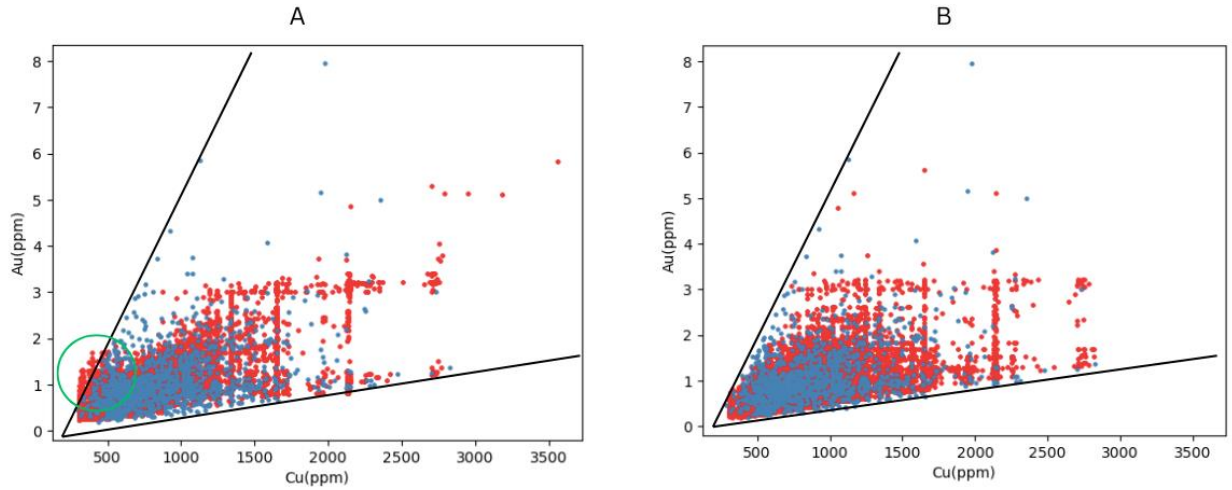


Figure 12. Bivariate Relationship Reproduction for Conventional hierarchical (A) and Hierarchical with acceptance-rejection (B) methods. Green circle highlights the difference between these two methods in preserving the linearity constraints

4.6.4 Cutoff Grade evaluations

To further validate the simulation results, cutoff grade curves are analyzed for both hierarchical and conventional co-simulation approaches. Figure 14 presents the tonnage, mean grade, and metal quantity variations as a function of cutoff grade for Copper (top row) and Gold (bottom row). These curves provide insight into the impact of the simulation methodologies on resource estimation and metal recovery potential.

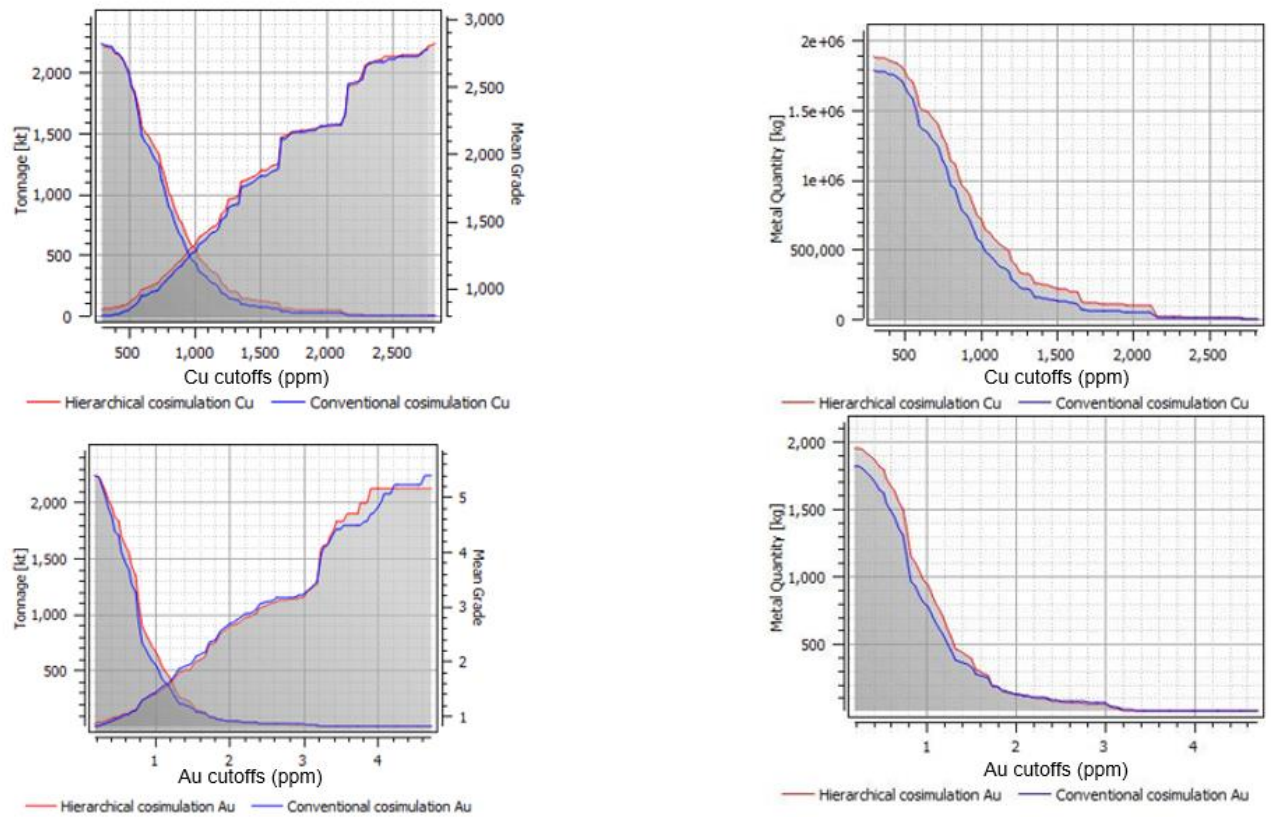


Figure 13. Cutoff grade curves for hierarchical with acceptance-rejection method (red) and conventional (blue) hierarchical co-simulation. (Top left) Tonnage and mean grade for Copper. (Top right) Metal quantity for Copper. (Bottom left) Tonnage and mean grade for Gold. (Bottom right) Metal quantity for Gold.

The hierarchical co-simulation with acceptance-rejection approach (red curves) closely follows the trends of the conventional method (blue curves) while exhibiting slight deviations in certain cutoff ranges. In the tonnage-grade curves (Figure 14, left column), both methods show similar trends, but the hierarchical approach with acceptance-rejection provides a more stable transition between different cutoff values, particularly in the mid-range cutoff grades. This suggests that enforcing linear constraints helps maintain more geologically realistic grade distributions.

The metal quantity curves (Figure 14, right column) for both Copper and Gold also indicate a strong alignment between the two methods, with the hierarchical approach with acceptance-rejection method preserving metal quantities effectively across varying cutoff values. This consistency further demonstrates that the hierarchical method does not introduce significant biases while improving the spatial relationships between simulated variables.

Overall, the cutoff grade analysis confirms that the hierarchical co-simulation method maintains resource estimates comparable to conventional techniques while enforcing additional constraints that enhance geological realism.

5. DISCUSSIONS AND CONCLUSIONS

5.1 Discussion

This research examined the use of hierarchical sequential Gaussian co-simulation with acceptance-rejection sampling for evaluating mine tailings. The objective was to enhance conventional geostatistics for correlated variables, particularly in preserving both bivariate associations and spatial distributions of Copper (Cu) and Gold (Au). Results indicate that the hierarchical approach outperforms conventional co-simulation techniques in maintaining statistical consistency while adhering to pre-defined linearity constraints.

A key finding of this study is the superior capability of the hierarchical method in reproducing essential statistical parameters and spatial correlations. The approach better preserves the mean values of Copper and Gold and maintains a higher correlation between the elements, ensuring more accurate resource estimates. This improvement is particularly beneficial for resource recovery, as more accurate estimations of metal distribution lead to more targeted and efficient reprocessing strategies. Furthermore, environmental monitoring is enhanced because the method provides a more realistic representation of the metal concentrations, which can inform better tailings management practices, such as determining the areas that may pose higher environmental risks due to metal leaching.

Given that resource recovery and environmental management rely on precise modeling of metal grades in mine tailings, the hierarchical approach presents a significant advantage over conventional methods by enabling more accurate estimations of tailings' economic value and environmental impact.

5.1.1 Key Challenges and Potential Solutions

1. Computational Cost

One notable limitation of hierarchical co-simulation is its higher computational demand due to the iterative acceptance-rejection process. The method requires multiple simulations to ensure values comply with the linearity constraints, which can slow down processing, especially for large-scale mining operations. In the current study, 100 realizations using the proposed method required approximately one month on a personal computer (Intel Core i7-8700H, 3.2 GHz, 16 GB RAM, no GPU acceleration). In contrast, the conventional hierarchical co-simulation required only 2–3 days.

Possible Solution: Optimization techniques, such as parallel computing and GPU acceleration, could be integrated to improve computational efficiency. For example, utilizing a workstation equipped with a 32-core processor or a GPU-enabled system could reduce computation time by an estimated factor of 8–20x. This implies that simulation time could be shortened from one month to approximately 1–

2 days, making the method significantly more practical for real-time applications, scenario testing, or larger-scale datasets.

2. Dependence on linearity constraints

The effectiveness of hierarchical co-simulation depends on the accuracy of the predefined linearity constraints. If the constraints do not correctly capture the true relationship between Copper and Gold, the method may introduce biases in the simulated data.

Possible Solution: More advanced machine learning techniques could be incorporated to dynamically adjust the constraints based on observed data patterns. Additionally, sensitivity analyses should be performed to evaluate the impact of different constraint formulations.

3. Scalability in Complex Geological Settings

While the hierarchical approach worked effectively for the Haveri mine tailings, its applicability to more geologically complex deposits remains uncertain. The assumption of a linear relationship between Copper and Gold may not hold in regions with nonlinear or multi-phase mineralization processes. As a result, applying a linearity constraint may be inadequate and could introduce bias.

Possible Solution: Future research should investigate extending the hierarchical co-simulation framework to accommodate nonlinear dependencies, such as by employing Gaussian mixture models, copula-based methods, or other advanced statistical techniques. These approaches could improve the flexibility of the simulation methodology and enhance its applicability across a broader range of geological environments.

In addition to addressing those challenges, another avenue for improving the efficiency and accuracy of tailings evaluation is the integration of supplementary data sources into the simulation process. It involves integrating historical processing plant data, such as metallurgical balances and recovery curves, into the resource modeling workflow. Such data can provide valuable prior information about metal grade distributions within the tailings, helping to constrain the simulation results more accurately. By combining plant performance data with limited drillhole information, it may be possible to reduce the number of required boreholes while maintaining estimation reliability. For example, if historical recovery rates for copper were consistently low in certain periods of plant operation, corresponding tailings deposited during those times could be expected to contain higher residual metal concentrations. Incorporating this knowledge into the simulation would allow more targeted drilling and improved resource characterization.

5.2 Conclusion

This study developed and validated a hierarchical sequential Gaussian co-simulation methodology enhanced with acceptance-rejection sampling for the evaluation of mine tailings. The proposed approach improves upon traditional co-simulation methods by enforcing linearity constraints between variables, preserving spatial continuity, and achieving more realistic bivariate relationships. Key contributions include the demonstration of improved resource estimation accuracy, better reproduction of spatial structures, and enhanced applicability to multivariate mining datasets.

The research findings demonstrate that this technique provides better results compared to traditional co-simulation practices through:

- **Preserving Statistical Integrity:** The hierarchical approach preserved original mean values, standard deviation and correlation coefficient of Copper and Gold which improved the accuracy of resource estimates.
- **Enforcing linearity Constraints:** By incorporating an acceptance-rejection sampling mechanism, the hierarchical method ensured that simulated values adhered to predefined linearity constraints, enhancing the realism of the results.
- **Improving Spatial Correlations:** Variogram analysis and LMC within the hierarchical approach maintained the natural metal distribution patterns which produced simulations with better geological validity.

This research provides results that improve the management of mine tailings by enabling more efficient resource recovery methods and improving environmental monitoring efforts. The proposed approach enables reliable estimation of metal distribution patterns, leading to better decision-making in mining operations and tailings reprocessing projects. More accurate estimates of metal recovery potential directly translate into optimized reprocessing and more effective resource extraction, enhancing the overall sustainability of mining operations.

Moreover, the methodology is designed to be applicable to active mining projects. In such cases, dynamic updating of the model would be required as new tailings are continuously deposited, and variations in tailings composition over time could affect the simulation accuracy. This adaptability is crucial in real-world mining environments where data availability and operational conditions can change over time. Additionally, the hierarchical approach can handle varying data quality, ensuring that even with limited or low-quality input data, the method still produces reliable resource estimates.

Future work should focus on enhancing the computational efficiency of the hierarchical method to handle large and complex geological datasets, while also ensuring its practicality under constraints like limited computational resources. Additionally, models of linearity constraints need further exploration to increase the method's adaptability across diverse geological settings. Several promising research directions include:

- Adapting the simulation framework to handle nonlinear relationships between variables, by incorporating advanced statistical methods such as copula models, Gaussian mixture models, or machine learning-based approaches, enabling accurate modeling of complex multi-phase mineralization processes.
- Using machine learning techniques to automatically infer and update linearity or nonlinear dependency constraints based on evolving datasets.
- Integrating real-time monitoring of active tailings facilities to dynamically update simulations as new deposition occurs.
- Incorporating historical and real-time processing plant data to improve prior models of metal grade distributions and reduce drilling requirements.

The hierarchical sequential Gaussian co-simulation method that uses acceptance-rejection sampling creates a significant improvement in geostatistical modeling of mine tailings by addressing key limitations of conventional methods to achieve enhanced resource estimation accuracy.

6. REFERENCES

- Abildin, Y., Madani, N., & Topal, E. (2019). A hybrid approach for joint simulation of geometallurgical variables with inequality constraint. *Minerals*, 9(1), 24.
- Madani, N., & Abulkhair, M. F. (2020). "Handling Linearity and Inequality Constraints in Hierarchical Sequential Gaussian Co-Simulation." *Mathematical Geosciences*, 52(6), 1375–1395.
- Abulkhair, S., & Madani, N. (2021). Assessing heterotopic searching strategy in hierarchical co-simulation for modeling the variables with inequality constraints. *Comptes Rendus. Géoscience*, 353(1), 115-134.
- Blannin, R., Frenzel, M., Tolosana-Delgado, R., Büttner, P., & Gutzmer, J. (2023). 3D geostatistical modelling of a tailings storage facility: Resource potential and environmental implications. *Ore Geology Reviews*, 154, 105337.
- Emery, X. (2005). Variograms of order ω : a tool to validate a bivariate distribution model. *Mathematical Geology*, 37, 163-181.
- Emery, X. (2005). "Simple and Ordinary Multi-Gaussian Kriging for Estimating Recoverable Reserves." *Mathematical Geology*, 37(3), 295–319.
- Emery, X. (2010). Iterative algorithms for fitting a linear model of coregionalization. *Computers & Geosciences*, 36(9), 1150-1160.
- Goulard, M., & Voltz, M. (1992). Linear coregionalization model: tools for estimation and choice of cross-variogram matrix. *Mathematical Geology*, 24, 269-286.
- Hosseini, S. A., & Asghari, O. (2019). Multivariate geostatistical simulation on block-support in the presence of complex multivariate relationships: iron ore deposit case study. *Natural Resources Research*, 28, 125-144.
- Karacan, C. Ö., Erten, O., & Martín-Fernández, J. A. (2023). Assessment of resource potential from mine tailings using geostatistical modeling for compositions: A methodology and application to Katherine Mine site, Arizona, USA. *Journal of Geochemical Exploration*, 245, 107142.
- Nwaila, G. T., Ghorbani, Y., Zhang, S. E., Tolmay, L. C., Rose, D. H., Nwaila, P. C., ... & Frimmel, H. E. (2021). Valorisation of mine waste-Part II: Resource evaluation for consolidated and mineralised mine waste using the Central African Copperbelt as an example. *Journal of Environmental Management*, 299, 113553.

- Parviainen, A., Soto, F., & Caraballo, M. A. (2020). Revalorization of Haveri Au-Cu mine tailings (SW Finland) for potential reprocessing. *Journal of Geochemical Exploration*, 218, 106614.
- Soto, F., Navarro, F., Díaz, G., Emery, X., Parviainen, A., & Egaña, Á. (2022). Transitive kriging for modeling tailings deposits: A case study in southwest Finland. *Journal of Cleaner Production*, 374, 133857.
- Tripodi, E. E. M., Rueda, J. A. G., Céspedes, C. A., Vega, J. D., & Gómez, C. C. (2019). Characterization and geostatistical modelling of contaminants and added value metals from an abandoned Cu–Au tailing dam in Taltal (Chile). *Journal of South American Earth Sciences*, 93, 183-202.
- Chiles, J.-P., & Delfiner, P. (2012). *Geostatistics: Modeling Spatial Uncertainty*. Wiley.
- Deutsch, C. V., & Journel, A. G. (1998). *GSLIB: Geostatistical Software Library and User's Guide*. Oxford University Press.
- Goovaerts, P. (1997). *Geostatistics for Natural Resources Evaluation*. Oxford University Press.
- Journel, A. G., & Huijbregts, C. J. (1978). *Mining Geostatistics*. Academic Press.
- Deutsch, C. V. (2017). *Geostatistical Reservoir Modeling*. Oxford University Press.
- Genton, M. G., & Hall, P. (2016). Robustness, quantile functions, and outlier detection in geostatistics. *Mathematical Geosciences*, 48(5), 561-582.
- Soto, F., Navarro, F., Díaz, G., Emery, X., Parviainen, A., & Egaña, Á. (2022). Transitive kriging for modeling tailings deposits: A case study in southwest Finland. *Journal of Cleaner Production*, 374, 133857.
- Tripodi, E. E. M., Rueda, J. A. G., Céspedes, C. A., Vega, J. D., & Gómez, C. C. (2019). Characterization and geostatistical modelling of contaminants and added value metals from an abandoned Cu–Au tailing dam in Taltal (Chile). *Journal of South American Earth Sciences*, 93, 183-202.