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**GEOSTATISTICAL SIMULATION OF ORE GRADE
IN A DEPOSIT WITH MULTI-CORRELATED METALS**

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Declaration

I, Ndou Tshimangadzo, student number 2027446471, declare that this thesis, submitted to the Department of Geology, Faculty of Natural and Agricultural Sciences at the University of the Free State, is my own independent work. This work has never been submitted to any other institution of higher education.

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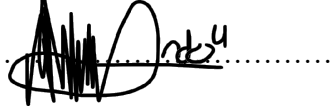
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Dedication

I dedicate this work to my four brothers and my mom, Ndou Khathutshelo for standing out as the most nurturing and encouraging. Their unwavering support in all my endeavors and daily motivation have been invaluable to me.

Abstract

Geostatistical simulation methods are increasingly used in mineral resources estimation. However, applying such methods to simulate the grades of metals that are strongly correlated within a deposit remains challenging. Therefore, it is desirable to develop improved geostatistical simulation methods for such a case. Previous research has explored transformation methods to remove or reduce the complexity of relationships among variables. Multivariate transformations, such as minimum/maximum autocorrelation factors (MAF) and projection pursuit multivariate transformation (PPMT), are widely applied in the field of geosciences to handle the correlation among variables prior to simulation with independent methods. This study evaluated the performance of two transformation methods, PPMT and MAF, within the Turning Bands Simulation (TBSIM) framework. The analysis focused on Fe and Al_2O_3 , which are strongly negatively correlated in the dataset. The assessments considered accuracy, time efficiency, and the effectiveness of the transformations in managing variable dependency. The results indicate that neither the MAF nor the PPMT, nor the TBSIM framework was able to fully reproduce the correlation among Fe and Al_2O_3 . Nonetheless, the MAF proved more effective than the PPMT, as it handled the complexity of correlated variables more consistently. The PPMT was able to reproduce only Al_2O_3 after back-transformation, while its performance for Fe was less reliable.

Keywords: Turning Bands Simulation (TBSIM), projection pursuit multivariate transform (PPMT), minimum/maximum autocorrelation factors (MAF), correlated variables.

Supervisor Declaration	iii
Chapter One: Introduction	1
1.1 BACKGROUND OF THE STUDY	1
1.2 PROBLEM STATEMENT	3
1.3 AIM AND SPECIFIC OBJECTIVE OF THE STUDY	3
1.4 RESEARCH HYPOTHESIS	4
1.5 SUMMARY OF METHODOLOGY	4
1.6 THESIS STRUCTURE	4
1.7 CONCLUSION	5
Chapter Two: Literature Review	6
2.1 JOINT MODELLING AND SIMULATION	8
2.2 DIRECT MULTIVARIATE SIMULATION	10
2.3 CHALLENGES ASSOCIATED WITH COMPLEX MINERAL DEPOSIT	11
2.4 DEALING WITH GEOLOGICAL DOMAINS	12
2.5 DEALING WITH UNCERTAINTY	12
2.6 CLASSIFICATION OF SIMULATED METAL GRADES	13
2.7 CONCLUDING REMARKS	14
Chapter 3: Research Methodology	15
3.1 STUDY AREA	15
3.1.1 Regional Geology	16
3.2 DATA ANALYSIS	18
3.2.1 Database	18
3.3 COMPOSITING	19
3.4 DECLUSTERING	23
3.5 HISTOGRAM	30
3.6 DATA TRANSFORMATION	35
3.6.1 Projection Pursuit Multivariate Transform (PPMT)	36
3.6.1.1 Normal score transformation	36
3.6.1.2 Data sphering	37
3.6.1.3 Projection pursuit	38
3.6.1.4 Back-transformation	39
3.6.2 Minimum/Maximum Autocorrelation Factor (MAF)	39
3.7 VARIOGRAM ANALYSIS	41
3.7.1 Experimental variogram	42
3.7.2 Variogram model	44

3.8 TURNING BAND SIMULATION	48
3.9 CONCLUSION	49
Chapter 4: Data Analysis Results	50
4.1 SIMULATION RESULTS.....	50
4.1.1 Statistical Validation	50
4.3 CONCLUSION	56
Chapter 5: Comparison and Results Discussion	57
5.1 CONCLUSION	60
Chapter 6: Conclusion and Recommendations	62
6.1 SUMMARY OF THE RESEARCH	62
6.2 LIMITATIONS.....	63
6.3 RECOMMENDATIONS	63

List of Figures

Figure 1.1: Flow chart of research methodology.....	5
Figure 2.1 Representation of multivariate complexity, (a) constraint, (b) heteroscedastic, (c) nonlinear.....	8
Figure 3.1 Summary of methodologies implemented in chapter 3	15
Figure 3.2: (2a) Simplified geological map of the Carájas region. (2b) Tectonostratigraphic column of the Carájas region (Holdsworth and Pinheiro 2000).....	20
Figure 3.3: Scatter plot showing the relationship between Fe and Al_2O_3	21
Figure 3.4: Distribution of drill holes.....	22
Figure 3.5: Histogram showing the distribution of sample length.....	25
Figure 3.6: Diagram showing clustered drillholes from the database.....	29
Figure 3.7: Drillholes in 3D, showing X, Y, and Z of the study area.....	30
Figure 3.8: Scatter plot showing the declustered mean of Fe.....	30
Figure 3.9: Scatter plot showing the declustered mean of Al_2O_3	31
Figure 3.10: Excel file showing data before PPMT transformation and after PPMT transformation.....	33
Figure 3.11: Scatter plot of normal transformation for Fe and Al_2O_3	34
Figure 3.12: Scatter plot of PPMT transformed data showing zero correlation between Al_2O_3 and Fe.....	35
Figure 3.13: Excel file showing data before and after applying MAF.....	35
Figure 3.14: Histogram showing positively skewed distribution of untransformed data (Al_2O_3)	36
Figure 3.15: Histogram showing negatively skewed distribution for untransformed data (Fe).....	36
Figure 3.16: Histogram showing normal distribution of PPMT(Fe).....	41
Figure 3.17: Histogram showing normal distribution of PPMT (Al_2O_3)	41
Figure 3.18: Histogram showing normal distribution of MAF(Fe).....	42
Figure 3.19: Histogram showing normal distribution of MAF(Al_2O_3)	42
Figure 3.20: Direct variogram for PPMT (Fe) and bar graph with number of samples on each point. Blue line represents major axis (azimuth 30°, dip 0°), green line represents semi-major axis (azimuth 25°, dip 0°), and red line represents minor axis (azimuth 0°, dip 0°)	44
Figure 3.21: Direct variogram of PPMT (Al_2O_3) and bar graph with the number of samples on each point. Blue line represents major axis (azimuth 30°, dip 0°), green line represents semi-major axis (azimuth 120°, dip 0°), and red line represents minor axis (azimuth 30°, dip 90°)	44
Figure 3.22: Direct variogram of MAF (Fe) and bar graph with the number of samples on each point. Blue line represents major axis (azimuth 30°, dip 0°), green line represents semi-major axis (azimuth 120°, dip 0°), and red line represents minor axis (azimuth 30°, dip 90°)	45
Figure 3.23: Direct variogram for MAF (Al_2O_3) and bar graph with number of samples on each point. Blue line represents major axis (azimuth 30°, dip 0°), green line represents semi-major axis (azimuth 120°, dip 0°), and red line represents minor axis (azimuth 30°, dip 90°)	44
Figure 3.24: Variogram model of PPMT (Fe) and bar graph representing the number of samples on each point. The blue line represents the major axis, the green line the semi-major axis, and the red line the minor axis.....	47

Figure 3.25: Variogram model of PPMT (Al_2O_3) and bar graph representing the number of samples on each point. The blue line represents the major axis, the green line the semi-major axis, and the red line the minor axis.....	47
Figure 3.26: Variogram model of MAF (Fe) and bar graph representing the number of samples on each point. The blue line represents the major axis, the green line the semi-major axis, and the red line the minor axis.....	48
Figure 3.27: Variogram model of PPMT (Fe) and bar graph representing the number of samples on each point. The blue line represents the major axis, the green line the semi-major axis, and the red line the minor axis.....	48
Figure 4.1: Declustered mean of Fe (a and c) in green line and Al_2O_3 (b and d) in green line. The red line in (a) is the back-transformed mean of PPMT-Fe. The black dotted line in (b) is the back-transformed mean for PPMT- Al_2O_3 . The red line in (c) is the back-transformed mean of MAF-Fe. The red line in (d) is the back-transformed mean of MAF- Al_2O_3	53
Figure 4.2: Correlation Coefficient for Fe and Al_2O_3 before transformation and back-transformation (a and b). the red line in (a and b) is the original correlation coefficient of Fe and Al_2O_3 . The green line in (a) is the correlation coefficient after back-transformation using PPMT. The green line in (b) is the correlation coefficient after back-transformation using MAF.	54
Figure 4.3: Original negative skewed distribution of Fe (a), and negative skewed distribution of five realizations from back-transformed data using PPMT-Fe (b, c, d, e, and f)	55
Figure 4.4: Original positive skewed distribution of Al_2O_3 (a) and positively skewed data of five realizations from back-transformed data using PPMT- Al_2O_3 (b, c, d, e, and f)	56
Figure 4.5: Original negatively skewed distribution of Fe (a), and negatively skewed data of five realization from back-transformed data from MAF-Fe (b, c, d, e, and f)	56
Figure 4.6: Original positively skewed data of Al_2O_3 (a), and positively skewed data of five realizations from back-transformed data using MAF- Al_2O_3 (b, c, d, e, and f)	57
Figure 5.1: (a) Original declustered mean of Fe in green line, back-transformed mean of PPMT-Fe in yellow line, and back-transformed mean of MAF-Fe in red line. (b) Original declustered mean of Al_2O_3 , back-transformed mean of PPMT- Al_2O_3 in black dotted line, and back-transformed mean of MAF- Al_2O_3	59
Figure 5.2: Original declustered correlation coefficients of Fe and Al_2O_3 in red line, correlation coefficients between PPMT-Fe and PPMT- Al_2O_3 in yellow line, and correlation coefficients between MAF-Fe and MAF- Al_2O_3 in red line.....	60

List of Tables

Table 3.1: Descriptive statistics of Al_2O_3 and Fe.....	21
Table 3.2: Descriptive statistics of sample length.....	24
Table 3.3: Strike, dip, and pitch of all semi-variogram maps.....	43
Table 3.4: Nugget effect, sill, and range of each axis of different transformed variable.....	49
Table 4.1: Declustered means of Fe and Al_2O_3 and back-transformed means of PPMT-Fe, PPMT- Al_2O_3 , MAF-Fe, and MAF- Al_2O_3	52
Table 5.1: Original declustered mean of Al_2O_3 and Fe, and back-transformed mean for both PPMT and MAF.....	59

Chapter One: Introduction

1.1 BACKGROUND OF THE STUDY

Mining industries have brought the field of geostatistics into attention, demanding an increase in accurate, realistic geological models for simulating ore grades of metals that exhibit correlations with each other within a deposit. For grade estimation, geostatistical simulation methods are becoming popular because they create new sets of data that behave like the original data, showing the original statistical properties like histogram and variogram, addressing the limitation of traditional methods (Caers and Zhang 2005; Hosseini and Asghari 2019). According to Dimitrakopoulos (2011) and Afzal et al. (2023) not only are geostatistical simulation methods developed for grade estimation, but they can also be used for understanding the uncertainty and differences in mineral characteristics in a deposit. In addition, geostatistical modeling frequently involves modeling continuous variables and geological domains, and it is applicable in different areas of earth sciences (Dagbert 2014; Watson et al. 1980).

A mineral deposit contains several metals or elements which are assumed to follow a multivariate normal Gaussian distribution, but geologically they tend to be non-Gaussian, which complicates resource estimation when using traditional methods (Boucher and Dimitrakopoulos 2012; Hosseini and Asghari 2019). Mineral deposits also contain multiple elements that tend to have non-linear patterns and complex relationships (Mahlooji et al. 2019). According to Hosseini and Asghari (2019), mineral resources estimation requires the understanding of the distribution of multiple correlated metals in a deposit. However, the complexity of correlated variables complicates geostatistical simulation methods, especially when using independent geostatistical simulation methods for grade estimation, unless transformation methods are used (de Figueiredo et al. 2021).

Geostatistical simulation methods for simulating grades of individual metals are, in general, straightforward, and easy to access (Chilès and Delfiner, 2012; Deutsch and Journel 1992; Dimitrakopoulos and Luo 2004; Godoy Marcelo 2003; Goovaerts 1997). However, according to Boucher and Dimitrakopoulos (2012), for simulating grades of multivariable deposits, they are limited more specifically to mineral deposits containing more than three variables. Currently, for simulating grades of metals that exhibit correlation with each other in a mineral deposit, co-simulation and joint simulation methods are popular. Moreover, previous research has trialed different co-simulation and joint simulation methods, but according to Boucher and Dimitrakopoulos (2009), Lopes et al. (2011), and Minniakhmetov and Dimitrakopoulos (2017) joint simulation methods are unsuitable for simulating grades of more than three metals in medium to large mineral deposits. Most co-simulation methods are unmanageable and inefficient for simulating grades of metals that exhibit correlation with each other. Grade data of such metals must be subjected to decorrelation, especially when dealing with more than two metals in a mineral deposit (Almeida and Journel 1994a).

Furthermore, because stochastic models are independent simulation methods (i.e., they can only simulate one metal at a time), they cannot be used for simulating multiple elements that exhibit correlation with each other in a mineral deposit (Dimitrakopoulos and Luo 2004). Transformation methods are becoming popular for handling the complexity of correlated variables so that elements can be simulated independently. Not only can transformation methods be applied in independent simulation methods, but previous research has trialed using transformation methods in co-simulation methods for simulating grades of at least three metals that exhibit correlation with each other in a mineral deposit of more than three variables (Dimitrakopoulos and Luo 2004).

1.2 PROBLEM STATEMENT

Geostatistical simulation methods are becoming increasingly popular for grade estimation, addressing the limitations of traditional methods. When simulating ore grade using geostatistical simulation, problems arise when a mineral deposit contains more than two metals exhibiting correlations that need to be simulated. Many researchers have trialed different geostatistical simulation methods for simulating grades of metals that exhibit correlation with each other in a deposit. Except for joint simulation and co-simulation methods, many researchers have trialed transformation methods based on independent simulation techniques. Research continues to develop new simulation methods for grades of metals that exhibit correlation with each other. However, literature lacks a comparison of the best methods that have been developed previously for simulating ore grades of metals that exhibit correlations with each other in a mineral deposit.

1.3 AIM AND SPECIFIC OBJECTIVE OF THE STUDY

This research aims to apply two different transformation methods in the geostatistical simulation of grades of metals that exhibit correlations with each other in a mineral deposit.

To achieve this aim, the following specific objectives are considered:

- 1) To determine which method, turning bands simulation (TBSIM) based on projection pursuit multivariate transform (PPMT) or TBSIM based on minimum/maximum autocorrelation factor (MAF), is better in terms of accuracy and time efficiency for simulating grades of metals that exhibit correlation with each other in a mineral deposit.
- 2) To compare the effectiveness of PPMT and MAF in handling the complexity of simulating grades of metals that exhibit high correlations with each other in a mineral deposit.

1.4 RESEARCH HYPOTHESIS

- 1) It was hypothesized that TBSIM-based on PPMT provides more accurate grade estimates, and it is more time efficient compared to TBSIM-based MAF for simulating grades of metals that exhibit correlation with each other in a mineral deposit.
- 2) It was hypothesized that PPMT more effectively handles the complexity of simulating grades of metals that are correlated with each other in a mineral deposit compared to MAF.

1.5 SUMMARY OF METHODOLOGY

Figure 1.1 illustrates the step-by-step methodology used in this research, beginning with data analysis and concluding with back-transformation.

1.6 THESIS STRUCTURE

This thesis is structured as follows:

1. Background of the study: This chapter presents the overview of the research topic; research aim and research questions that were answered based on different methods.
2. Literature Review: The chapter reviews previous relevant studies.
3. Research Methodology: This chapter explains the database preparation, simulation approaches and application of PPMT and MAF.
4. Data Analysis results: This chapter presents statistical, spatial and validation outcomes from simulation results.
5. Comparison and Results discussion: This chapter compares the performance of both PPMT and MAF based on TBSIM.

6. Conclusion and Recommendations: This chapter summaries the key findings, highlights strength and limitations of PPMT, MAF, and TBSM, and provide recommendations based on the results.

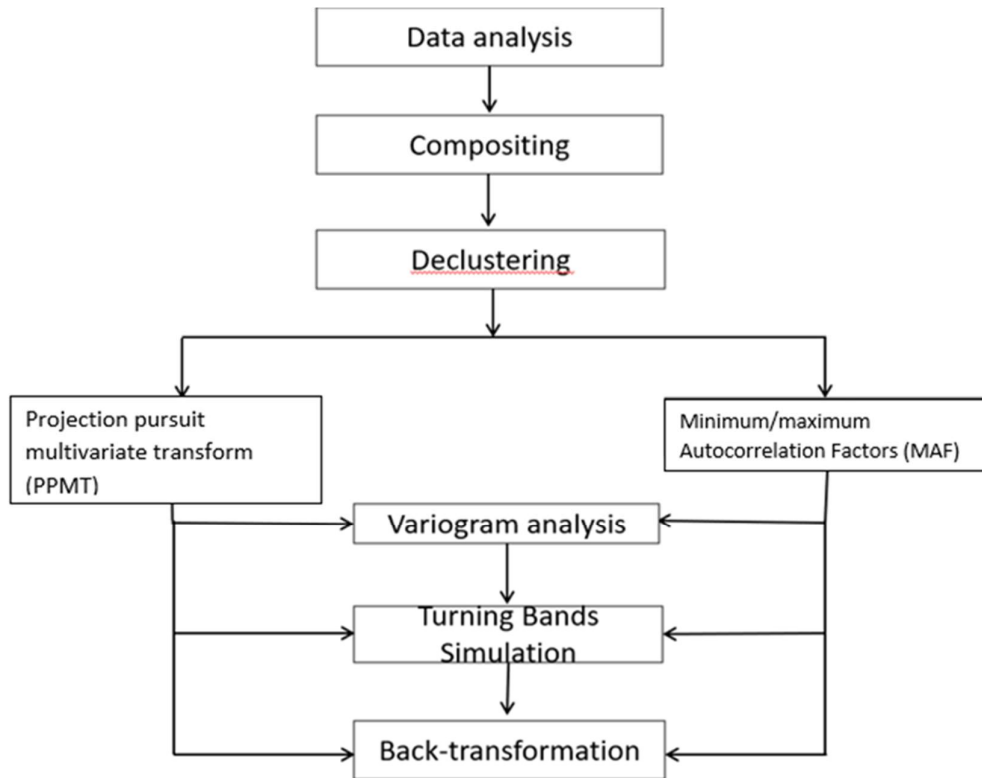


Figure 4.1: Flow chart of research methodology

1.7 CONCLUSION

Geostatistical simulation of grades of correlated metals in a mineral deposit remains challenging. To address the challenge, this evaluated two of the best-ranked transformations: PPMT and MAF within the TBSIM framework. The next chapter reviews previous research on transformation methods and Geostatistical simulation algorithms to situate this study within the existing body of knowledge.

Chapter Two: Literature Review

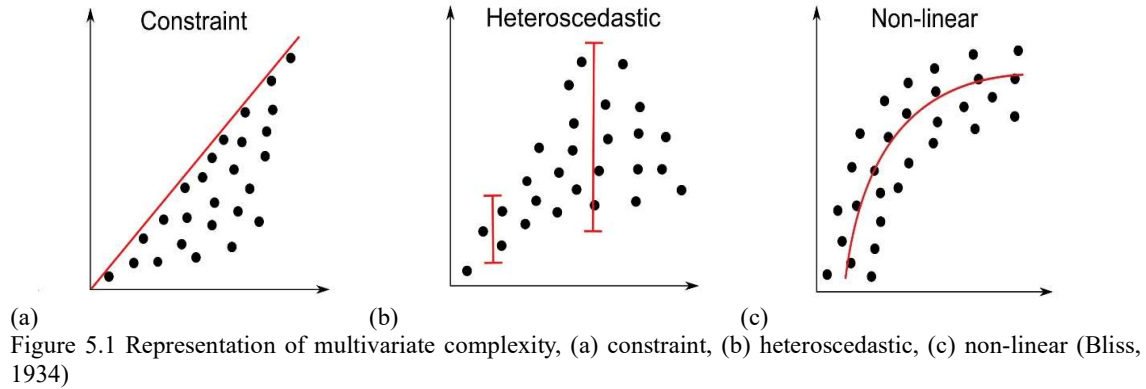
Geostatistical simulation methods have been increasingly used as a powerful tool for simulating spatial attributes, addressing the limitations of traditional methods (Chilès and Delfiner, 2012). However, not every geostatistical simulation technique could be applied to all problems such as simulating correlated metals, simulating uncertainty, simulating post-mineralization, and modelling geological domains (Yunsel and Ersoy 2011). Metal grades in a mineral deposit can be influenced based on different rock types, mineralized zones, alteration zones, and minerals that host each element. These factors affect correlation between elements and guide the choice of geostatistical simulation methods.

Before the development of geostatistical simulation methods for ore grade estimation, traditional geostatistical methods have been popular for ore grade estimation (Paithankar and Chatterjee 2018). Conventional methods like kriging and its variants that are statistically based on variograms fail to capture the complexity that arises from correlated metals. However, even though sequential indicator simulation can handle the complexity that arises among correlated metals, it loses accuracy in ore grade estimation when based on indicator kriging (Emery 2004). The limitations for ore grade simulations when using traditional geostatistical methods like kriging include: (1) smoothing effect, (2) reducing the range of variation, (3) overestimation of low-grade correlated metals, and underestimation of high-grade correlated metals (Dagbert 2014). Kriging-based techniques are well understood but not only that they fail to accurately capture the grade estimation of correlated metals, they also fail to accurately capture uncertainty of the ore grade model of a mineral deposit (Dagbert 2014; Goovaerts 1997; Isaaks 1989).

For ore grade estimation, geostatistical simulation methods fail to capture the complexity that arises from multi-correlated metals. However, the approach of removing correlations among metals in multivariate simulation has been gaining popularity over joint simulation methods due to its accuracy and more computational efficiency as the number of metals to be simulated increase (Rondon 2012).

In geostatistics, it is important to use transformation methods for ore grade estimation because it handles complexity and speeds up the processes of multivariate geostatistical simulation (Mueller Ferreira 2012), but it is very challenging (Barnett et al. 2014). Principal components analysis (PCA) has been popular for de-correlation of metals, but its limitations include (Erten and Deutsch 2021): (1) Decorrelation of metals, but it cannot handle the complexity of correlation among metals, (2) Cannot determine the correlation of two metals that are located far from each other, (3) the variogram of PCA-transformed data is quite different from the variogram of the original data, but new transformation methods have been developed.

Transformation methods gaining popularity for decorrelating variables include projection pursuit multivariate transformation (PPMT), minimum/maximum autocorrelation factor (MAF), normal score transformation, and stepwise conditional transformation. However, unlike PCA, these transformation methods are based on how metals are correlated in one location and how metals are correlated from one location to another (Mueller and Ferreira 2012). Moreover, normal score transformation can change correlated metals to follow normal Gaussian only at a lag-zero, but it does not handle the complexity among variables including, non-linearity, heteroscedasticity, and constraints (Figure 2.1) (Bliss 1934; Deutsch Journal 1998).



2.1 JOINT MODELLING AND SIMULATION

Geostatistical simulation methods for simulating ore grade of individual metals are easy to use and more efficient (Chilès and Delfiner 2012; Deutsch and Journel 1992; Dimitrakopoulos and Luo 2004; Godoy Marcelo 2003; Goovaerts 1997; Remy et al. 2009), but for joint modelling they are too difficult to use in a mineral deposit that contains more than three correlated metals of interest. However, Boucher and Dimitrakopoulos (2009) jointly simulated grades of correlated metals using joint direct block simulation with MAF. According to Boucher and Dimitrakopoulos (2009), *dbmafsim* is more efficient for simulating grades of multi-correlated metals but it cannot handle more than two variables. However, regardless of joint models not handling more than two correlated variables (Boucher and Dimitrakopoulos 2009; Lopes et al. 2011), Boucher and Dimitrakopoulos, (2012) trialed joint models using direct block simulation and MAF (*dbmafsim*) and sequential Gaussian co-simulation (SGCOSIM) for simulating grade of five correlated metals. In conclusion, *dbmafsim* compared to SGCOSIM was found to be more useful for two reasons: (1) MAF was more efficient at reducing correlation before simulation, and (2) only 10 independent metals were fitted into MAF rather than two sets of 15 acceptable variograms and cross variograms (Boucher and Dimitrakopoulos, 2012).

In addition, different researches Carvalho and Dimitrakopoulos (2019), and Van Der Grijp and Minnitt (2015), have trialed using complex high-order or multi point univariate simulation

methods to independently simulate the grade of metals that exhibit correlation independently, but according to Minniakhmetov and Dimitrakopoulos, (2017) they are limited during the back-transformation processes. To address these limitations, Minniakhmetov and Dimitrakopoulos (2017) developed a framework named high-order joint simulation from high-order simulation (Dimitrakopoulos et al. 2010; Mustapha and Dimitrakopoulos 2011). Minniakhmetov and Dimitrakopoulos (2017) used diagonal domination condition for high-order cumulants as a transformation method and variables were simulated using high-order joint simulation. This proposed framework worked more accurately but: (1) it overestimates the relationship between metals, (2) for the method to be more effective, training images are required. Moreover, Minniakhmetov and Dimitrakopoulos (2017) suggested that further research should be done to improve decorrelation transformation by using a non-linear transformation instead of linear model.

Geostatistical simulation is first applied at a detailed point support across the grid, and the results are averaged within the selective mining units to produce the simulation of the grade produced at the scale of direct block (Andre and Journel, 2004). However, Boucher and Dimitrakopoulos (2009, 2012), and Emery and Ortiz (2011) mentioned that direct block simulation does not use fine grids to divide blocks when compared to traditional methods and it is becoming more popular in mining industries and widely accepted in academic application (Boucher et al. 2005; Boucher and Dimitrakopoulos 2012; de Freitas Silva and Dimitrakopoulos 2016; Hosseini et al. 2017). To address the limitation of traditional geostatistical simulation methods, Hosseini and Asghari (2019) extended direct block simulation to multivariate direct block simulation (MDBSIM) to reproduce the complex relationships among the correlated variables. According to Hosseini and Asghari (2019), MAF cannot handle the complexity which arises from correlated variables and PPMT cannot address

correlations among variables. However, Hosseini and Asghari (2019) combined PPMT and MAF for decorrelating metals. According to the results, Hosseini and Asghari (2019) concluded that MDBSIM is more effective and simpler for simulating cross-correlated metals from block support at point-support data.

Furthermore, high-order joint simulation has been used for jointly simulating the grade of multivariate correlated metals based on different transformations, such as PCA (David 1988), normal score transformation (Leuangthong and Deutsch 2003; van den Boogaart et al. 2017), PPMT (Barnett et al. 2014), uniformly weighted exhaustive diagonalisation with Gauss iterations (U-WEDGE) transformation (Mueller and Ferreira 2012), and MAF transformation (Boucher and Dimitrakopoulos (2009, 2012); Rondon 2012; Dimitrakopoulos and Fonseca 2003; van den Boogaart et al. 2017).

2.2 DIRECT MULTIVARIATE SIMULATION

According to de Figueiredo et al. (2021), the correlation of multiple metals depends on linear correlation coefficients, but metals are not symmetrically distributed showing nonlinear and heteroscedastic properties, and so linear correlation coefficients fail to reproduce the complex relationships among metals. To overcome such limitation for grade simulation, Leuangthong and Deutsch (2003) proposed stepwise conditional transformation (SCT) and simulated transformed variable using Gaussian simulation. However, using SCT for multi-correlated variables has some limitations, including: (1) it becomes less precise at capturing and replicating the statistical characteristics of the distribution when dealing with a high number of variables, and (2) the correlations among metals depend on the distribution of variables during transformation processes (Leuangthong and Deutsch, 2003). To overcome SCT limitation, Barnett et al. (2014) introduced PPMT which was found to be more accurate for a high number

of observations and a commodity with less than three metals. In addition, de Figueiredo et al. (2021) developed a new direct multivariate simulation (DMS) framework based on SCT. A comparison between the SCT and PPMT using direct multivariate simulation was carried out, and de Figueiredo et al. (2021) concluded that the proposed framework can be more useful for simulating grade of complex multivariate deposits with strong non-linear distribution.

When simulating grades of metal that exhibit correlation, the distance between metals is of fundamental importance. During geological modelling for correlated metals, the distance between metals helps in transforming correlated metals into uncorrelated metals (Mueller and Ferreira, 2012). According to Doyen (2007), sequential gaussian simulation (SGS) is popular for simulating metal grades with accurate grade estimates because it can incorporate real-world data (i.e., no transformation is required) directly into simulation. Simulating metal grades that exhibit correlation with each other using SGS is not straightforward; hence, normal score transformation can be applied. de Figueiredo et al. (2021) developed a new DMS algorithm that can be applied to several deposits. de Figueiredo et al. (2021) compared DMS with PPMT based on non-conditional and conditional simulations for simulating metal grades that exhibit correlation with each other in a mineral deposit. According to de Figueiredo et al. (2021) DMS showed lower errors compared to PPMT, and DMS based on SCT can be used for data that show complex multivariate distributions with strong non-linear behaviors of metals.

2.3 CHALLENGES ASSOCIATED WITH COMPLEX MINERAL DEPOSIT

The complexity of mineral deposits with non-Gaussian and non-linear metal grade distributions drives scientists to create geostatistical simulation techniques that can faithfully capture the complexity of relationships among multiple elements in a mineral deposit. Complex mineral deposits with several correlated elements are particularly challenging when simulating metal

grades, which can be addressed by developing existing multivariate models. However, for simulating grades of more than two metals that exhibit correlation with each other in a deposit, Mahlooji et al. (2019) trialed SGS based on three different transformation methods namely SCT, PPMT, and MAF. The results of the different transformation methods were compared, and SGS based on PPMT yielded the most accurate grade estimate compared to those based on SCT and MAF.

2.4 DEALING WITH GEOLOGICAL DOMAINS

When modelling geological domains, ore grade is impacted by distinct characteristics, including lithology and rock types. To model two continuous metals and one categorical metal, Madani and Maleki (2023) developed a joint simulation approach that combines multi-Gaussian and plurigaussian methods. Two continuous metals were transformed based on PPMT and Gaussian anamorphosis and simulated based on plurigaussian. According to Madani and Maleki (2023), when simulating metal grades that exhibit correlation, plurigaussian produces inaccurate grade estimates based on the two transformations because it fails to manage the complexity of relationships among metals, hence further investigation should be done.

2.5 DEALING WITH UNCERTAINTY

Developing joint geostatistical simulation methods for metal grade that exhibit correlation with each other decreases grade uncertainty. According to Almeida and Journel (1994b) and Emery and Silva (2009), grade uncertainty can be decreased better by using co-simulation methods than by independent simulation methods. Hence, Almeida and Journel (1994b) mentioned that co-simulation methods that do not rely on transformation methods tend to be complex when simulating metal grades that exhibit correlation and turn to be more inefficient when more than two elements are considered. Minniakhmetov and Dimitrakopoulos (2017) developed diagonal

domination conditions as a transformation method, and metals were simulated independently using higher order simulation. For accurate grade estimate when simulating metal grade to assess uncertainty based on joint simulation methods that have been developed, Minniakhmetov and Dimitrakopoulos (2017) concluded that further research can be done focusing on improving decorrelation condition by increasing cross cumulants and using non-linear transformation.

Furthermore, according to Hosseini et al. (2017), not only are traditional methods limited to handling uncertainty but they are also limited (1) for changing true data obtained from drill holes into a useful way for further modelling, (2) for handling the complexity that arises from having multiple elements when making a decision on which one to select for extraction (multiple correlated metals). Hosseini et al. (2017) developed direct block sequential co-simulation for managing such limitations based on normal score transformation. Hosseini et al. (2017) concluded that direct block sequential co-simulation is: (1) very simple to use, (2) it can improve the accuracy of predicted recoverable resources by taking into consideration both scale effect and correlation among metals, (3) and it also helps in understanding how elements change in different parts of an orebody whether on a small scale or large scale.

2.6 CLASSIFICATION OF SIMULATED METAL GRADES

Geostatistical simulations are well known for classifying metal grades. In situations where the mineral deposit contains more than two elements, it is difficult to simulate the grade of such elements using traditional methods. To address the problem Battalgaży and Madani (2019) used three simulation methods to simulate multiple correlated metals. These methods include turning bands co-simulation (TBCOSIM) based on multi-Gaussian transformation, TBSIM based on normal transformation score, and TBSIM based on PPMT (Battalgaży and Madani (2019)). Among the three methods, TBSIM based on PPMT produced the most accurate grade

estimates (Battalgazy and Madani 2019). According to Battalgazy and Madani (2019), PPMT based on TBSIM can produce accurate grade estimate when simulating grade of multiple correlated metals not only at local correlation scales (i.e., part of a deposit) but also at global correlation scales (i.e., at the deposit scale).

2.7 CONCLUDING REMARKS

Several geostatistical simulation methods have been developed for simulating the grades of metals that exhibit correlations with each other in a mineral deposit. While single-variable simulations are more straightforward, multi-correlated variables that exhibit complex relationships complicate the use of co-simulation methods and joint-simulation methods. Previous research focused on developing new geostatistical simulation approaches for correlated metals, often relying on widely used transformation methods. Despite this, studies continue to outline the limitations of these transformation methods, but more studies are being developed based on the transformation methods. According to the literature, transformation methods like normal score and SCT can only handle the correlation of metals at a lag zero, but they cannot handle the complexity of relationships among variables. Similarly, PPMT does not fully account for correlations between metals and MAF and does not adequately represent the multivariate complexity of correlated variables. Nonetheless, both PPMT and MAF remain popular for de-correlating highly correlated meals. This literature underscores the need for practical comparison between PPMT and MAF in terms of their performance in multivariate geostatistical simulation.

Chapter 3: Research Methodology

This chapter presents the methodology adopted for this research. It describes how the research was designed including sources of data, study area, regional geology of the study area, and methods employed to achieve research questions. The methods are outlined step by step in Figure 3.1.

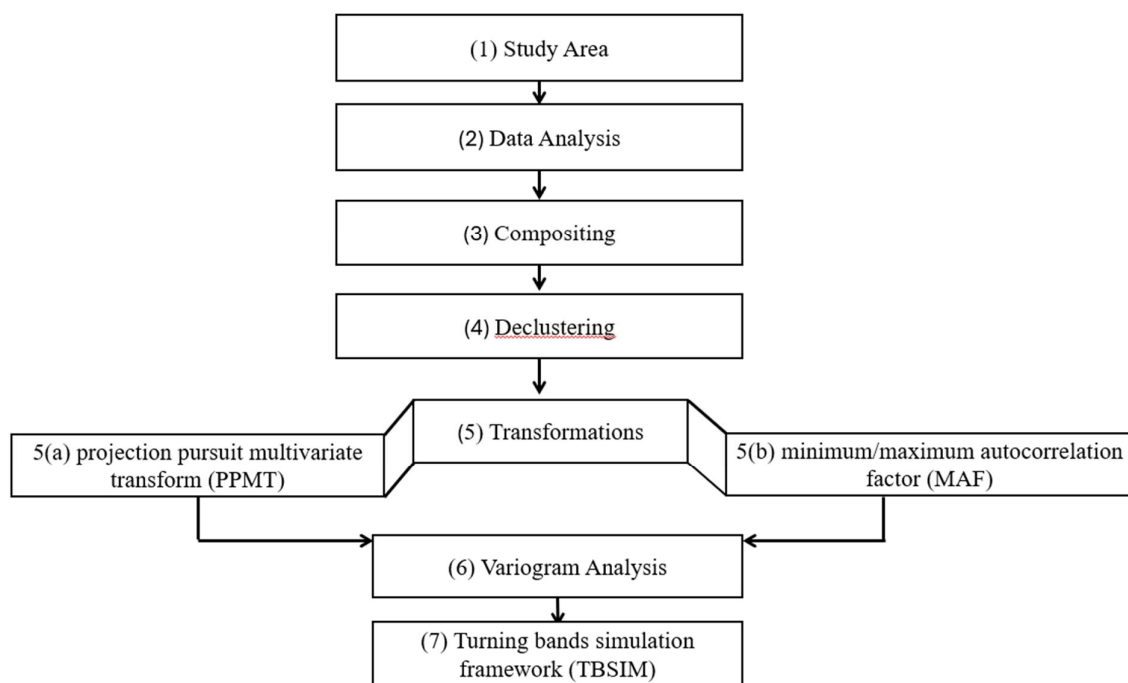


Figure 6.1 Summary of methods implemented in this study.

3.1 STUDY AREA

This study used data from the Carajás mine, the biggest iron ore mine in the world, which is situated in the Northern Brazilian state of Pará. The lithostructure and geology at the Carajás mine are defined by the Parauapebas and Carajás formations, which contain volcanic rocks and ironstones, and are among the metavolcanic and metasedimentary rocks. The Carajás deposits were discovered with the highest content of iron, which is 66%, making the Fe primary commodity of economic interest. The Carajás mine also include manganese, copper, tin,

aluminium, and gold (Paradella et al. 2015). The Carajás deposit is found within an Archaean iron formation with volcanic rocks that have been weathered between depths of 100 m and 150 m. In addition, the Carajás deposits also contain iron oxide, which is observed along the banded iron formations (BIFs) to total depth of 500 m.

Therefore, the Carajás mine is characterized by multiple metals in complex mineralization, which makes it a nonlinearly complex geological deposit. The complex interrelationships among metals in a deposit provide challenges for ore grades to be simulated accurately. The Carajás mine shows multi-correlated metals, thereby providing an opportunity to explore how multiple metals can be simulated using multivariate geostatistical simulation methods.

3.1.1 Regional Geology

The Carajás mineral province is divided into two Archaean tectonic blocks, namely the Southern Rio Maria granite-greenstone terrane and the northern Itacaiúnas shear belt (Souzas et al. 1997). The region surrounding the Carajás deposit is highly dominated by metavolcano-sedimentary rock and Meso to Neo-Archaean basement, which includes igneous rock and metamorphic complexes (Lobato et al. 2005). However, the iron ore at Carajás mine is hosted by the Carajás iron formation, which is found within mafic volcanic rocks of the Grão Pará Group (Figueiredo et al. 2019) (see Figure 3.2).

The Grão Pará Group represents a classic greenstone belt sequence consisting of volcanic and sedimentary rocks, dated between 2.8 and 2.7 billion years ago, with interbeds of BIFs (Lobato et al. 2005). The lower unit of the Grão Pará Group, known as the Parauapebas Formation, consists of basalt and basaltic andesites with minor basic to intermediate pyroclastic rocks. The upper unit of the Grão Pará Group consists of amygdaloidal facies with BIF and basic tuff intercalations. Large iron ore concentrations are found in the BIF of the Carajás Formation,

which comprises the middle portion of the Grão Pará Group (Lobato et al. 2005). The Grão Pará Group is exposed to both the northern and southern sides of a synclinal structure called the Carajás fold, with a shear zone known as the Carajás shear zone located along the central axis of the fold. The iron ore deposit at the Carajás mine is formed along the northern side of the fold known as the Serra Norte (Northern Range) deposits, and along the southern side of the fold known as the Serra Sul (Southern Range) deposits forming two zones of mineralization (Lobato et al. 2005).

The Serra Norte consists of nine deposits, namely N1-N9, in which some of the nine deposits are divided into two deposits. At the Serra Norte iron ore deposit, the protore is classified as jaspilite, which includes bedding-parallel quartz veins and early hydrothermal alteration, namely, the least altered jaspilite (Lobato et al. 2005). Lobato et al. (2005) defined iron ore as an advanced stage of hydrothermally altered and mineralized jaspilite, which consists of porous hard and hard ore. In addition, hard ore is made of quartz and hematite vein type. Transformation of hydrothermal hard ore from jaspilite includes the development of different stages of porosity that are characterized by high-grade soft ore type (Lobato et al. 2005, 2019). N4 and N5 deposits consist of basalts that exhibit hydrothermal alteration, characterized by strong chloritization and hematitization, particularly near the contact zone with the ore (Lobato et al. 2005). The N4 deposit is divided into two deposits, N4E and N4W, separated by a north-south-oriented fault.

At the Carajás mine, concentrations of phosphorus, aluminum, and manganese increase near the contacts with mafic volcanic wall rocks and dikes, as well as beneath the ferricrete cover. Iron ores are categorized according to the sequence of oxide formation (oxide paragenesis) as well as the specific textures and mineralogical characteristics of both the oxide minerals and

associated gangue minerals like quartz and carbonate. Hematite-martite and hematite are two most common iron types recognized at the Carajás mine (Lobato et al. 2005). Hematite-martite ore type is found along the N4W and N deposit and hematite ore type is found within the N5E deposit

3.2 DATA ANALYSIS

This research was based on data from 188 drill holes in the Carajás deposit, comprising 5,767 samples. The dataset included five elemental concentrations: phosphorus (P), iron (Fe), aluminum (Al_2O_3), manganese (Mn), and silica (SiO_2) obtained from unpublished dataset. From the five elements, the research focuses on two elements (Fe) and (Al_2O_3). Except for Fe and Al_2O_3 , as shown in Table 3.1, all elements show less correlation with one another. Fe exhibits a low coefficient of variation, suggesting homogeneous grades while Al_2O_3 shows high coefficient variation reflecting strong relative variability and heterogeneity. A Pearson correlation of -0.80 shows that the availability of Al_2O_3 is highly controlled by Fe; therefore, an increase in Fe will lead to a decrease in Al_2O_3 (Figure 3.3)

3.2.1 Database

Grade simulation requires different steps, including data gathering and organization of data (drill-hole) to create a model. For the database creation in this study, only 188 drill holes with depths ranging from 0 to 371.08 m were used (Figure 3.4). Due to proprietary restrictions, information regarding their spatial coverage cannot be disclosed. The database creation required three files: survey files, collar files, and assay files. Micromine software was used to create the database. However, the errors encountered during drill hole database validation included: (1) survey beyond hole depth, (2) intervals beyond hole depth, and (3) missing

intervals. Errors (1) and (2) were rectified based on the collar file, but error (3) cannot be corrected because the intervals were not recorded when recording data in the Excel file.

3.3 COMPOSITING

The depth of the drill holes differs across the study area because mineralized horizons occur at varying depth, ore bodies vary in thickness, and sampling intervals along the holes are adjusted accordingly. In mining, during resource estimation, drillholes that are assayed at different length increase uncertainty. Elements that occur in high concentrations can be assayed over short intervals, which may not be captured accurately during simulation, as most software assumes that drillhole data is collected at a constant support length (Dagbert 2014). Compositing is employed to ensure that all samples have the same weight (Palmer 2024). Compositing is a linear-weighted averaging method in which the composite value is determined by summing the products of each sample's length and its measured value, then dividing that sum by the total length of all the samples used in the calculation. Compositing can be employed to obtain values for different purposes such as orebody interception, lithological grouping, standardized downhole interval, bench composite, high-grade zone, and composite based on minimum length and grade criteria (Dagbert 2014).

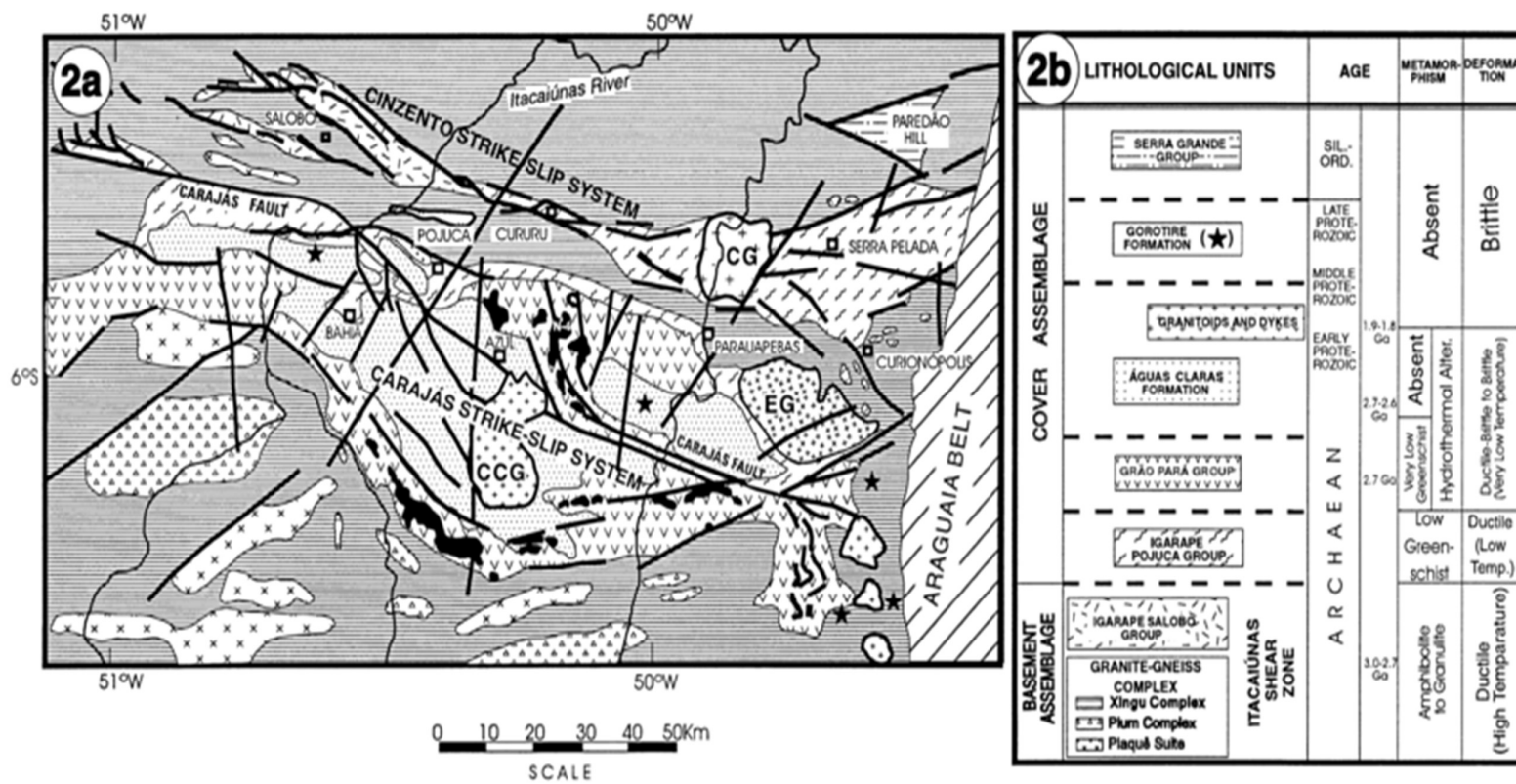


Figure 3.2: (2a) Simplified geological map of the Carajás region. (2b) Tectonostratigraphic column of the Carajás region (Holdsworth and Pinheiro 2000).

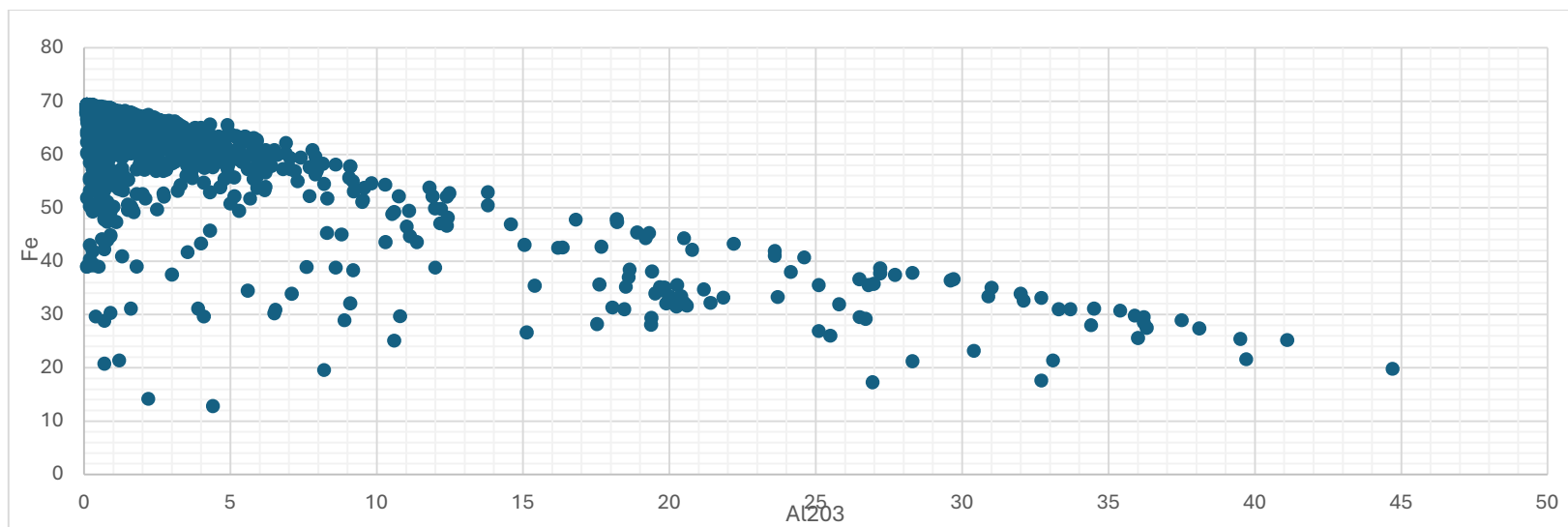


Figure 3.3: Scatter plot showing the relationship between Fe and Al_2O_3 .

Table 3.1: Descriptive statistics of Al_2O_3 and Fe.

Variables	Number samples	Number of drill holes	Minimum	Maximum	Mean	Mode	Median	Range	Coefficient of variation
Fe	5767	188	4.8	69.4	60.51069	67.8	66.6	64.6	0.11
Al_2O_3	5767	188	0.07	44.7	1.774442	0.5	0.8	44.63	2.33

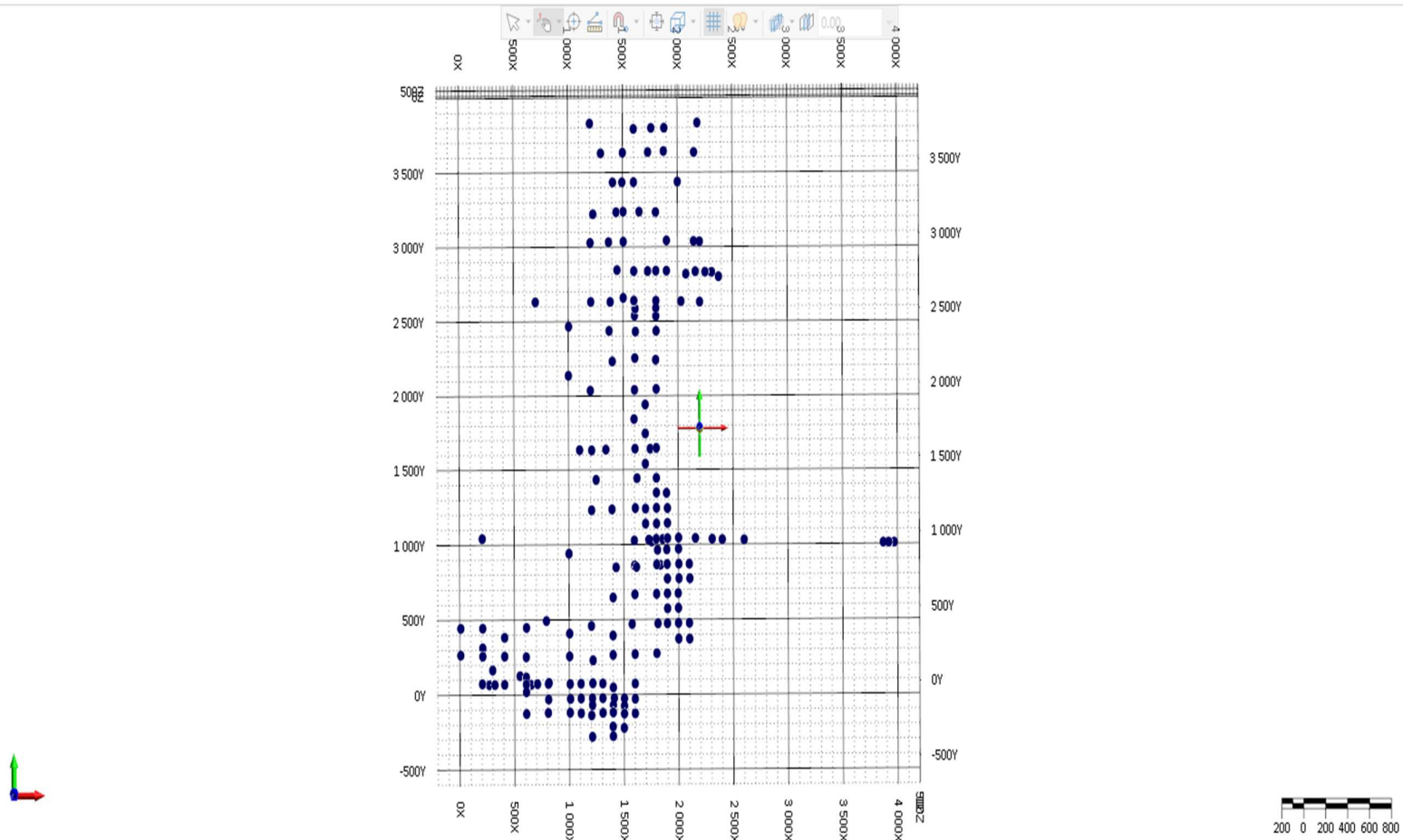


Figure 3.4: Collar positions of the 188 drill holes were selected for this study.

Compositing was done based on two methods: downhole compositing and bench compositing, which is the most popular in open pit mining operations. However, compositing in this study was done based on downhole composite because bench composite is based on bench height in open pit, which is not justified in this study. In addition, the bench composite has some drawbacks in drill holes that are inclined because the actual composite length will be different from the bench height (Dagbert 2014). Downhole composite is done based on the length of the drillhole from the top to the bottom, in which the length of the composited drillholes is always the same. This study used 5766 samples with assay depths ranging from 0.010 m to 133.17 m. Figure 3.5 shows the distribution of assay length with the statistics shown in Table 3.2 below. Most of the sample lengths ranged 2–4 m. Based on the statistics shown in Table 3.2 below, all sample lengths had a mode of 3.00 and a mean of 3.7. A 3-m interval was used for compositing, based on the median of all sample lengths.

Table 3.2: Descriptive statistics of sample length.

Min value (m)	Max value (m)	Mean	Variance	Standard deviation	Coeff. Of variance	mode
0.01	133.170	3.701	36.1335	6.011	2	3

3.4 DECLUSTERING

In mining, it is natural to collect samples randomly for resource estimation. According to Pyrcz and Deutsch (2002), random sampling mostly occurs in an area of interest, leading to data clustering. However, during the stage of mining, it is very important to start mining in an area of high grade, which influences the random sampling of clustered data. In addition, areas that are sampled more densely than others will have more weight, and this will influence statistics. Declustering is well known and applied in clustered data, and the processes of declustering are done based on software tools and algorithms (Pyrcz and Deutsch, 2002). Declustering is done based on two assumptions (Pyrcz and Deutsch, 2002): (1) samples must accurately represent

all possible values in the area of interest and be collected evenly across space, without overrepresenting certain locations; and (2) understand the nature of clustering.

Declustering includes three methods: (1) polygonal declustering, (2) cell declustering, and (3) kriging weight declustering. Polygonal declustering has some drawbacks: if two samples are close to each other and they are collected next to the boundary of the study area, they will be assigned the same weight, which can mislead the results (Dubois and Saisana, 2002). Kriging weight declustering is also known for being time-consuming compared to cell declustering and polygonal declustering. Kriging weight declustering consists of a string effect which causes samples to have uneven weights. Samples that are close to the boundary can end up gaining more weight compared to other samples, even though they are far from each other (Pyrz and Deutsch, 2002).

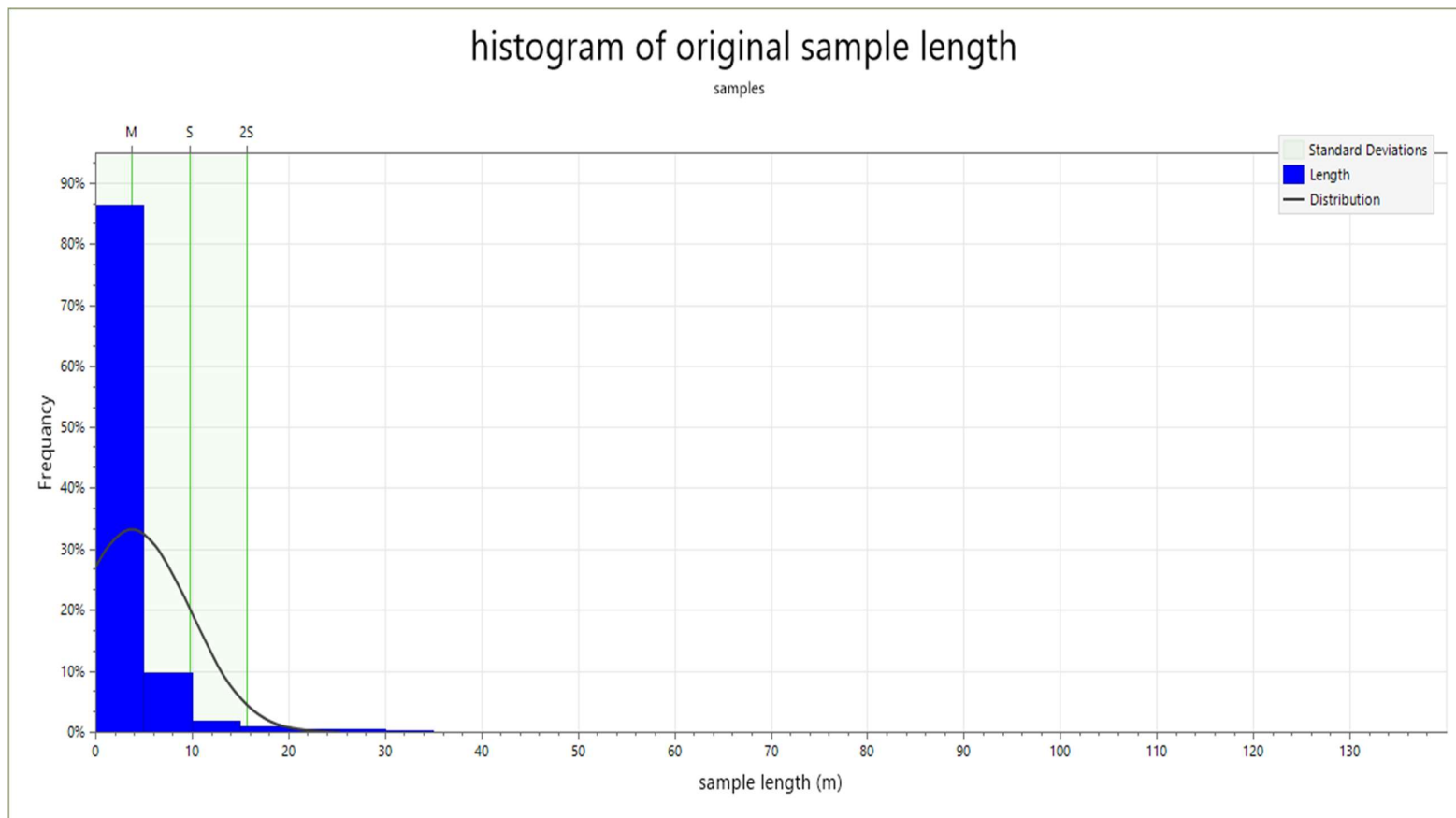


Figure 3.5: Histogram showing the distribution of sample length.

Cell declustering is the most common method applied in resource estimation as it is more robust compared to polygonal declustering and kriging weight declustering (Pyrz and Deutsch, 2002). Cell declustering splits a study area into rectangular cells using a moving window system in which each cell is assigned a weight that is inversely proportional to the number of samples within the same window. Because of the drawbacks of cell declustering, the results can change depending on the choice of the size and starting point of grid cells, and since there is no exact rule for picking them, the outcome can be a bit uncertain (Dubois and Saisana 2002). Cell sizes are selected based on a rule of thumb, which depends on the type of clustering data. In areas where samples are unevenly collected, cell sizes are created for each cell size to accommodate only one sample (Dubois and Saisana 2002; Pyrcz and Deutsch 2002). In areas with high or low-grade concentrations, cell sizes can be selected to calculate weights that either minimize or maximize the overall average value of the dataset. If the cell size is too small, each sample ends up in its own cell, resulting in all samples being weighted equally, just like using the raw data. If the cell size is too large, all the samples fall into a single cell, again leading to equal weighting (Pyrz and Deutsch, 2002).

This study was based on 188 drillholes that are clustered (Figure 3.6) and the cell de-clustering method (Dagbert, 2014) was used to assign all drillholes with equal weight.

Cell declustering was done based on the following steps using Micromine software:

Step 1: divide the volume of the area of interest into a grid cell.

Step 2: from each occupied cell, count the number of data available.

Step 3: assign a weight to each data point based on how many data points fall within the same cell. From an occupied cell, each cell must be assigned the same weights where all weights must be greater than zero and sum to one. However, Dagbert (2014) emphasized that it is of

importance to consider that the cell size for de-clustering only defines the grid for assigning de-clustering weight which is not the same as the cell size for geological modelling.

The study area (Figure 3.7) was visualized in 3D and it extends approximately 4000 m along the X-axis, 3500 m along the Y-axis, and 500 m along the Z-axis. The minimum drillhole spacing within the area was 10 m. Cell declustering was done based on the maximum and minimum distances of x, y, and z with an increment of 10 m. The increment distance was selected based on the minimum distance between drill holes. An optimum cell dimension of 460 m x 460 m x 91m was selected, as it resulted in the lowest stable declustered mean and standard deviation for both Fe and Al₂O₃. The mean of actual values before declustering was hindered the raw mean, which was always greater than the mean of all samples after declustering. Figures 3.8 and 3.9 show scatter plots of Fe and Al₂O₃ after declustering with the lowest declustered mean and standard deviation. After declustering, the declustered mean was calculated for Fe and Al₂O₃, which remained unchanged from the raw mean. In addition, after declustering the mean is expected to change if there is a significant clustering in the dataset. However, in this case it is assumed that the drillholes were not close enough to cause substantial spatial bias in which the mean after declustering remains the same.

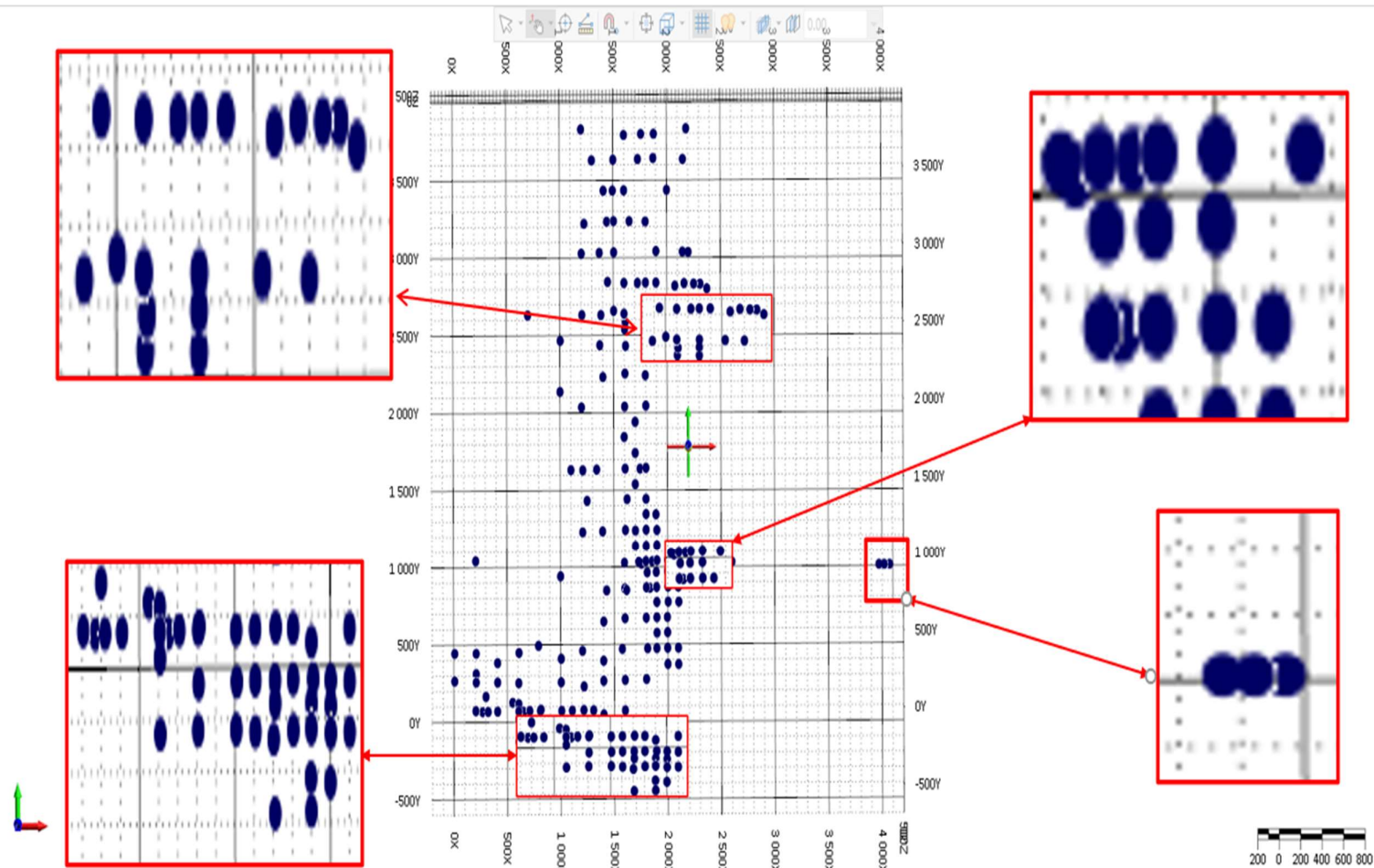


Figure 3.6: Diagram showing clustered drillholes from the database.

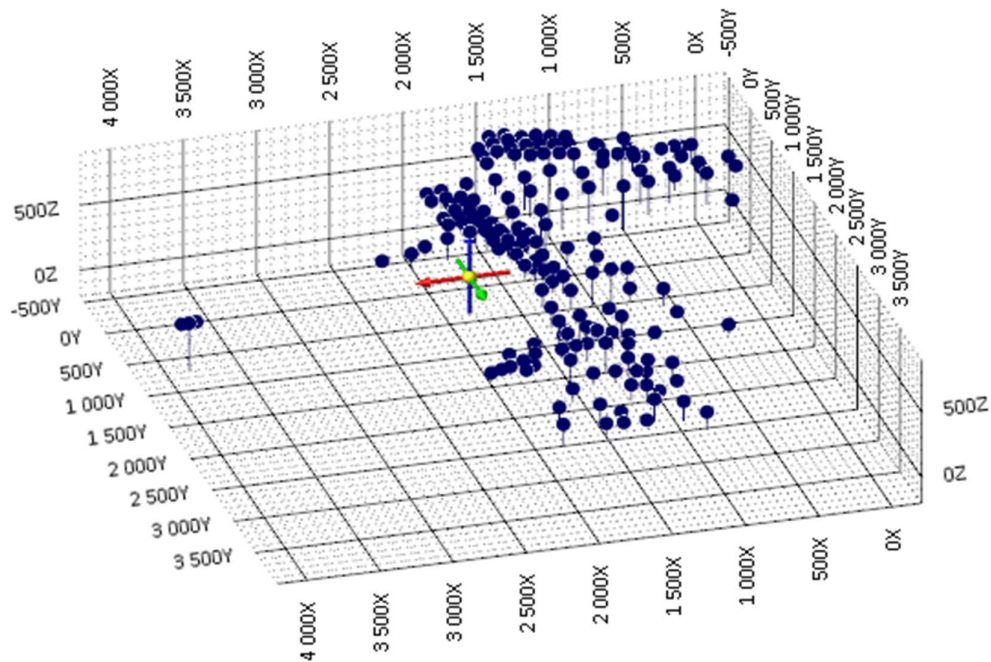


Figure 3.7: Drillholes in 3D, showing X, Y, and Z of the study area.

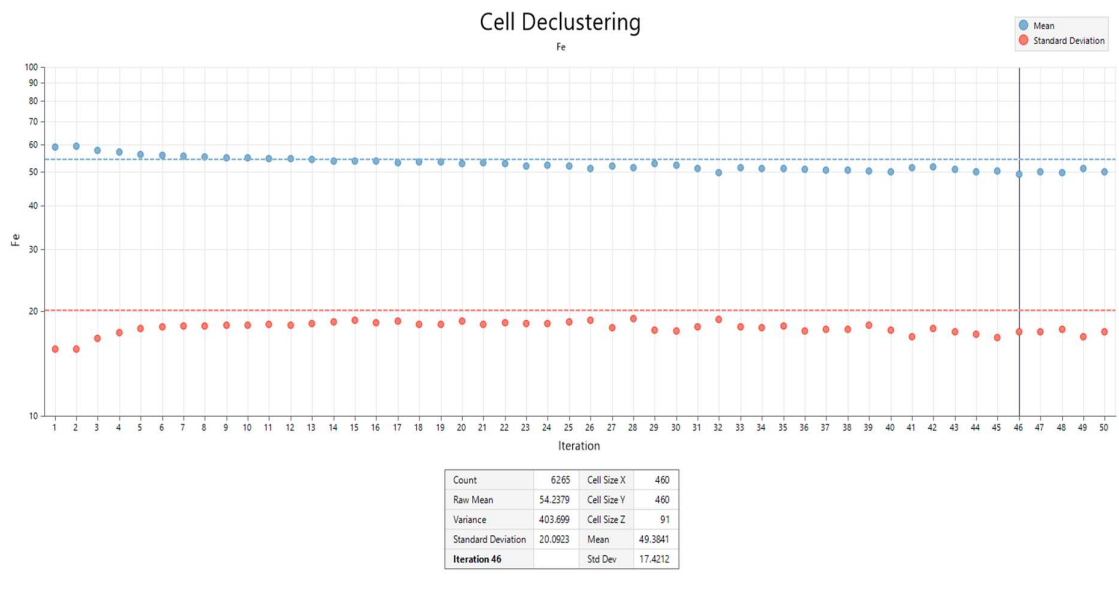


Figure 3.8: Scatter plot showing the declustered mean of Fe.

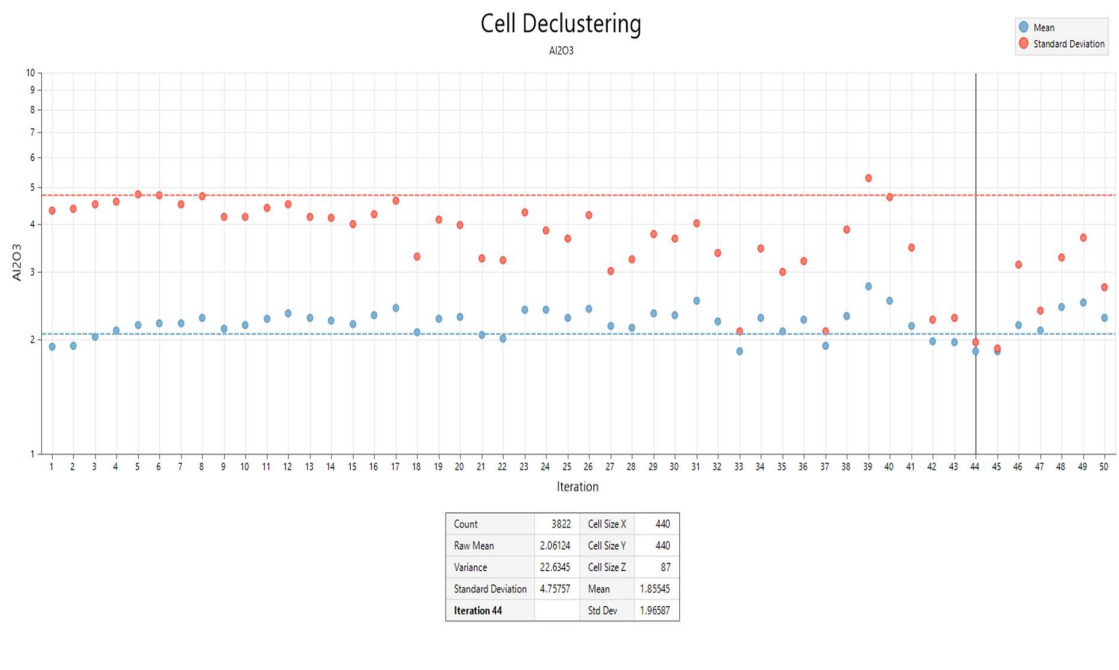


Figure 3.9: Scatter plot showing the declustered mean of Al_2O_3 .

3.5 HISTOGRAM

A histogram is a type of graph that allows for visual interpretation of numeric data by indicating the number of data that lie within a range of values called a class or bin or series of intervals. Histograms are one of the basic statistical tools used for data analysis (Dagbert, 2014). Histograms help in determining statistical properties of the data to understand all potential factors that may have effects in resources estimation. According to Dagbert (2014), not only are histograms important but normal distributions are important in the history of geostatistics. In addition, positively skewed distribution indicates that most of the data are concentrated on the left (Figure 3.14) of original data set. Positively skewed lognormal distribution shows that the mean > median > mode.

However, Dagbert (2014) mentioned that earth science data values are positive and positively skewed. Moreover, not all science data are considered positive and positively skewed, (see Figure 3.15). Figure 3.15 shows positive data which is negatively skewed, showing that all data

are concentrated on the left. Negative skewed distribution shows that the mean < median < mode.

With the help of histograms, two characteristics can be determined: outliers and bimodal distributions. Outliers are data values that are much lower or higher than most data values but in geostatistics outliers are values which are significantly distanced from most of the data values. Figures 3.10 and 3.11 show the distribution of untransformed Fe and Al₂O₃ data, indicating that there are no outliers and a bimodal distribution of the data. Dagbert (2014) indicated that geostatistical simulation methods require the use of transformation methods to create a histogram of normal distribution for data, which will reduce extreme values (outliers) that influence resource estimation. Normal distribution was first introduced by Abraham de Moivre in 1733 to estimate the results of a bimodal distribution when the number of trials is large (Dagbert, 2014). Statistically, bimodal distribution is referred to as two relatively most common values that are not adjacent to one another. According to Dagbert (2014) the normal distribution is characterized by a zero mean and a standard deviation of one. Transformed data using PPMT for both Al₂O₃ and Fe shows a normal distribution of zero mean and standard deviation of one (Figures 3.12, 3.13, 3.14, and 3.15)

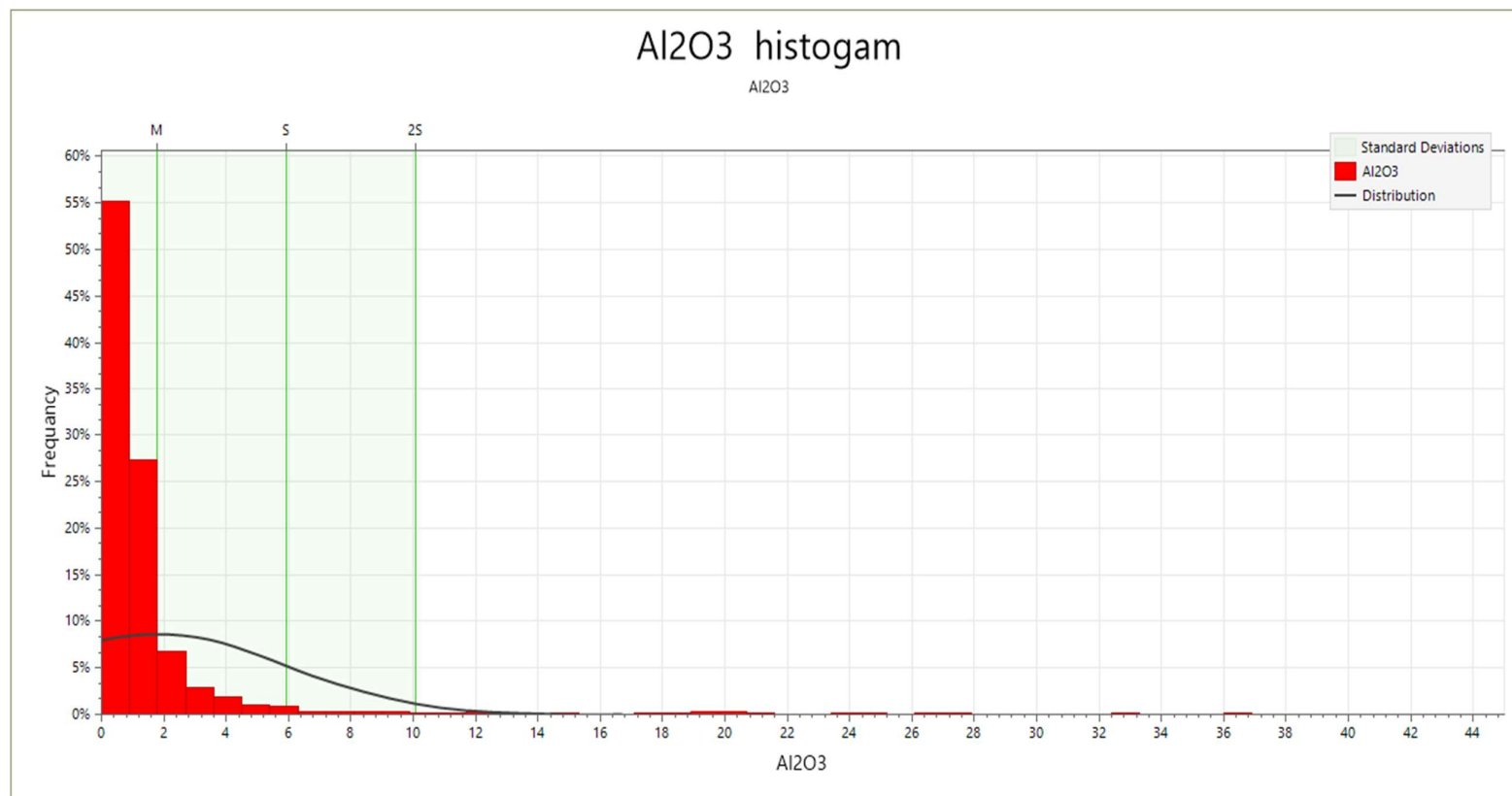


Figure 3.10: Histogram showing positively skewed distribution of untransformed data (Al₂O₃).

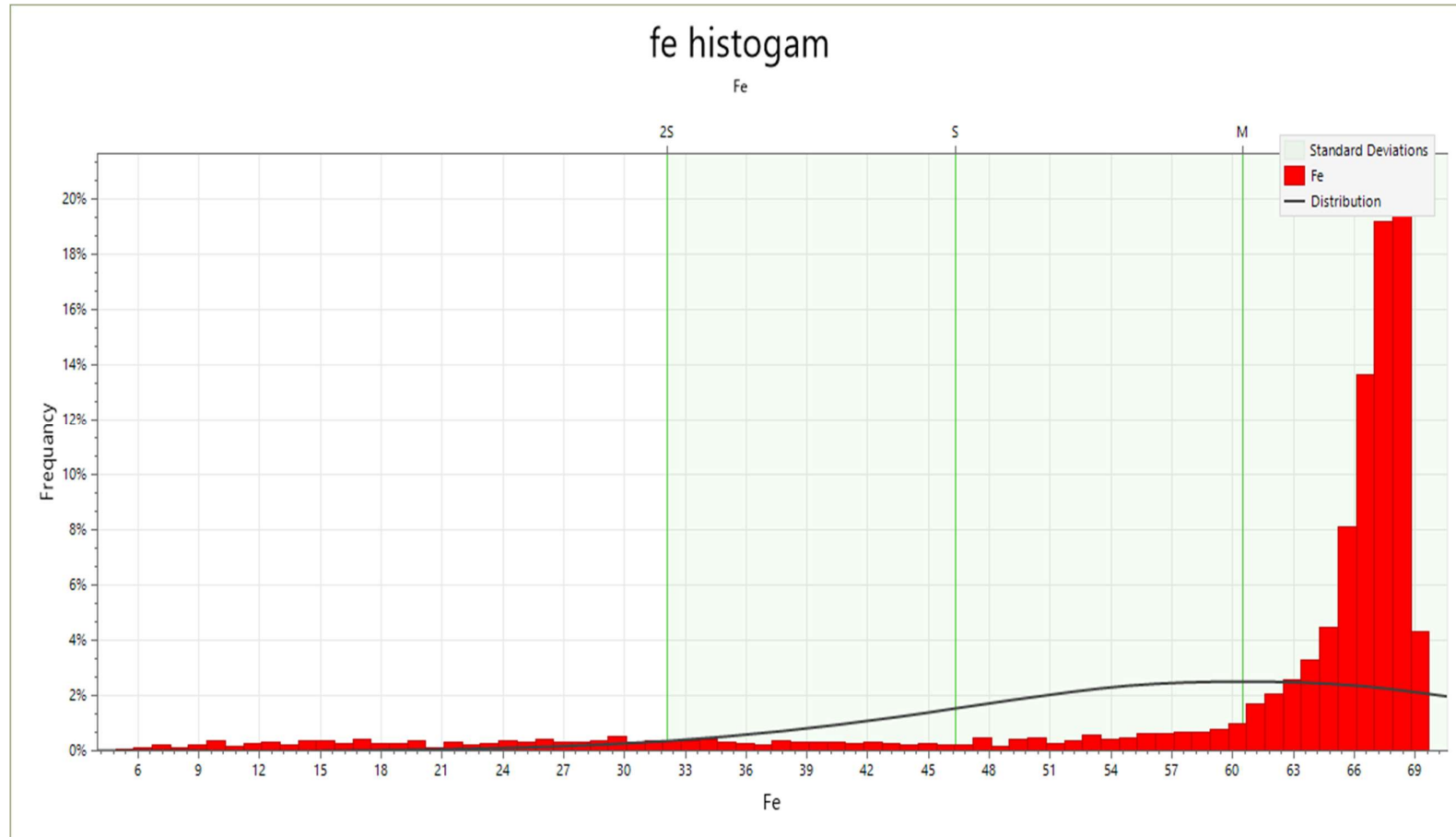


Figure 3.11: Histogram showing negatively skewed distribution for untransformed data (Fe).

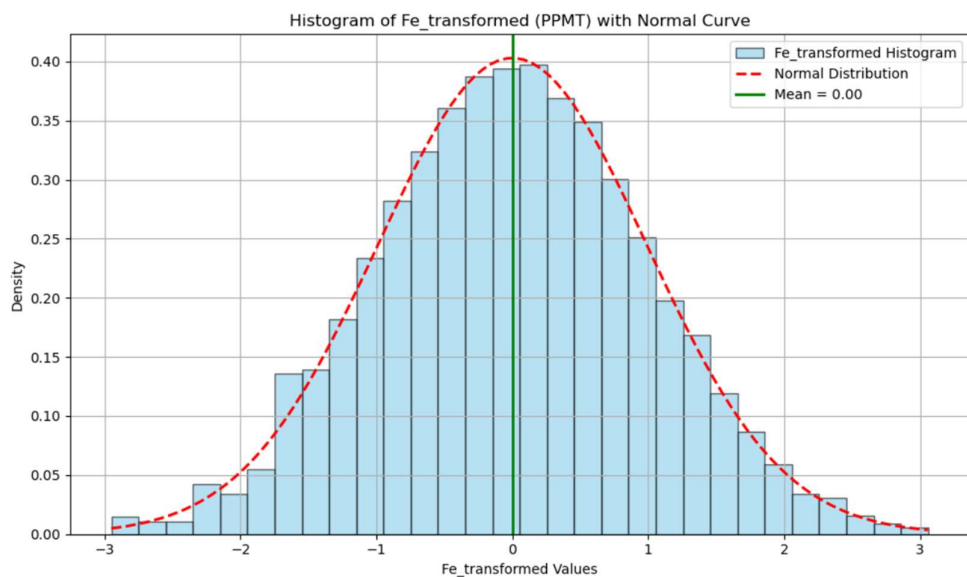


Figure 3.12: Histogram showing normal distribution of PPMT(Fe).

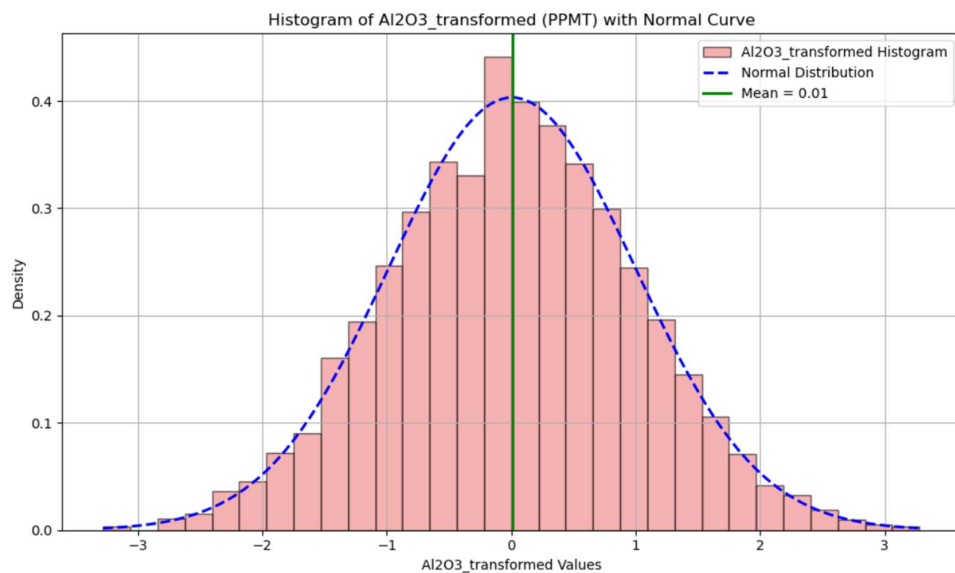


Figure 3.13: Histogram showing normal distribution of PPMT(Al₂O₃)

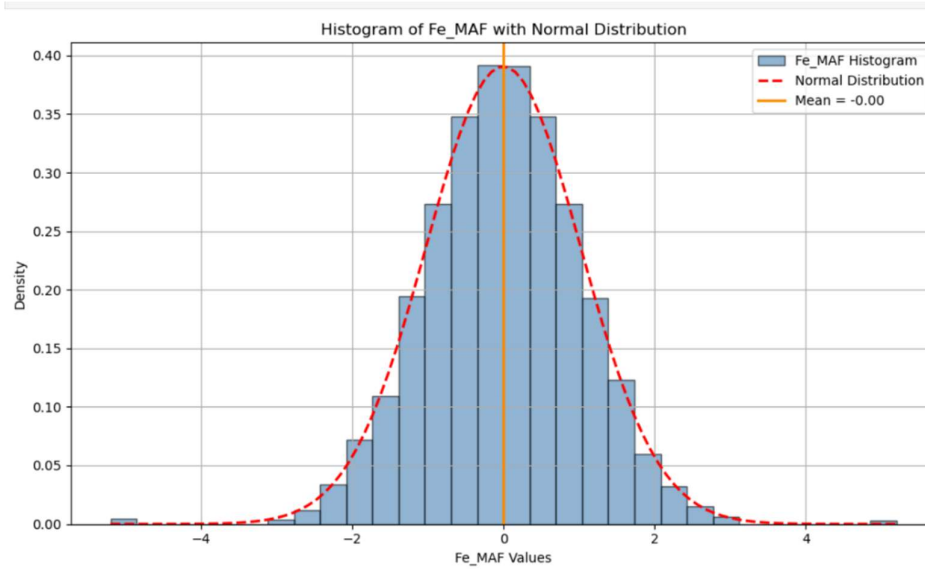


Figure 3.14: Histogram showing normal distribution of MAF(Fe)

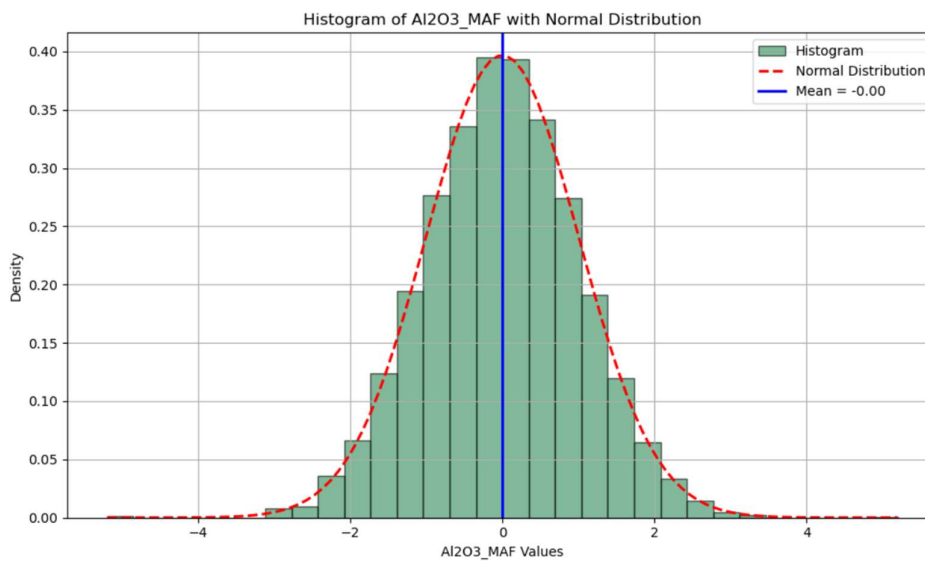


Figure 3.15: Histogram showing normal distribution of MAF(Al_2O_3)

3.6 DATA TRANSFORMATION

Transformation methods play an important role in geostatistical simulation for the preparation of multivariate models. Metals that exhibit strong correlation fail to meet the statistical assumption required when simulating values of multivariate normality. This research trialed

two transformation methods, namely projection pursuit multivariate transform (PPMT) and minimum/maximum autocorrelation factor (MAF).

3.6.1 Projection Pursuit Multivariate Transform (PPMT)

Before PPMT, Friedman and Tukey (1974) introduced projection pursuit density estimation (PPDE) for determining projection of high-dimensional data. However, Barnett et al. (2014) developed PPMT for analyzing multivariate data. The idea of PPMT is to determine the direction on which multidimensional data can be projected to reveal the features of the data. PPMT was found to be more effective for decorrelating assay grades compared to principal components analysis and factor analysis for several reasons including (Abildin et al. 2022): handling the complexity among variables, namely (1) nonlinearity, (2) heteroscedastic relationships and (3) geological constraints. PPMT is performed based on forward and backward transformation. Forward transformation involves converting correlated variables into uncorrelated ones with normal distribution considering the complexity between metals. Back-transformation includes transforming simulated data back into normal data. PPMT is done through three steps (Barnett et al., 2014): (1) normal score transformation, (2) sphering, and (3) projection pursuit.

3.6.1.1 Normal score transformation

Normal score transformation is applied to obtain values with mean of zero and variance of one (Battalgazy and Madani 2019). Normal score transformation is applied to each metal data before applying projection pursuit to normalize data and mitigate heteroscedasticity, the by ensuring approximate homoscedasticity and second order stationary in the transformed space to provide accurate results after applying projection pursuit (Barnett et al. 2014). The transformation is ranked-based, with tides values assigned identical transformed scores through

average ranking to preserve equality among identical observations following multi-gaussian assumption (Figure 3.17). Normal score transformation is applied based on equation 2 (Deutsch and Journal 1998):

$$z_i = G^{-1}(F_i(Y_i(u))) \dots\dots\dots (Eq\ 2)$$

where G^{-1} is standard normal cumulative distribution function, F_i is cumulative distribution function of the original variables, and $z_i(u)$ and $Y_i(u)$ are normal score value.

3.6.1.2 Data sphering

Although data sphering procedure in the PPDE relies on the covariance matrix, it is highly sensitive to outliers, which can significantly affect the results (Barnett et al. 2014). Before employing projection pursuit, Friedman (1987) advised applying changes that make each variable more normally distributed. The goal of projection pursuit is to find intricate patterns in multivariate data; this additional preprocessing step lessens the impact of the features of individual variables. Applying normal score transformation on each variable was demonstrated to improve the efficiency and result of the projection pursuit process, even though multivariate outliers may still have an impact on data covariance. Projection pursuit requires variables to be centered with unit variance and an orthogonal covariance matrix, which can be done using data sphering (Friedman 1987).

Normal score transformation consists of a covariance matrix, which is identical to the sample correlation variables matrix (Battalgazy and Madani, 2019). For two variables, the matrix (V) is determined using equation 3.

$$V = Corr\{z_1(u), z_2(u)\} \dots\dots\dots (Eq3)$$

where V is a matrix of both Al_2O_3 and Fe, $z_1(u)$ and $z_2(u)$ represent the transformed values of Al_2O_3 and Fe. After determining the matrix (V) for both variables, spectral decomposition is

considered as a next step for V to derive orthogonal eigenvectors matrix (M_1), which is associated with underlying diagonal eigenvalues matrix E_1 :

$$V = M_1 E_1 M_1^T \dots\dots\dots (\text{Eq 4})$$

Step four includes calculating sphering transformation using (equation 5) after determining spectral decomposition of matrix (V) at u :

$$\varphi_i(u) = z_i(u) M_1 E_1^{-1/2} M_1^T \dots\dots\dots (\text{Eq 5})$$

where $\varphi_i(u)$ is a normal score standard distribution.

3.6.1.3 Projection pursuit

After determining the matrix (V) for both variables, projection pursuit is applied. Normal score is transformed to standard Gaussian, which turns to be equal to projection as shown in equation 6.

$$\varphi_i(u)' = \tau' \dots\dots\dots (\text{Eq 6})$$

where τ' is projection and $\varphi_i(u)'$ is standard gaussian.

Transformation using projection pursuit was achieved including the Gram-Schmidt algorithm to calculate orthogonal matrix (see equation 7).

$$\omega = [(\alpha, \phi_1, \phi_2 \dots \dots \dots \phi_{k-1})] \dots\dots\dots (\text{Eq 7})$$

where ω is the orthogonal matrix, α is projection index, ϕ is orthogonal factor and ϕ_{k-1} is the last orthonormal vector.

Therefore, Gaussian standard projection is determined by normal score transformation using equation 8.

$$G(\varphi_i(u)\omega) = [\tau' \varphi_i(u) \phi_1, \varphi_i(u) \phi_2 \dots \dots \dots \varphi_i(u) \phi_{k-1}] \dots\dots\dots (\text{Eq 8})$$

where $G(\varphi_i(u)\omega)$ is a Gaussian standard projection.

Although PPMT consists of multiple complex steps, all of them are carried out using a single program, making the processes straightforward and fast. Figure 3.16 shows the original data

before transformation and after transformation using PPMT. Figures 3.17 and 3.18 show the scatter plots of normal transformation and PPMT, respectively.

3.6.1.4 Back-transformation

After simulation, the results were transformed back to their original assay values. Back-transformation is performed by applying inverse of the normal score transformation, data sphering, and projection pursuit to simulated realizations, converting values from the standardized normal space back to their original assays. Identical transformed values result from tied observations in the original data are assigned identical assay values during back transformation.

3.6.2 Minimum/Maximum Autocorrelation Factor (MAF)

MAF is used for transforming correlated metal grades into uncorrelated factors and for transforming them back to the original scale after simulation. This can be done based on the following steps: (1) transforming original data into normal score; (2) determining uncorrelated factors from MAF using correlated metal, and (3) back-transformation (Figure 3.19).

MAF was constructed using lag zero ($h=0$) covariance following the global correlation between Fe and Al₂O₃ because Fe and Al₂O₃ were measured at the same sample locations. Non-zero lag distance was not considered in this study as the objective of MAF in this study was to decorrelate variables measured at the same location before simulation.

	K	L		K	L
1	Al2O3	Fe	1	PPMT_Fe	PPMT_Al2O3
2	0.90	65.90	2	0.379793891	-0.211116996
3	0.90	66.70	3	0.436171244	-0.211116996
4	0.50	67.70	4	0.506642934	-0.307689246
5	0.70	67.60	5	0.499595765	-0.259403121
6	3.70	61.40	6	0.062671285	0.464888753
7	on	28.90	7	-2.227658652	
8	on	41.70	8	-1.325621015	
9	0.70	68.50	9	0.563020286	-0.259403121
10	0.90	68.70	10	0.577114624	-0.211116996
11	0.30	69.20	11	0.61235047	-0.355975371
12	0.70	68.40	12	0.555973117	-0.259403121
13	0.30	69.10	13	0.605303301	-0.355975371
14	0.40	68.70	14	0.577114624	-0.331832309
15	0.80	68.20	15	0.541878779	-0.235260059
16	0.90	68.20	16	0.541878779	-0.211116996
17	1.00	67.60	17	0.499595765	-0.186973934
18	0.90	68.00	18	0.527784441	-0.211116996
19	1.20	67.30	19	0.478454258	-0.138687809
20	1.10	67.10	20	0.46435992	-0.162830871

Figure 3.16: Excel file showing data before PPMT transformation and after PPMT transformation.

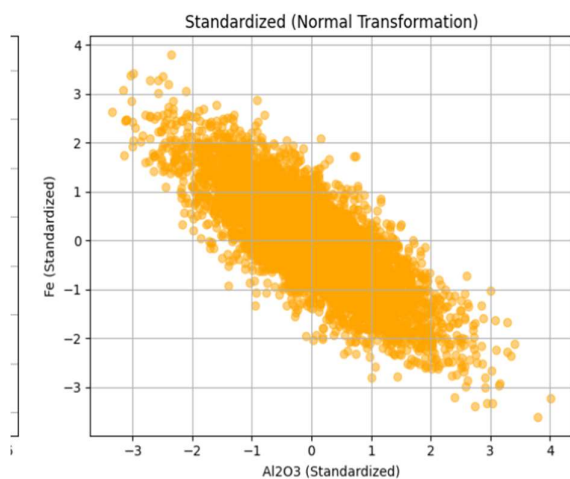


Figure 3.17: Scatter plot of normal transformation for Fe and Al₂O₃.

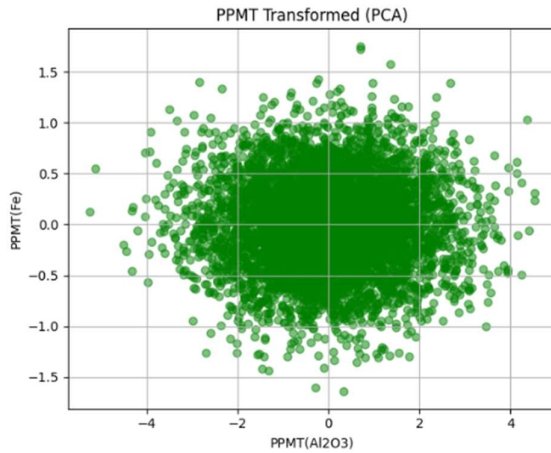


Figure 3.18: Scatter plot of PPMT transformed data showing zero correlation between Al_2O_3 and Fe.

	K	L
1	Al2O3	Fe
2	0.90	65.90
3	0.90	66.70
4	0.50	67.70
5	0.70	67.60
6	3.70	61.40
7	on	28.90
8	on	41.70
9	0.70	68.50
10	0.90	68.70
11	0.30	69.20
12	0.70	68.40
13	0.30	69.10
14	0.40	68.70
15	0.80	68.20
16	0.90	68.20
17	1.00	67.60
18	0.90	68.00
19	1.20	67.30
20	1.10	67.10

(a) data before MAF

	M	N
1	Fe_MAF	Al2O3_MAF
2	-0.213504957	0.230633481
3	0.062595297	0.230633481
4	0.58625571	-0.615822469
5	0.519131042	-0.154881792
6	-0.756747709	1.42459407
7	-1.471879345	
8	-1.184686933	
9	1.339189542	-0.154881792
10	1.647633532	0.230633481
11	2.522893136	-1.269115456
12	1.231358017	-0.154881792
13	2.346736425	-1.269115456
14	1.647633532	-0.902577431
15	1.028302709	0.037004071
16	1.028302709	0.230633481
17	0.519131042	0.415078963
18	0.843243055	0.230633481
19	0.350476057	0.612029921
20	0.239125733	0.525842714

(b) Data after MAF

Figure 3.19: Neutral academic wording showing data before and after applying MAF.

3.7 VARIOGRAM ANALYSIS

Variograms are a graphical tool that describes how data values change over distance and direction. They are used to characterize correlated data by comparing differences between samples against distances. Variograms help in determining variogram maps, which explain the anisotropy and directional continuity of data. The experimental variogram is calculated based on the dataset, which aids in fitting the variogram model (Barnes,2003). Variograms are aligned

with parameters called nuggets, sill, and range. Nuggets are influenced by the type of values in which they describe the difference between the values of samples at a separation distance of zero. A sill is defined as a value at which a variogram levels off or flattens. In experimental variograms, from the point where different values increase until they become negligible, a point where all values become constant is called the sill. A sill is considered the amplitude of a variogram. Range is the maximum distance at which the sill is attained. The distance beyond each range value shows that all samples are uncorrelated.

To evaluate the spatial directional continuity and anisotropy of the data, semi-variogram maps were generated using Micromine, as shown in Appendix 3.1. For each transformed variable, anisotropy was assessed along three orthogonal directions corresponding to the major, semi-major, and minor axes (Table 3.3).

Table 3.3: Strike, dip, and pitch of all semi-variogram maps.

	Major axes	Semi-major axes	Minor axes
PPMT (Fe)	344	64.7	90
PPMT (Al ₂ O ₃)	66.8	66.3	83.3
MAF (Fe)	344	64.3	90
MAF (Al ₂ O ₃)	60	68.2	82.2

3.7.1 Experimental variogram

Through the analysis of semi-variogram maps, direct variograms were created, considering the direction of continuity, to fit the experimental variograms. Direct variogram is referred to as a type of variogram in which pairs of samples are selected based on the distance and direction in which they are separated. For each transformed variable, experimental variograms were constructed along three principal axes of anisotropy, including major axis, semi-major axis, and minor axis. Variograms are statistically defined using equation 9.

$$2\gamma(h) = \frac{1}{n(h)} \sum_{j=1}^{n(h)} (z(x) - z(x+h))^2 \dots\dots\dots \text{Equation 9}$$

where $\gamma(h)$ is the variogram at lag distance h , $n(h)$ is number of data pairs separated by lag h , $z(x)$ is the value of a variable at a location x , $z(x+h)$ is the value of the variable at a location $x + h$. The experimental variograms for each variable are shown in Figures 3.20, 3.21, 3.22, and 3.23, whereas all three individual variograms of each variable are shown in Appendix 3.2.

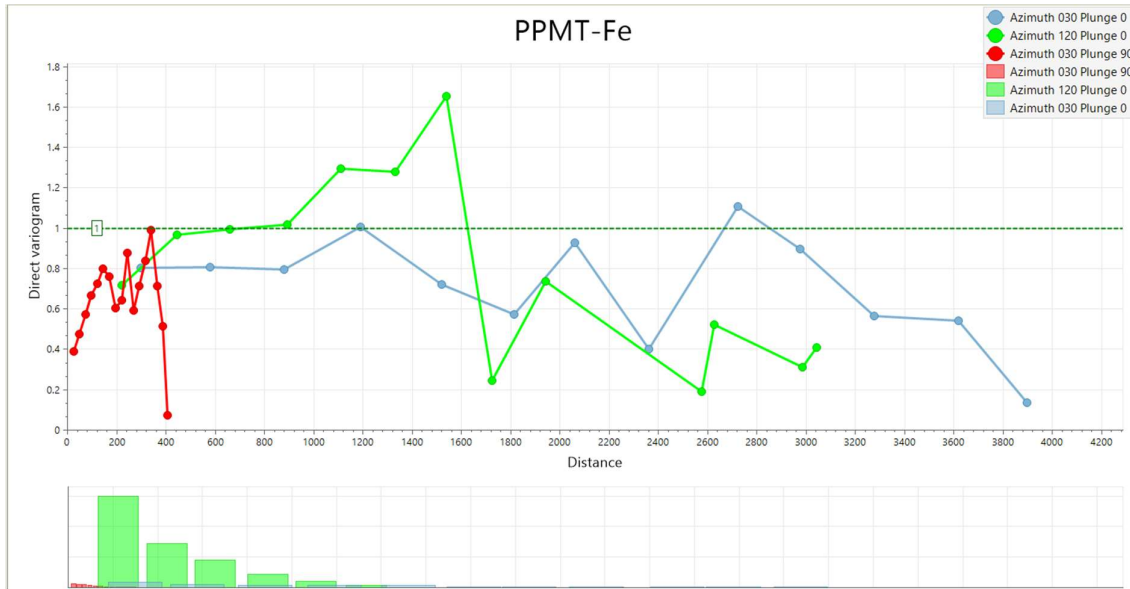


Figure 3.20: Direct variogram for PPMT (Fe) and bar graph with number of samples on each point. Blue line represents major axis (azimuth 30°, dip 0°), green line represents semi-major axis (azimuth 120°, dip 0°), and red line represents minor axis (azimuth 30°, dip 90°).

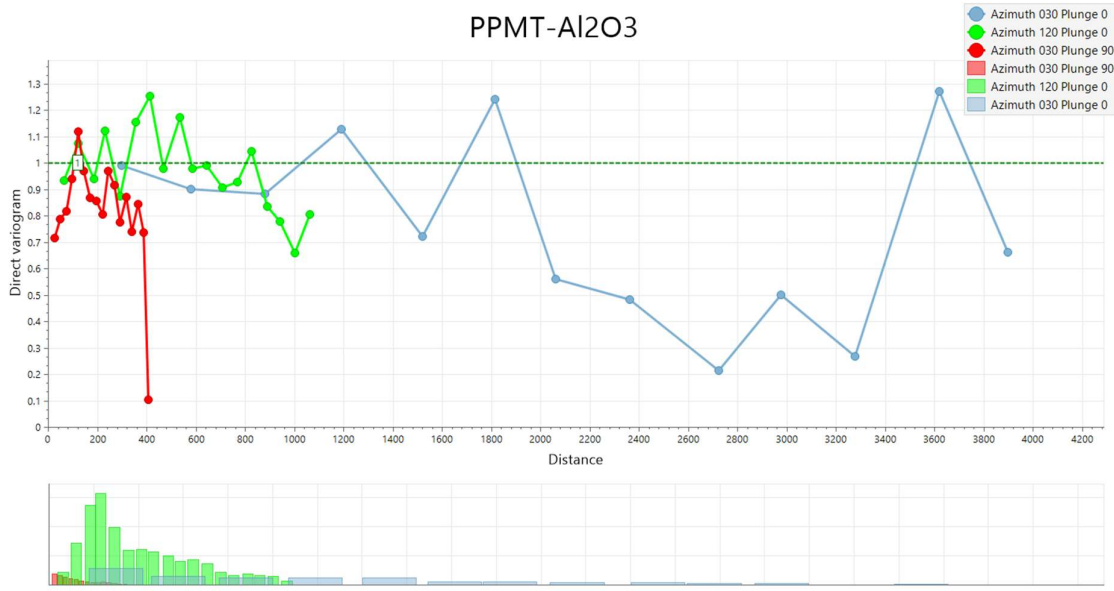


Figure 3.21: Direct variogram of PPMT (Al_2O_3) and bar graph with the number of samples on each point. Blue line represents major axis (azimuth 30°, dip 0°), green line represents semi-major axis (azimuth 120°, dip 0°), and red line represents minor axis (azimuth 30°, dip 90°).

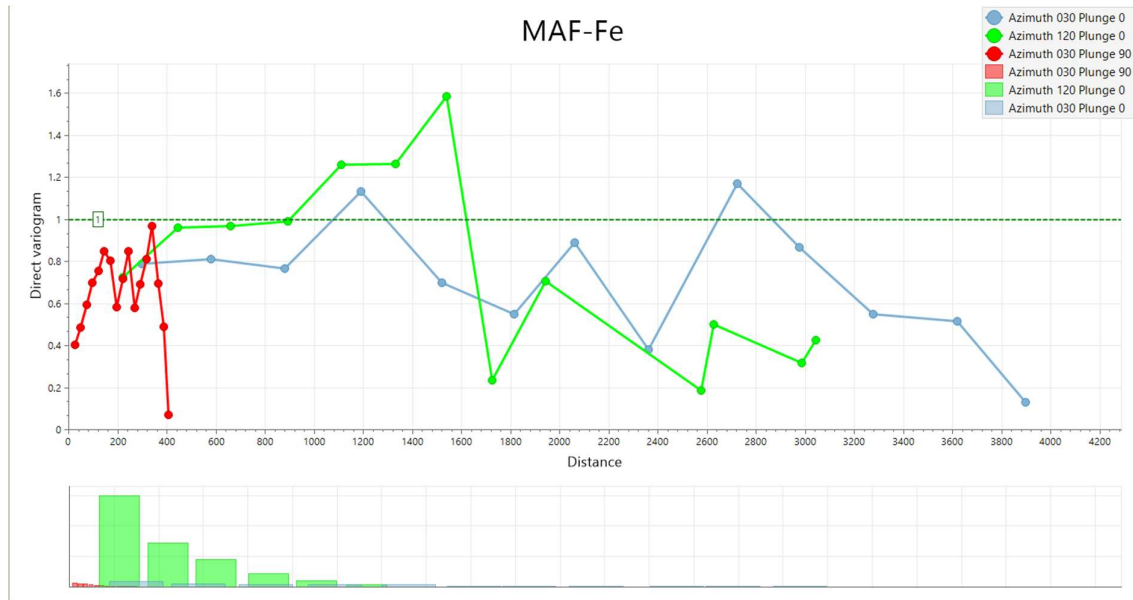


Figure 3.22: Direct variogram of MAF (Fe) and bar graph with the number of samples on each point. Blue line represents major axis (azimuth 30°, dip 0°), green line represents semi-major axis (azimuth 120°, dip 0°), and red line represents minor axis (azimuth 30°, dip 90°).

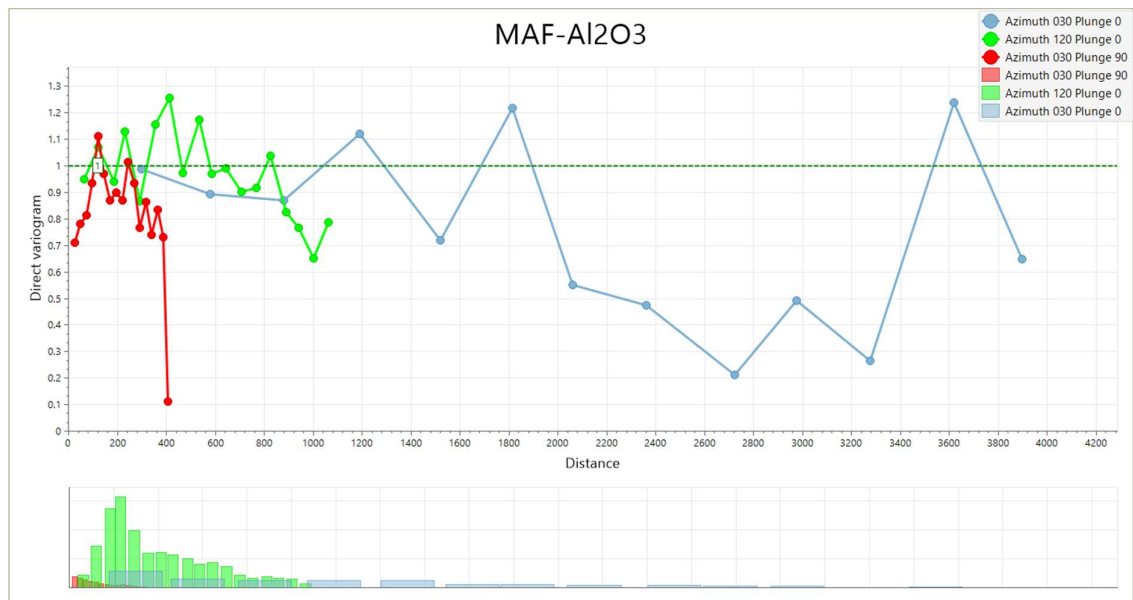


Figure 3.23: Direct variogram for MAF (Al₂O₃) and bar graph with number of samples on each point. Blue line represents major axis (azimuth 30°, dip 0°), green line represents semi-major axis (azimuth 120°, dip 0°), and red line represents minor axis (azimuth 30°, dip 90°).

3.7.2 Variogram model

Once experimental variograms were created, variogram models were fitted per axis for each variable. However, before fitting variogram models, a single downhole variogram was created

to generate the nugget effect. Dagbert (2014) indicates that a downhole variogram effectively captures the nuggets effect and short-range continuity by analyzing data points collected along drill holes without taking directional orientation into account (Appendix 3.3). Downhole variogram statistically estimates accurate nugget effect contributing to determining the sill and range that will be used in simulation using turning bands. After determining the nugget effect from downhole variogram, variogram models were fitted (Figures 3.24, 3.25, 3.26, and 3.27) for three axes (In which two axes are shown in APENDIX) of each variable using the same nugget effect to estimate the sill and range (Table 3.4). Variogram models of two axes per variable are shown in (Appendix 3.4). According to literature, for simulation purposes, the nugget effect, sill, and range from the major axes are used, as they are considered more accurate than those from the semi-major and minor axes (Figure 3.24, 3.25, 3.26, 3.27).

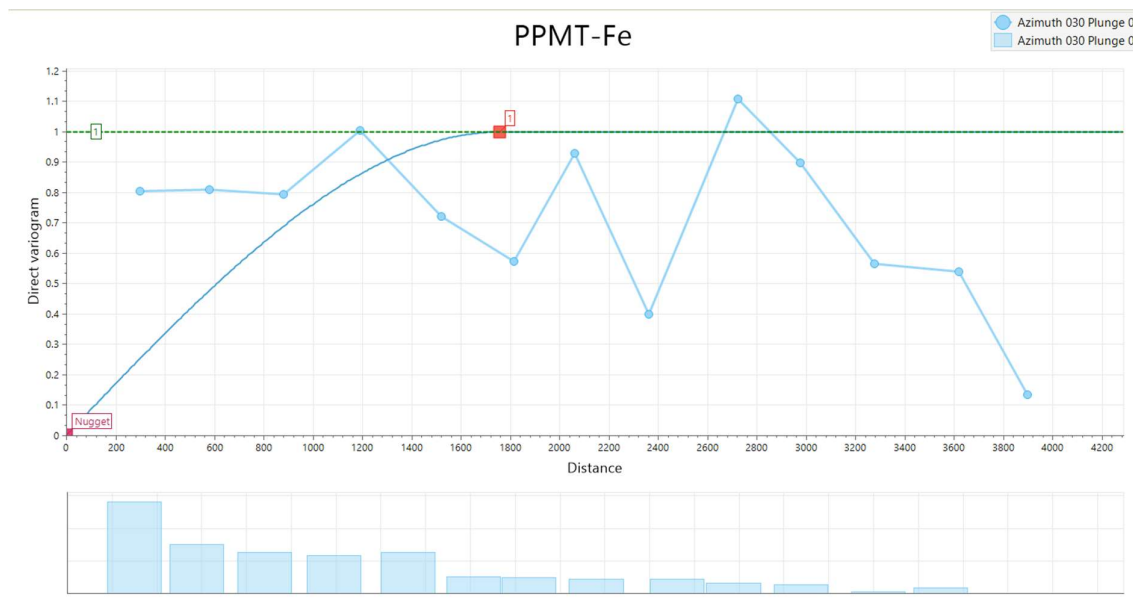


Figure 3.24: Variogram model of PPMT (Fe) and bar graph representing the number of samples on each point. The blue line represents the major axis.

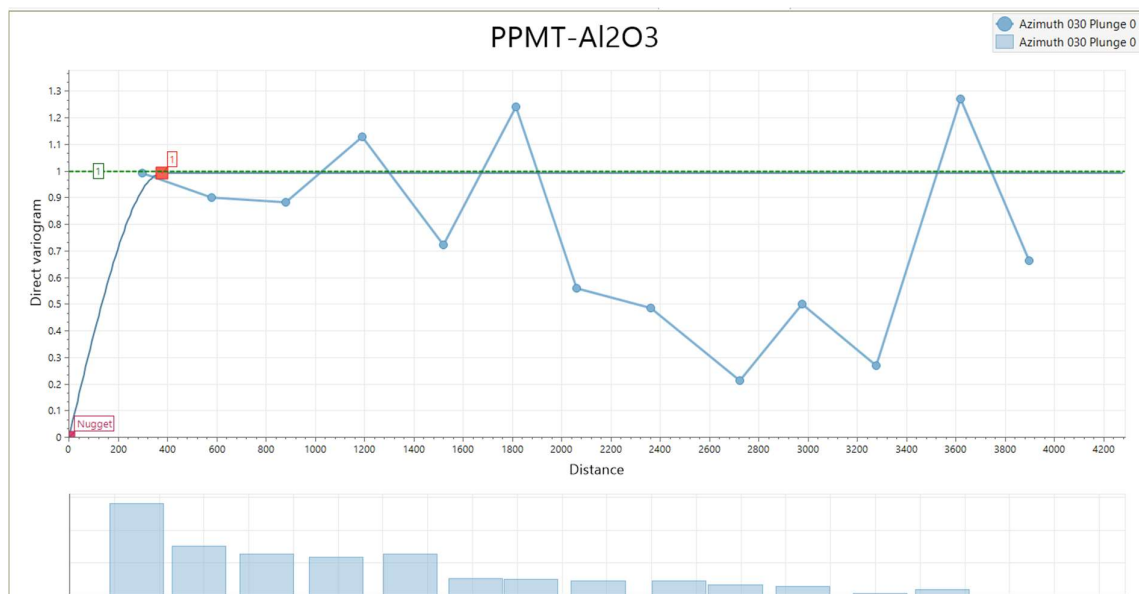


Figure 3.25: Variogram model of PPMT (Al_2O_3) and bar graph representing the number of samples on each point. The blue line represents the major axis.

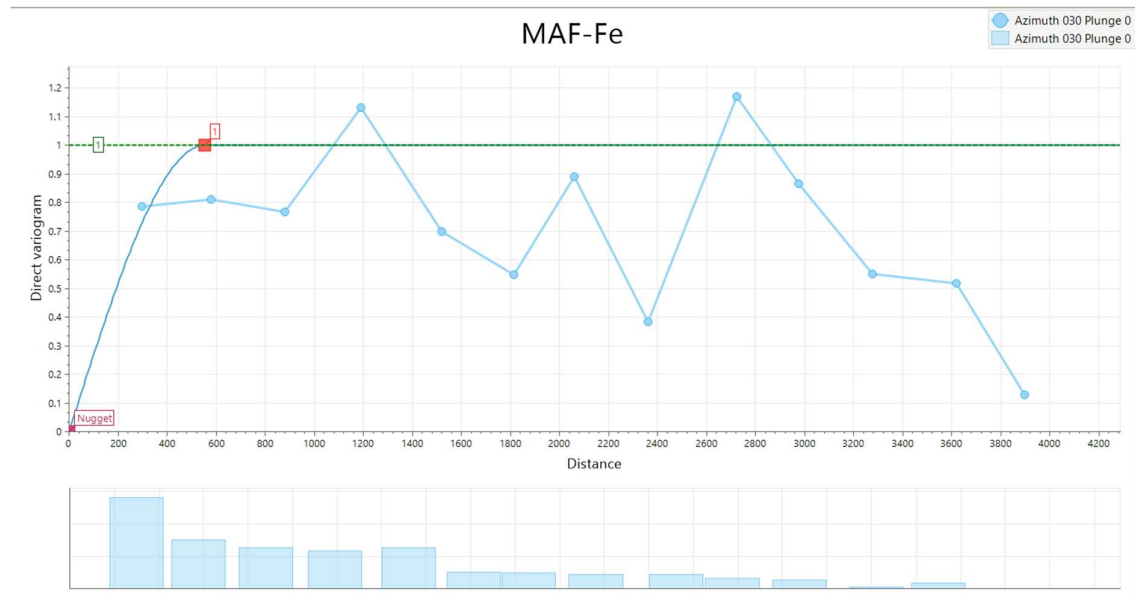


Figure 3.26: Variogram model of MAF (Fe) and bar graph representing the number of samples on each point. The blue line represents the major axis.

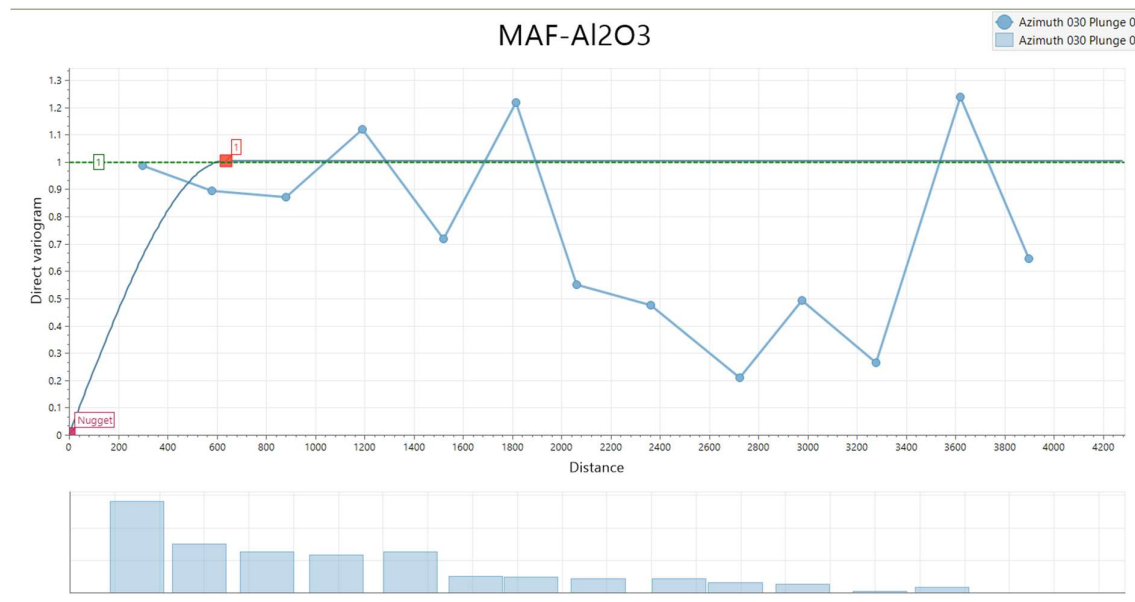


Figure 3.27: Variogram model of PPMT (Fe) and bar graph representing the number of samples on each point. The blue line represents the major axis.

Table 3.4: Nugget effect, sill, and range of each axis of different transformed variables.

		Nuggets effect	Range	Sill	Model type
PPMT Fe	Major axes	0.004171	1759.00	1.005	Spherical
	Semi-major axes	0.004171	561.00	1.002	Spherical
	Minor axes	0.004171	574.00	1.002	spherical
PPMT Al₂O₃	Major axes	0.0178	326.00	0.988878	Spherical
	Semi-major axes	0.0178	213.00	0.99178	Spherical
	Minor axes	0.0178	78.00	0.98678	spherical
MAF Fe	Major axes	0.00400	553.00	1.046	Spherical
	Semi-major axes	0.00400	535.00	1.04	Spherical
	Minor axes	0.00400	127.00	1.042	spherical
MAF Al₂O₃	Major axes	0.014512	637.00	1.02151	Spherical
	Semi-major axes	0.014512	117.00	1.01051	Spherical
	Minor axes	0.014512	100.00	1.01251	spherical

3.8 TURNING BAND SIMULATION

Simulation of correlated variables is common in geology, and it requires geostatistics methods (Emery and Lantuéjoul, 2006). However, the literature focuses on using co-simulation methods for simulating grade of correlated variables. Except for sequential gaussian simulation (SGS) and sequential indicator simulation (SIS), turning band simulation (TBSIM) has been proven as one of the simulation methods that produces accurate results compared to SGS (Paravarzar et al. 2015). This research used TBSIM, which is non-conditional simulation to compare accuracy, time efficiency, and effectiveness in handling the complexity of simulating metal grades that exhibit high correlation within a mineral deposit, focusing on elements relevant to mineralization.

The turning bands method is the earliest method for 3-D simulation, which was first initiated by Matheron (1973) and was developed early in the 1970s by A. Journé. The turning bands method produces unconditional simulation results based on variogram or covariance models that assume that spatial continuity is the same in all directions. In addition, the turning bands method provides a series of 2D and 3D simulations at the central processing unit time (CPU)

of a one-dimensional simulation (Emery and Lantuéjoul 2006). According to Emery and Lantuéjoul (2006), the turning band method builds up a simulation in three dimensions and two dimensions by combining many simulations in one dimension. In this study, a turning bands simulation was performed using MATLAB software with a code created by Emery and Lantuéjoul, (2006).

3.9 CONCLUSION

This chapter presented the methods used to prepare the data for the turning bands simulation of Al_2O_3 and Fe. Histogram analysis of the original data was used to identify outliers and understand the distribution of the original data. Data transformation was performed, including both projection pursuit (PPMT) and minimum/maximum autocorrelation factor (MAF) to capture the relationships and to address correlation among variables. Variogram maps were generated to determine the direction of continuity; hence, experimental variograms were determined using direct variogram. Variogram models were fitted to estimate nugget, sill, and range, while nuggets for each transformed variable were estimated using a downhole variogram. Overall, the methods effectively prepared the data for further simulation using turning bands.

Chapter 4: Data Analysis Results

Chapter three presented the methodological framework adopted in the study, including methods like data analysis, compositing, declustering, variogram analysis, and the turning bands method for simulation. Variogram analysis is the final methodological process that provides the necessary parameters (nugget effect, sill, and range) to proceed with the simulation. This chapter details the results and analysis addressing the research objectives of this research.

4.1 SIMULATION RESULTS.

After performing variogram analysis, the turning bands simulation was carried out on a grid of 43 m x 38 m x 30 m using nugget effect, sill, and range from major axes for each variable. Four simulations were carried out, including TBSIM on PPMT-Fe, TBSIM on PPMT-Al₂O₃, TBSIM on MAF-Fe, and TBSIM on MAF-Al₂O₃. For the TBSIM, 100 realizations were produced for each transformed variable. After simulation, PPMT-Fe, PPMT-Al₂O₃, MAF-Fe, and MAF-Al₂O₃ were back-transformed to their original states before transformation.

4.1.1 Statistical Validation

The results obtained from the TBSIM are suitable for further statistical analysis. However, validation is important because it helps in comparing the results obtained with the original data to evaluate the methods used (Battalgazy and Madani 2019; Madenova and Madani 2021). Declustering, variogram modelling (including nugget effect, sill, and range), model size (grid size), number of realizations produced, and software used for simulation are some of the criteria that can influence the model not to reproduce input data (Leuangthong et al. 2004).

Validation, including (1) comparing the overall mean of 100 realizations for back-transformed data with the original declustered mean before transformation and simulation, (2) comparing

the correlation between variables after transformation and after simulation, and (3) histogram reproduction of back-transformed data, was conducted. The first step involved validation of the mean of original assays with the mean of back-transformed data (Figure 4.1). The original declustered mean of Fe was determined to be 54.238. After TBSIM and back-transformation, the mean of PPMT-Fe was 54.958, and the mean of MAF-Fe was 54.524. In comparison, the original declustered mean of Al_2O_3 was 2.061, and after simulation and back-transformation, the mean of PPMT- Al_2O_3 was 2.061, and the mean of MAF- Al_2O_3 was 2.052 (Table 4.1).

Table 4.1: Declustered means of Fe and Al_2O_3 and back-transformed means of PPMT-Fe, PPMT- Al_2O_3 , MAF-Fe, and MAF- Al_2O_3 .

	PPMT-Fe	PPMT- Al_2O_3	MAF-Fe	MAF- Al_2O_3
Declustered mean	54.238	2.061	54.238	2.061
Back-transformed mean	54.958	2.061	54.524	2.052

The second step involved validation of correlation coefficients after simulation. How transformation handles complexity between variables was determined by comparing the correlation coefficient of untransformed data with back-transformed data (Madenova and Madani 2021). The original correlation coefficient for Fe and Al_2O_3 was -0.80. After back-transformation, the correlation coefficients for PPMT-Fe and PPMT- Al_2O_3 and for MAF-Fe and MAF- Al_2O_3 were -0.007 and -0.003, respectively (Figure 4.2).

Thirdly, validation involved histogram reproduction to verify whether the back-transformed data reproduces the original weight. However, during the simulation processes, more than 25 realizations were produced. According to (Leuangthong and Deutsch 2003), it is impractical to validate histogram reproduction using all realizations generated. The literature suggests that a few realizations can be randomly selected for histogram reproduction validation. When validating histogram reproduction, factors such as the shape of the histogram, range of the simulated values, and summary statistics (mean, median, and variance) should be considered.

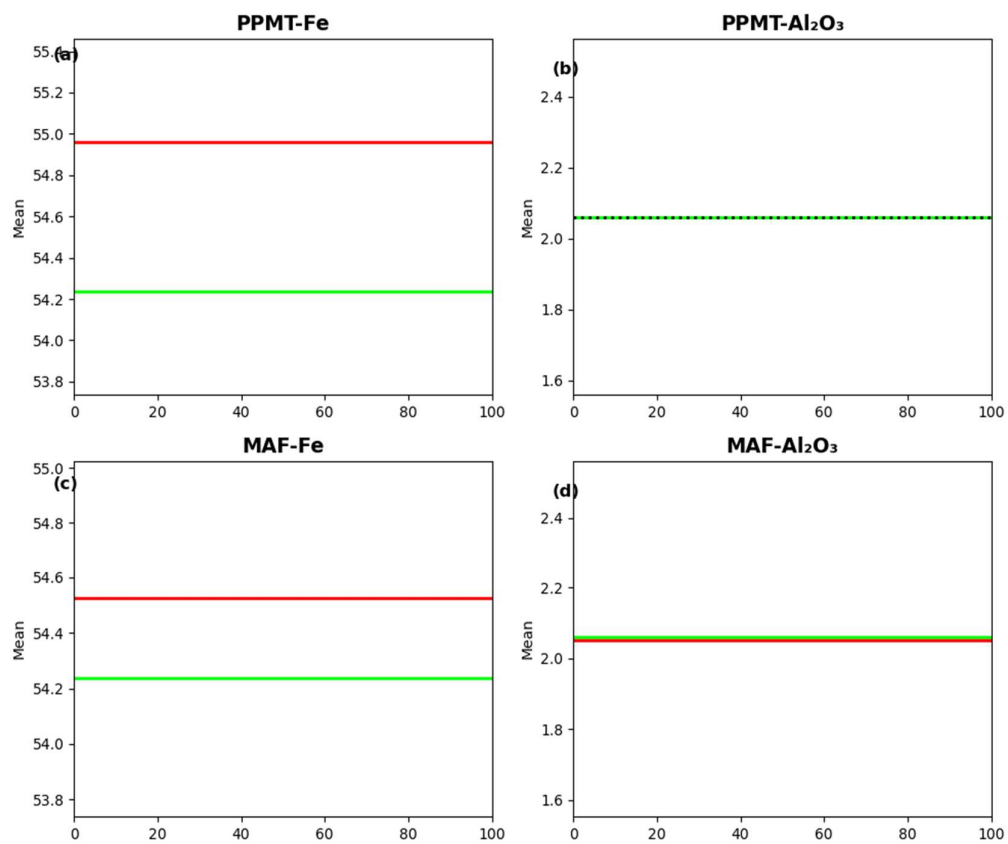


Figure 4.1: Declustered mean of Fe (a and c) in green line and Al₂O₃ (b and d) in green line. The red line in (a) is the back-transformed mean of PPMT-Fe. The black dotted line in (b) is the back-transformed mean for PPMT-Al₂O₃. The red line in (c) is the back-transformed mean of MAF-Fe. The red line in (d) is the back-transformed mean of MAF-Al₂O₃.

Comparison of Original and Back-Transformed Correlations (PPMT & MAF)

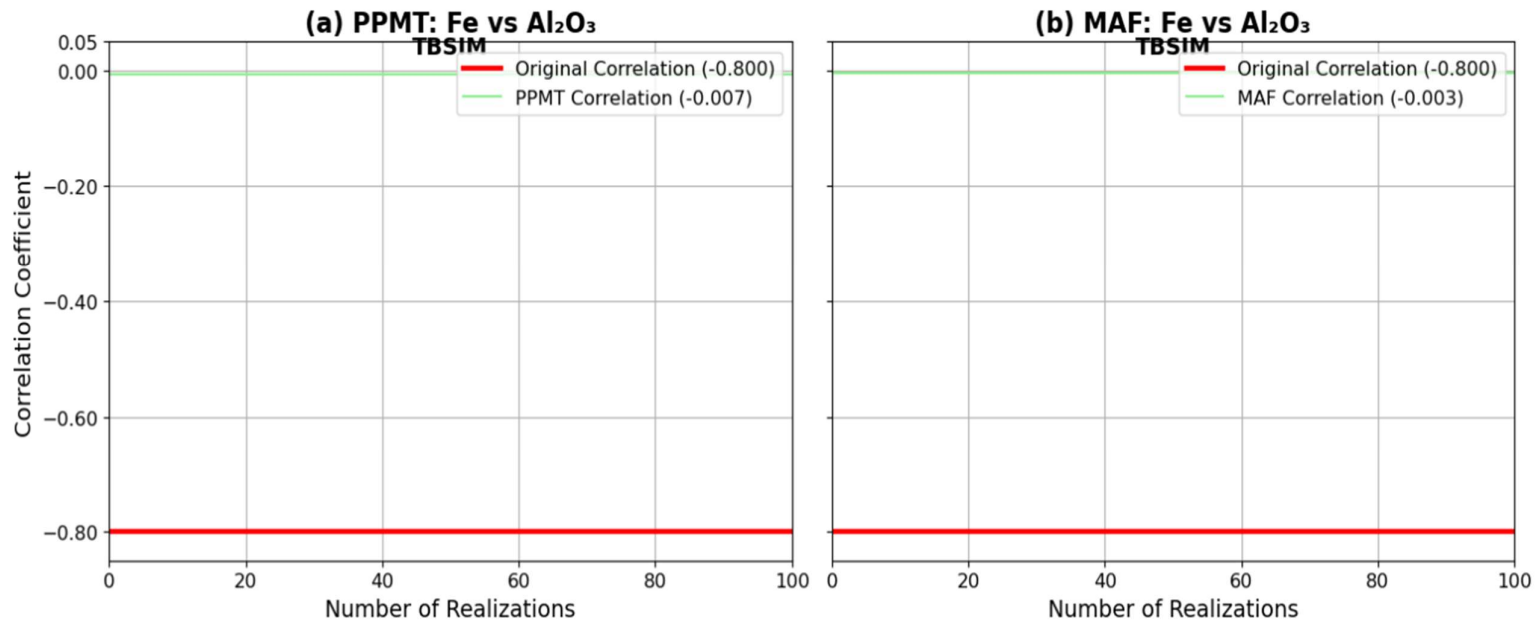


Figure 4.2: Correlation Coefficient for Fe and Al₂O₃ before transformation and back-transformation (a and b). the red line in (a and b) is the original correlation coefficient of Fe and Al₂O₃. The green line in (a) is the correlation coefficient after back-transformation using PPMT. The green line in (b) is the correlation coefficient after back-transformation using MAF.

From each transformed variable, five realizations were randomly selected for histogram validation and compared to the histogram of the original data set. For Fe, in both transformations, realizations 45, 46, 54, 71, and 84 were selected randomly. For Al_2O_3 , in both transformations, realizations 9, 19, 20, 38, and 47 were selected. Statistical validation was performed by examining the range, mean, median, and variance. For PPMT-Fe and MAF-Fe, when compared to the original statistical distribution, all selected realizations showed different means, medians, variances, and ranges (Figures 4.3 and 4.5). Similarly, for Al_2O_3 in both transformations, the original statistics were not reproduced. However, only PPMT- Al_2O_3 exhibited a histogram shape that more closely resembled the original histogram. None of the transformations reproduced the target histogram, as the simulated data showed different weights compared to the original data distribution.

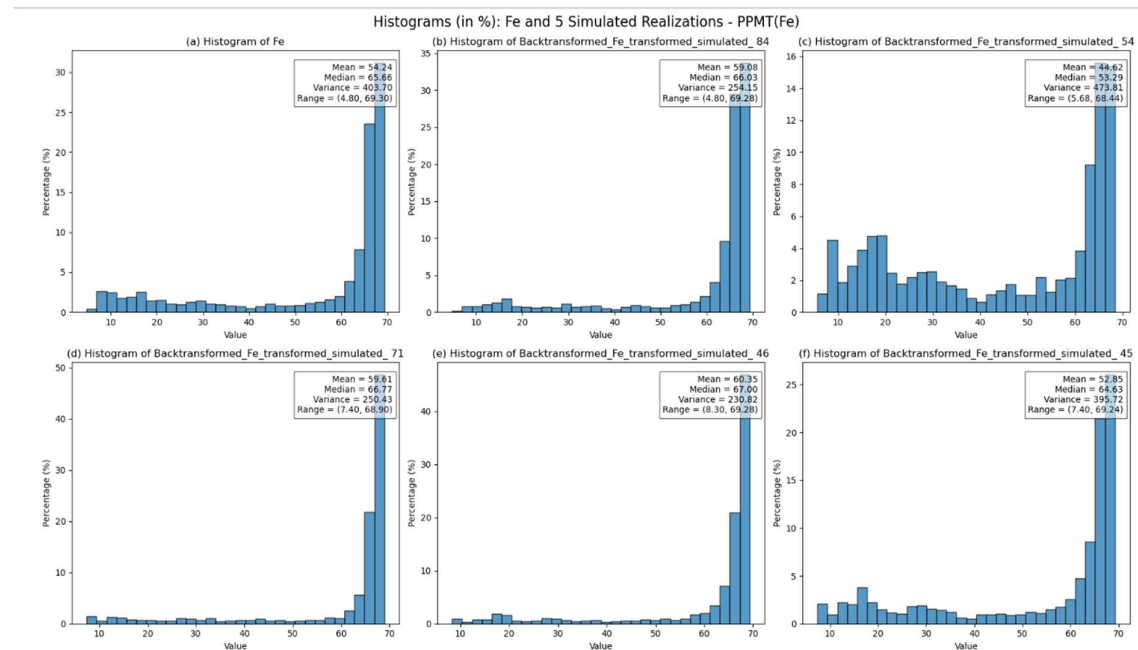


Figure 4.3: Original negative skewed distribution of Fe (a), and negative skewed distribution of five realizations from back-transformed data using PPMT-Fe (b, c, d, e, and f).

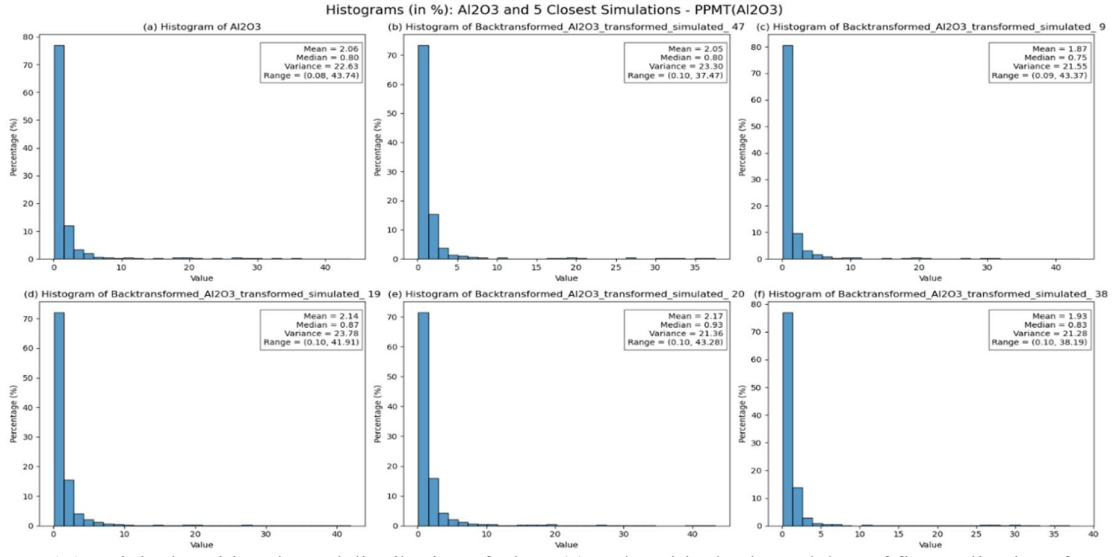


Figure 4.4: Original positive skewed distribution of Al_2O_3 (a) and positively skewed data of five realizations from back-transformed data using PPMT- Al_2O_3 (b, c, d, e, and f).

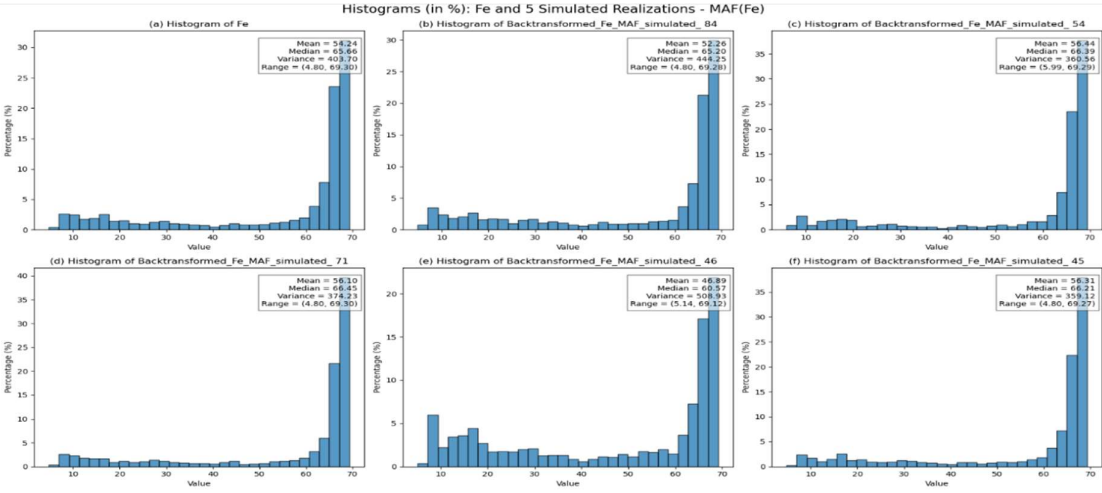


Figure 4.5: Original negatively skewed distribution of Fe (a), and negatively skewed data of five realization from back-transformed data from MAF-Fe (b, c, d, e, and f).

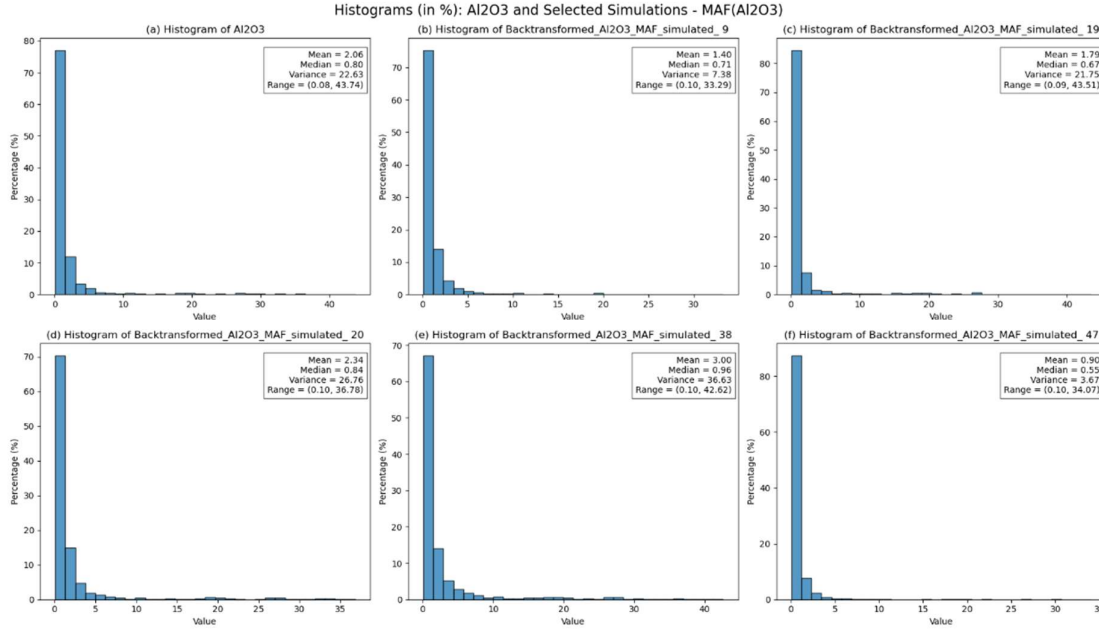


Figure 4.6: Original positively skewed data of Al₂O₃ (a), and positively skewed data of five realizations from back-transformed data using MAF- Al₂O₃ (b, c, d, e, and f).

4.3 CONCLUSION

For each transformed variable (PPMT-Fe, PPMT-Al₂O₃, MAF-Fe, and MAF-Al₂O₃), 100 realizations were produced using the turning bands simulation. All simulated variables were back-transformed to their original values for validation. The statistical validation illustrated that the means of all back-transformed data closely matched the original declustered means. The correlation coefficients of back-transformed data were lower compared to those of the original data. However, this indicated some loss of relationship of the original data between variables, either during transformation, simulation, or back-transformation. In addition, statistical validation indicated that there were some complexities during the transformation and simulation processes.

Chapter 5: Comparison and Results Discussion

Based on the findings in Chapter Four, this chapter addresses the research questions by comparing the results obtained in Chapter Four. The comparison focuses on two transformations: the projection pursuit multivariate transform (PPMT) and the minimum/maximum autocorrelation factor (MAF). The declustered means of the original data are compared with the means of the back-transformed PPMT and MAF values, thereby evaluating how effectively each transformation handled the complexity among correlated variables. In addition, the ability of both transformations to preserve correlations among variables is assessed by comparing the correlations among declustered data with those of the back-transformation data.

For decorrelating purposes, the PPMT and MAF were used for two variables, namely Fe and Al_2O_3 , which are highly correlated. Simulation was conducted on a grid measuring 43 m x 38 m x 30 m within a search ellipsoid of 4000 m. For each transformed variable, 100 realizations were generated and subsequently back-transformed to their original state. The mean of back-transformed assays was calculated and compared to the original declustered mean. As shown in Table 5.1, none of the transformations were able to reproduce the original declustered mean. However, the MAF produced a Fe mean that was closer to the original declustered mean compared to that of the PPMT, as illustrated in Figure 5.1a. PPMT more accurately reproduced the mean of Al_2O_3 than MAF Figure 5.1b.

Table 5.1: Original declustered mean of Al_2O_3 and Fe, and back-transformed mean for both PPMT and MAF.

	PPMT-Fe	PPMT- Al_2O_3	MAF-Fe	MAF- Al_2O_3
Original declustered mean	54.238	2.061	54.238	2.061
Back-transformed mean	54.958	2.061	54.524	2.052

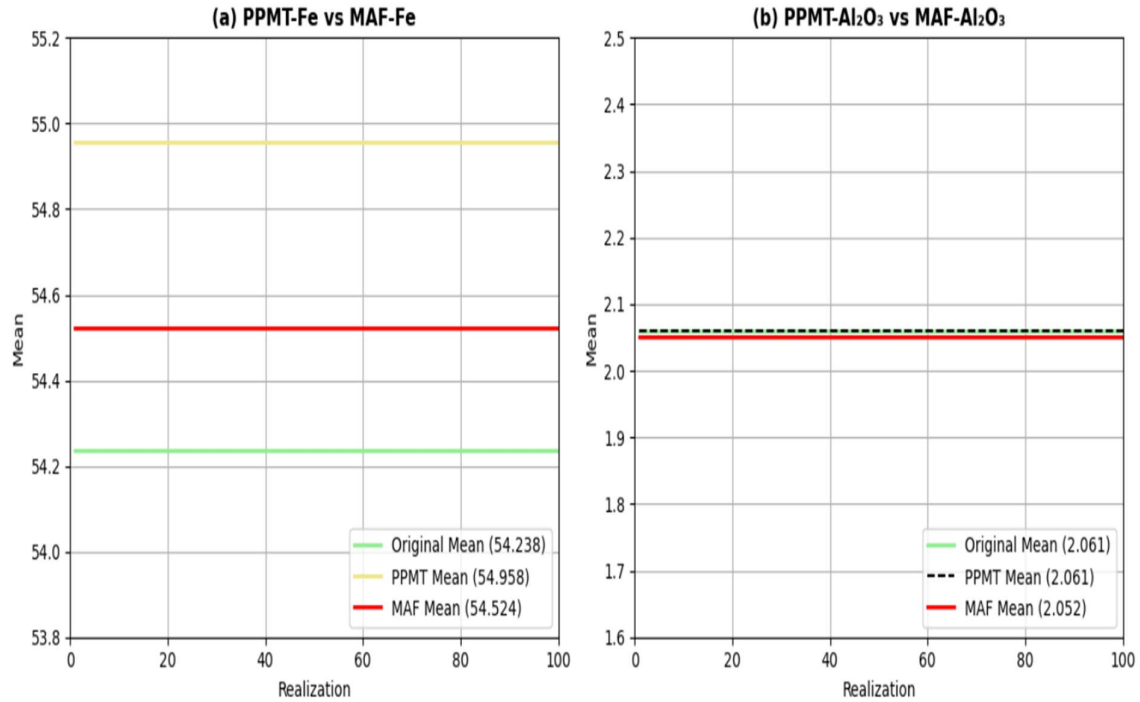


Figure 5.1: (a) Original declustered mean of Fe in green line, back-transformed mean of PPMT-Fe in yellow line, and back-transformed mean of MAF-Fe in red line. (b) Original declustered mean of Al_2O_3 , back-transformed mean of PPMT- Al_2O_3 in black dotted line, and back-transformed mean of MAF- Al_2O_3 .

The correlation coefficients for all transformations were calculated from 100 realizations. Both the PPMT and MAF transformations were unable to preserve the correlation among variables after back-transformation (Figure 5.2). According to Hosseini and Asghari (2019), MAF is unable to handle the complexity of correlated variables, whereas PPMT cannot address the correlation among variables. The results obtained from this research indicate that both the MAF and PPMT can handle the complexity of correlated variables, but neither can handle the correlation between variables. When comparing the two transformations, MAF appeared to better capture the complexity of correlated variables than PPMT.

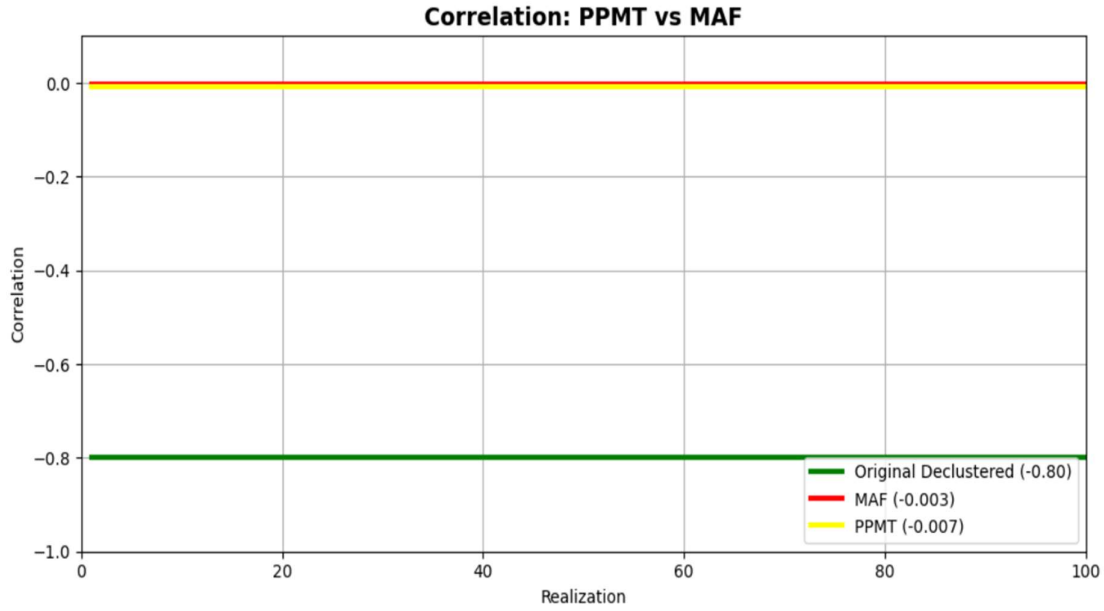


Figure 5.2: Original declustered correlation coefficients of Fe and Al_2O_3 in red line, correlation coefficients between PPMT-Fe and PPMT- Al_2O_3 in yellow line, and correlation coefficients between MAF-Fe and MAF- Al_2O_3 in red line.

Not only can transformation methods fail to preserve correlations, but according to (Battalgazy and Madani, 2019) the Turning Bands Simulation (TBSIM) produces weaker correlations among variables. These findings are consistent with the results of the present study, where the correlations were also found to be zero. Unlike independent simulation methods, co-simulation methods can maintain correlations between multiple variables by explicitly considering their interactions within the simulated space. Abildin et al. (2019), Battalgazy and Madani (2019), Eze et al. (2019), and Maleki and Madani (2016) all concluded that independent simulation methods fail to preserve correlation between variables because they do not account for inter-variable relationships during the simulation process.

Before conducting the simulation, several decisions must be made, including the application of declustering, variogram analysis, the number of realizations to generate, and the software to be used. Such parameters can influence the ability of the simulated data to reproduce the original data (Boisvert et al. 2010, Leuangthong et al. 2004). Studies by Boucher et al. (2005), Boucher

and Dimitrakopoulos (2009), Desbarats and Dimitrakopoulos (2000), Rondon (2012), and Dimitrakopoulos and Fonseca (2003) concluded that MAF is generally more accurate than other transformation methods in handling the complexity of correlated variables.

However, in the present study, the PPMT was able to reproduce the declustered mean of Al_2O_3 after back-transformation (Table 1). Similarly, Madenova and Madani (2021) reproduced the exact mean of Al_2O_3 using normal score transformation with Sequential Gaussian Co-Simulation. These findings suggest that Al_2O_3 may be one of the easiest variables to simulate, regardless of the simulation or transformation methods applied. With advancements in technologies and the availability of simulation tools in various software packages, transformation methods such as the PPMT and MAF have become increasingly popular and are now widely implemented within these software platforms. In this research, both the PPMT and MAF were implemented using Python, an advanced programming language, making the process straightforward and time-efficient for both methods.

5.1 CONCLUSION

Geostatistical simulations have become increasingly popular for modelling the grade of multiple variables in ores. Among the available transformation techniques, the PPMT and MAF methods are widely recognized for their ability to decorrelate correlated variables, enabling their independent simulation using univariate geostatistical methods. In this research, both the PPMT and MAF were applied in conjunction with TBSIM to assess their accuracy and computational efficiency in simulating correlated variables. Although PPMT has often been ranked as one of the most effective transformation methods, the results in this research indicate that MAF achieved better accuracy than PPMT. Nevertheless, both transformation methods demonstrated limitations, as neither of them was able to preserve the correlation between two

strongly correlated variables after back-transformation. These findings also highlight the challenges of using independent simulation approaches when maintaining inter-variable relationships is essential.

Chapter 6: Conclusion and Recommendations

Multivariate transformations, such as minimum/maximum autocorrelation factors (MAF) and projection pursuit multivariate transform (PPMT), are popular in the field of geosciences to handle correlations among variables for further simulations using independent methods. These transformation techniques are increasingly being incorporated into geostatistical simulation algorithms, providing a way to overcome the limitations of traditional kriging methods. This research aimed to evaluate the performance of two popular transformation methods, PPMT and MAF, using the Turning Bands simulation (TBSIM) algorithm to compare their accuracy, effectiveness, and time efficiency using identical search neighbourhoods and number of realizations to have fair results.

6.1 SUMMARY OF THE RESEARCH

Although geostatistical simulation methods have become popular for decades, independent simulation methods cannot be used when modeling the grades of correlated metals in an ore deposit, because they simulate variables independently. Therefore, this research compared PPMT and MAF within the TBSIM, broadening the range of approaches applicable in mineral resource modeling. The workflow incorporated compositing, declustering, data transformation, and variogram analysis, followed by simulation. These steps provided the structural framework for assessing the performance of the two transformations. By constructing the PPMT and MAF, the research highlighted their relative strengths and limitations, offering practical insights for improving ore grade modeling and quantifying uncertainty in mineral resource estimation.

Transformations like PPMT and MAF are typically applied where there are strong correlations among variables. This study utilized ore grade data from the Carajás mine, recognized as the

world's largest iron ore mine. The focus was on Fe and Al_2O_3 , which showed a strong negative correlation of -0.80. The findings of this research show that both MAF and PPMT can manage the complexity caused by correlated variables, but MAF can handle this complexity more effectively than PPMT.

6.2 LIMITATIONS

Nonetheless, some limitations remain. Previous research has shown that the PPMT cannot capture the correlation among variables while the MAF cannot handle the complexity among variables. According to the results of this research, neither of these two transformations reproduced the correlation among the studied variables. This is not solely due to the transformation methods. Previous research found that independent simulation algorithms do not consider the relationship between variables, as variables are simulated independently. PPMT reproduced Al_2O_3 marginally better than Fe after back-transformation. The 100 realizations produced did not match the statistics of the original data. The distributions of the original data were not modelled by the distributions of back-transformed realizations, thus introducing more bias into the results. This bias can lead to uncertainty. In conclusion, neither PPMT, MAF, nor TBSIM can reproduce the correlations among variables.

6.3 RECOMMENDATIONS

Because independent simulation methods cannot handle correlations among variables, it is recommended that future studies use joint simulation methods, such as co-simulation, to improve correlation reproduction. In practice, MAF can be used for correlated variables over PPMT by applying other independent simulation methods such as Sequential Gaussian Simulation (SGS) and Sequential indicator Simulation (SIS). Furthermore, rigorous validation should be conducted to ensure the reliability of back-transformed results.

Overall, this research contributes to understanding the strengths and weaknesses of transformation methods in geostatistical simulation and emphasizes the need for advanced joint approaches to improve multivariate resource modelling.

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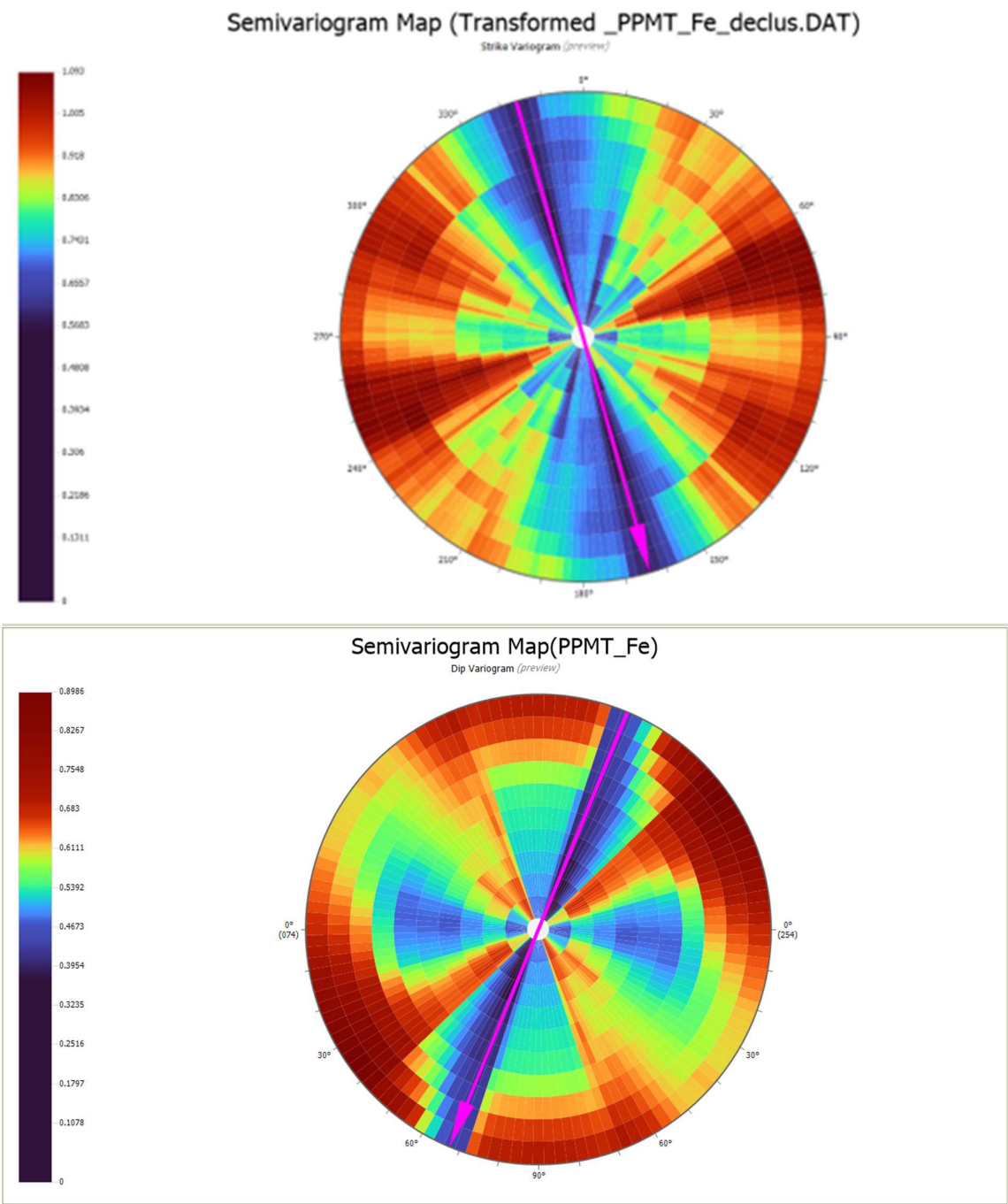
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APPENDICES

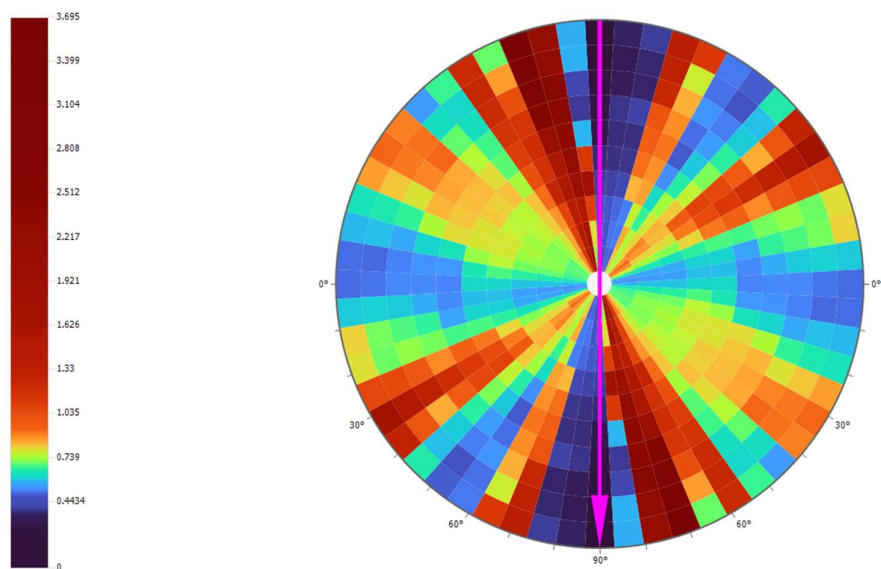
Appendix A

Appendix 3.1: Semi-variogram maps representing continuation direction of PPMT-Fe, PPMT-Al₂O₃, MAF-Fe, and MAF-Al₂O₃ analyzed along three directions: strike, dip, and pitch.



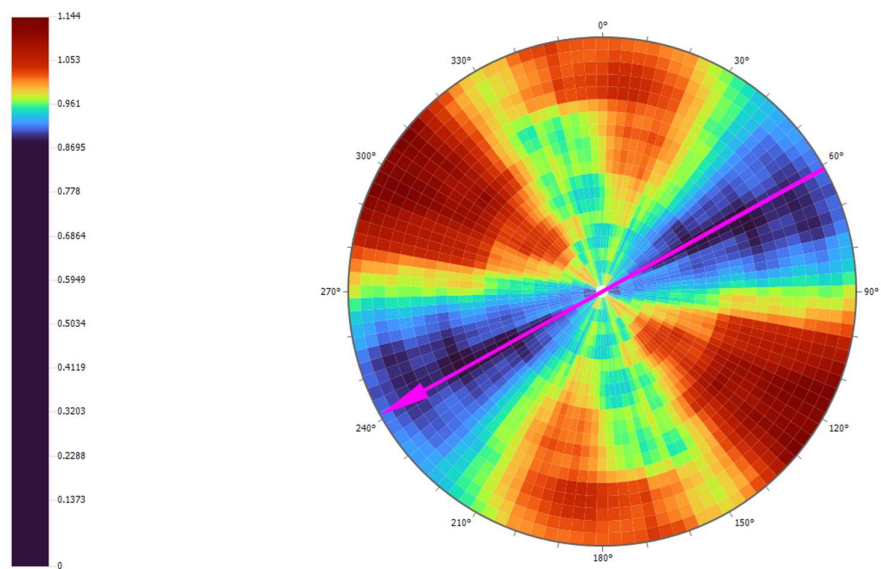
Semivariogram Map(PPMT_Fe)

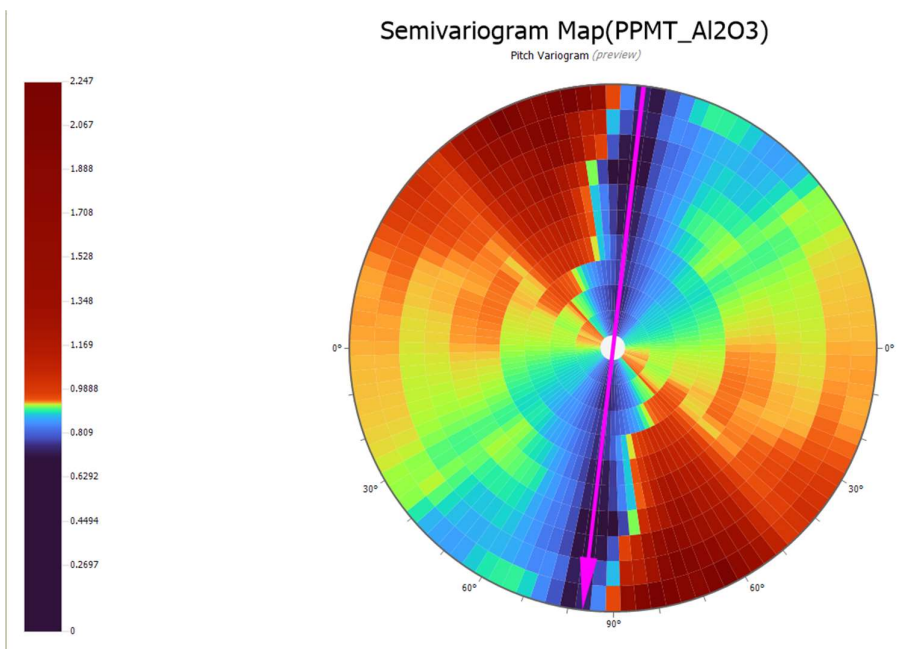
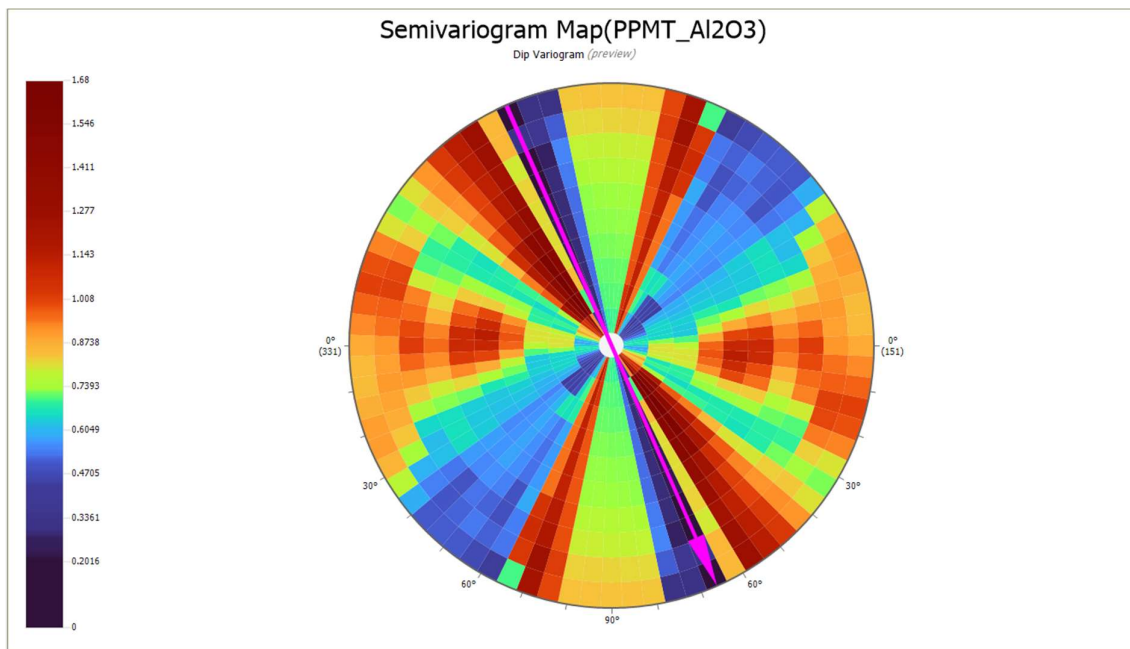
Pitch Variogram (preview)



Semivariogram Map(PPMT_Al2O3)

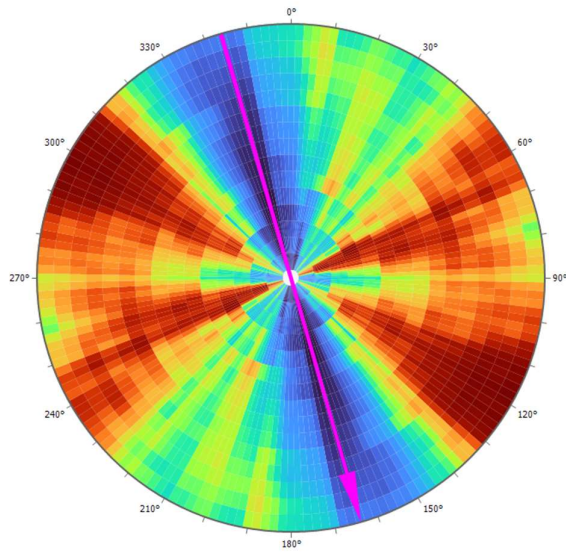
Strike Variogram (preview)





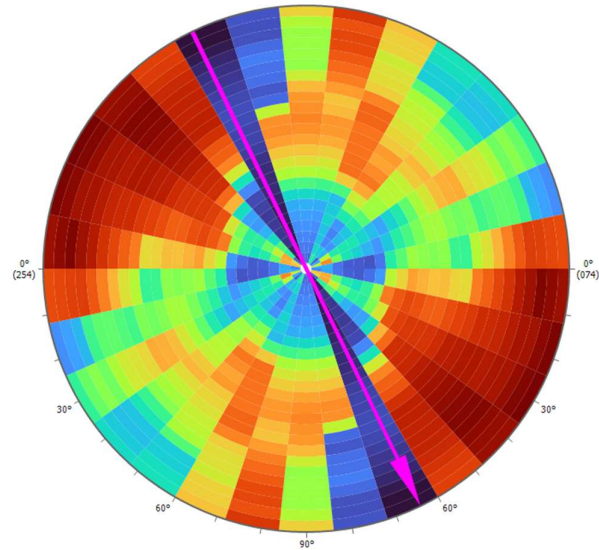
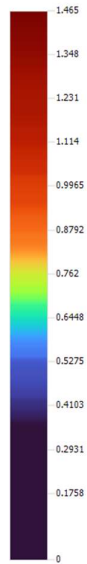
Semivariogram Map(MAF_Fe)

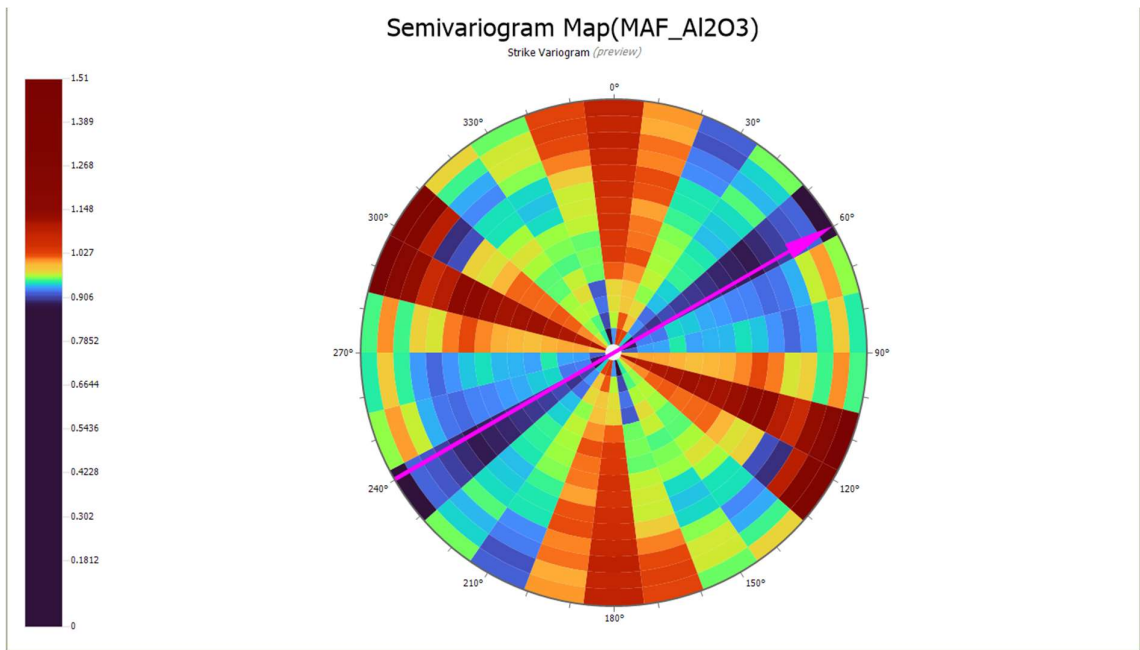
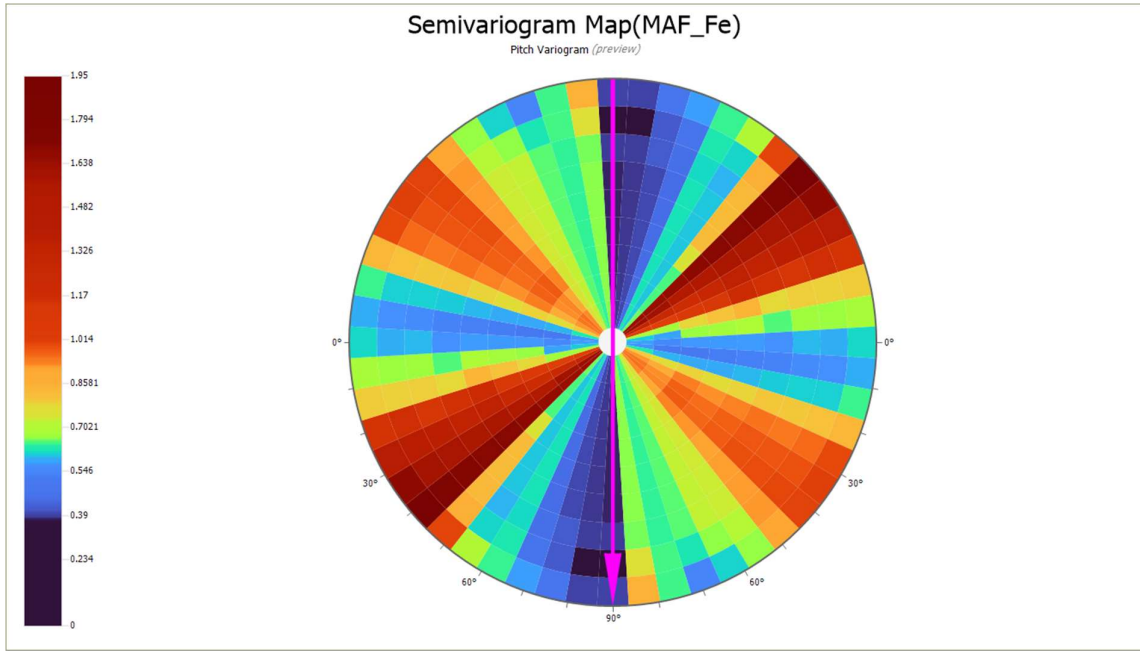
Strike Variogram (preview)



Semivariogram Map(MAF_Fe)

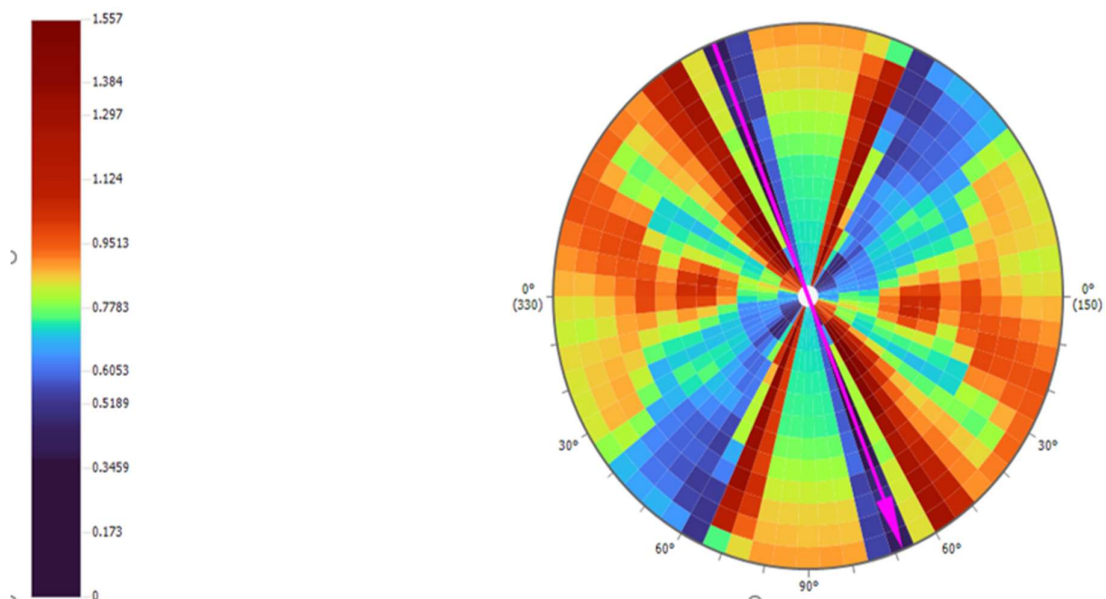
Dip Variogram (preview)





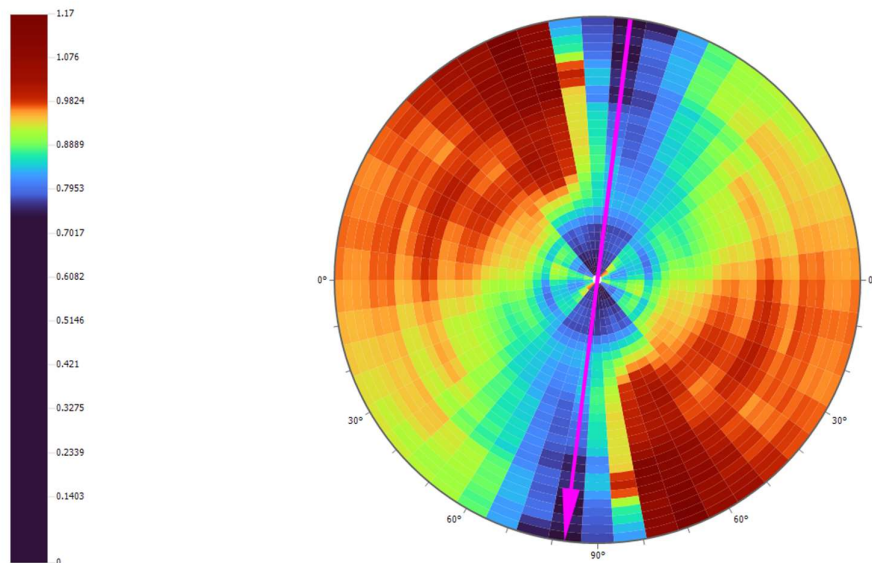
Semivariogram Map(MAF_AI2O3)

Dip Variogram (preview)



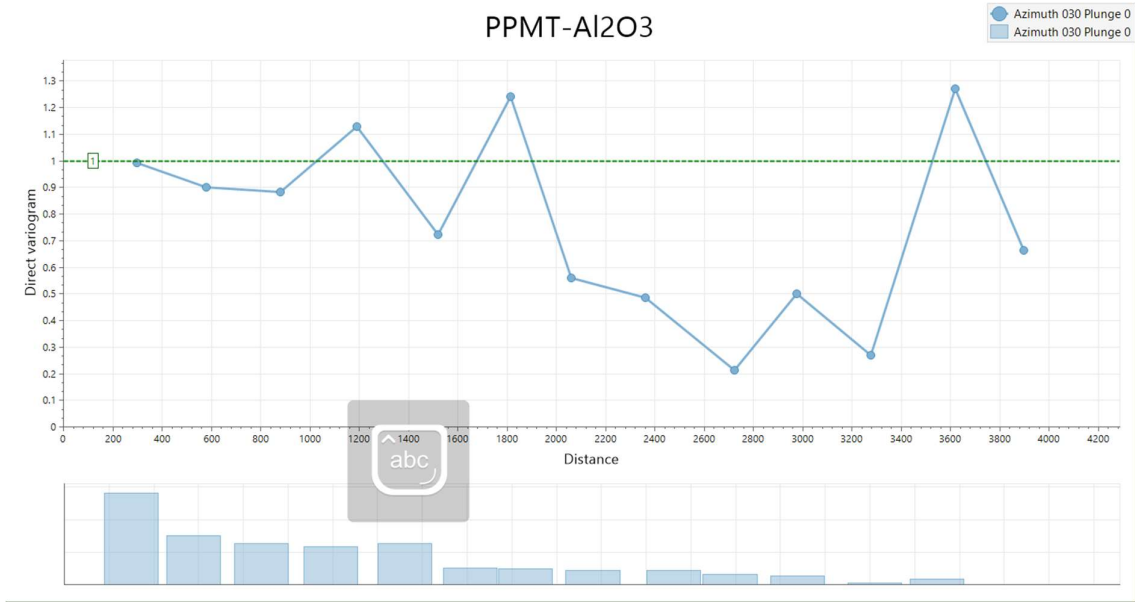
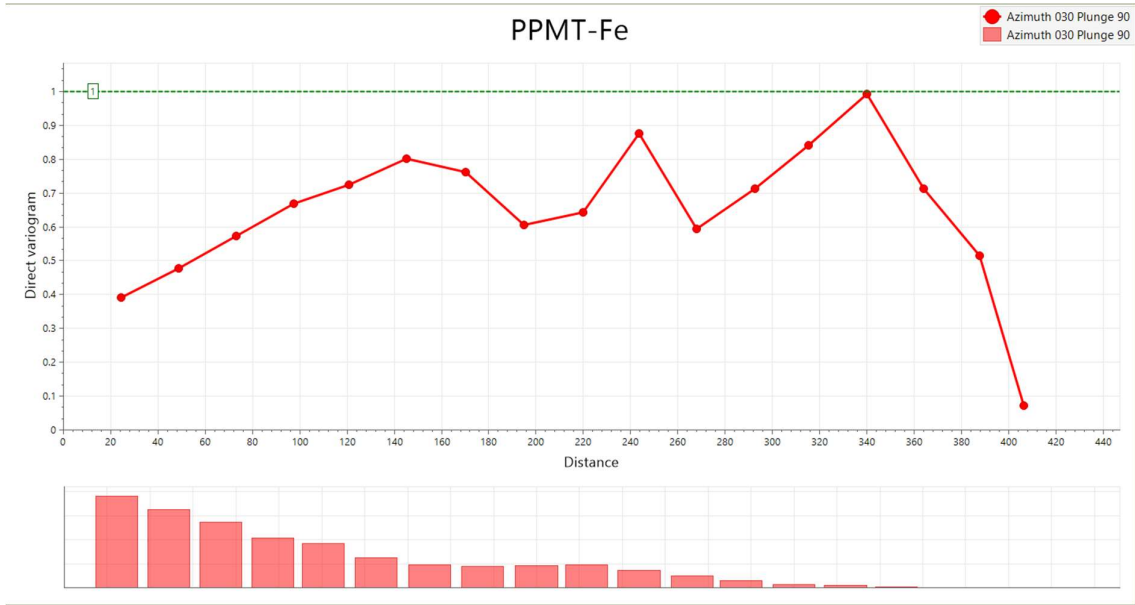
Semivariogram Map(MAF_AI2O3)

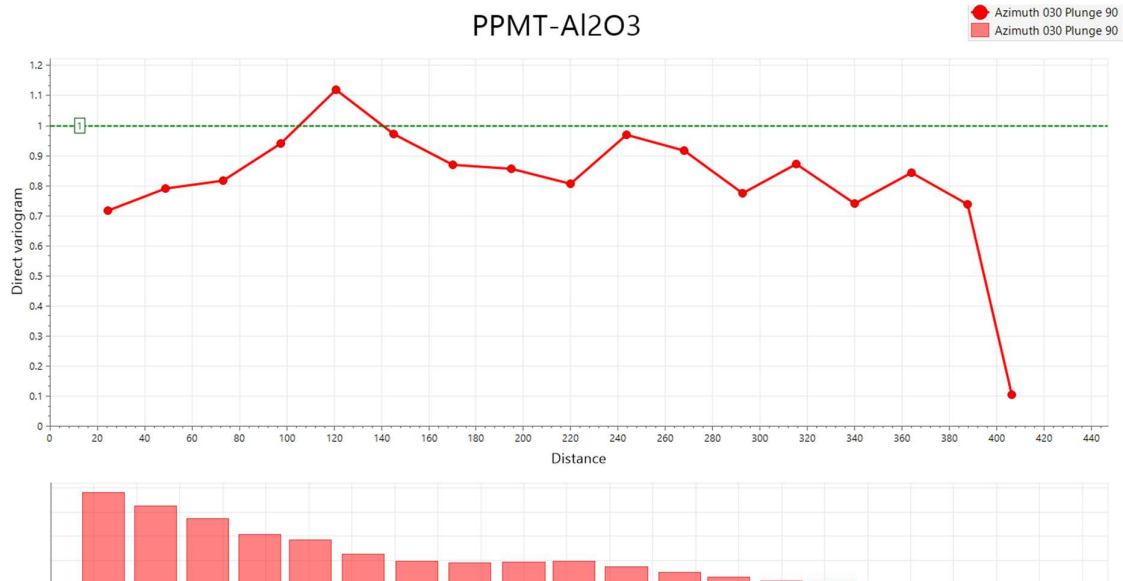
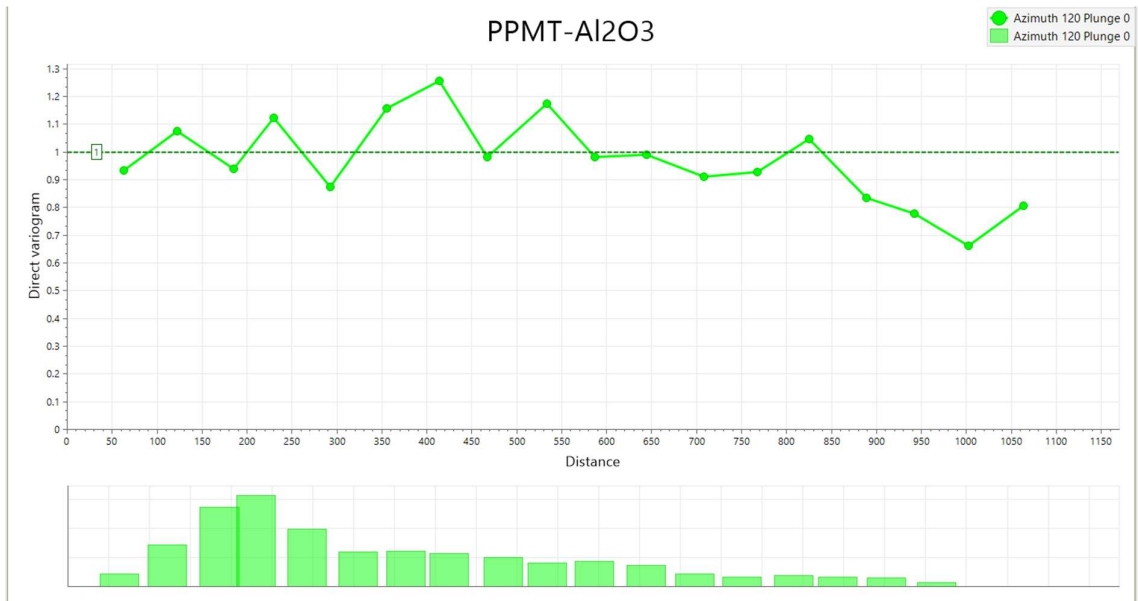
Pitch Variogram (preview)

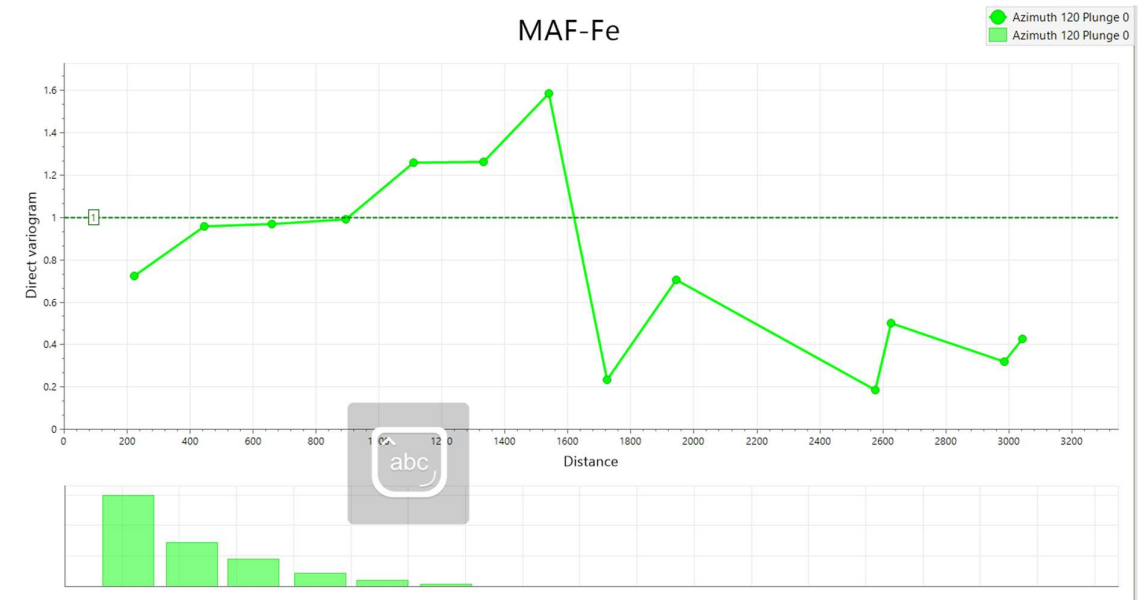
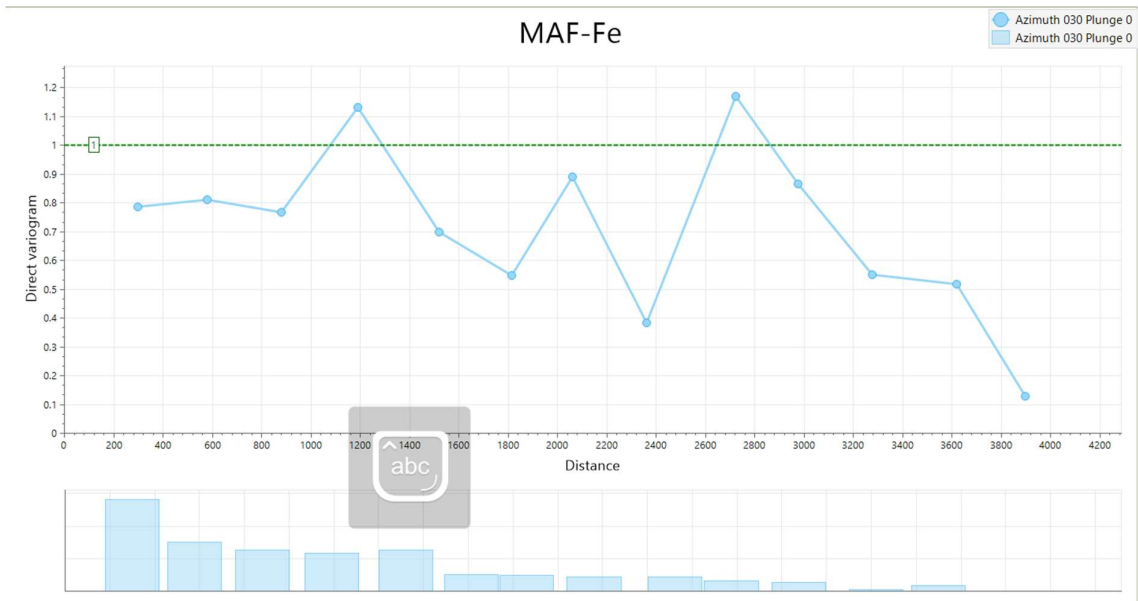


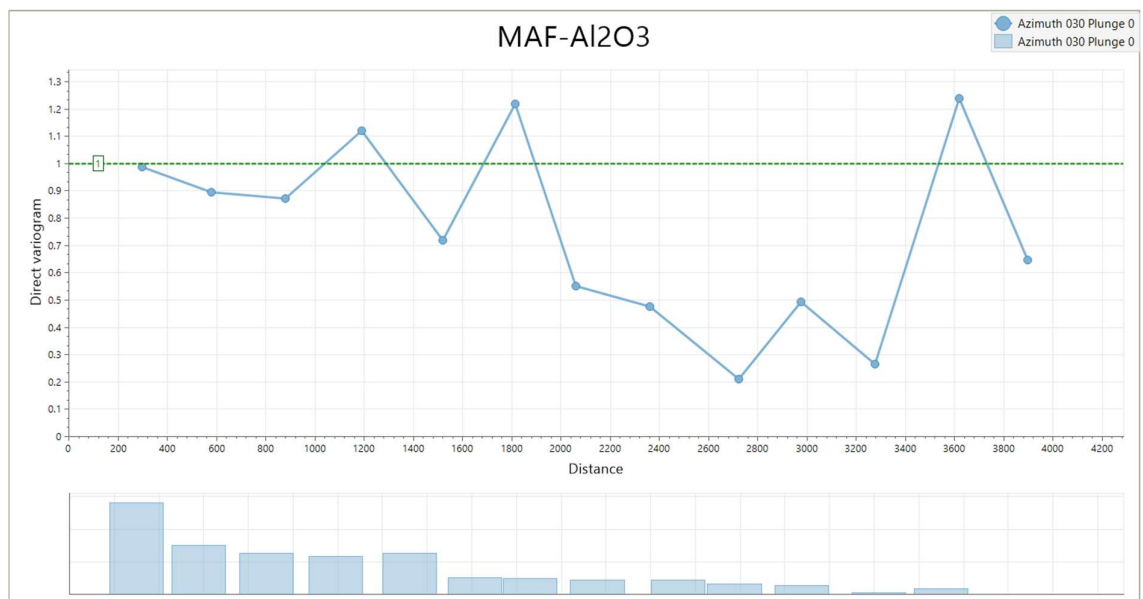
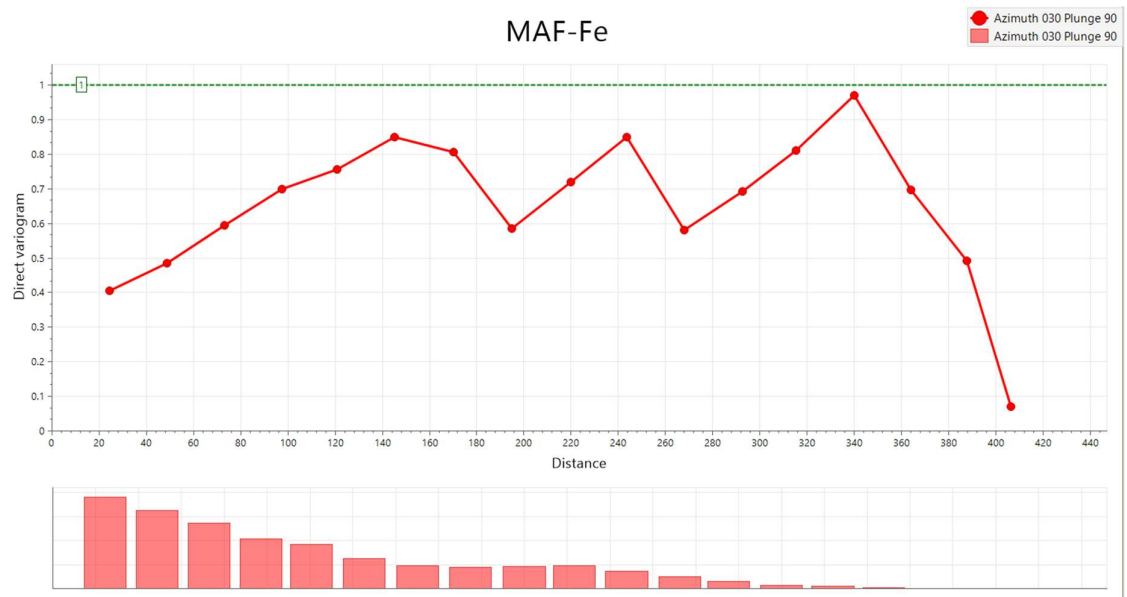
Appendix 3.2: Direct variogram of each transformed variable including major axis (blue), semi-major axis (green), and minor axis (red).

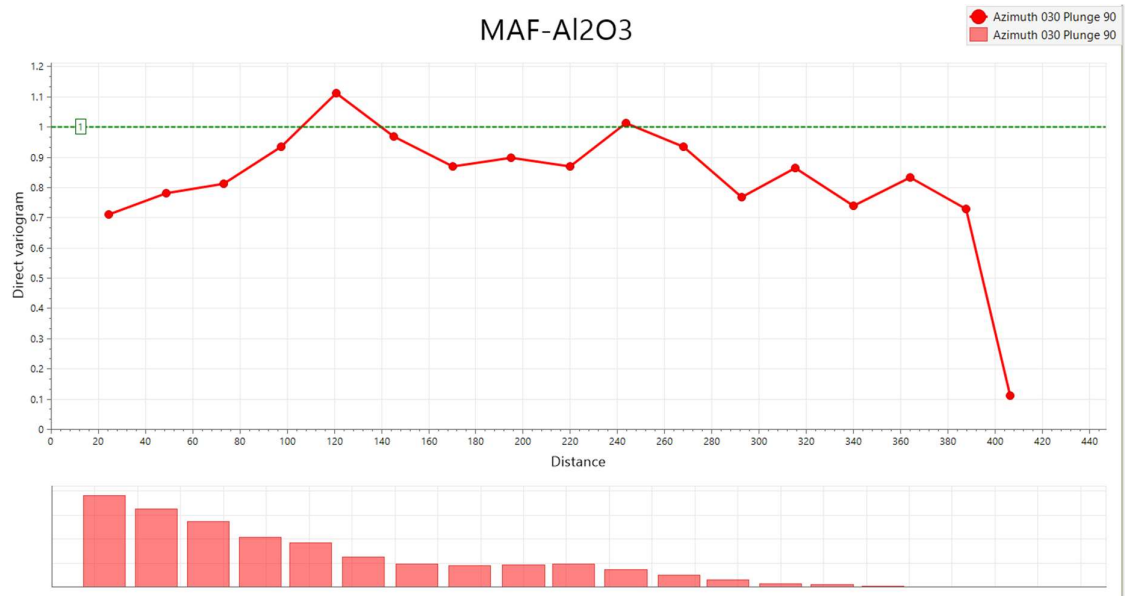
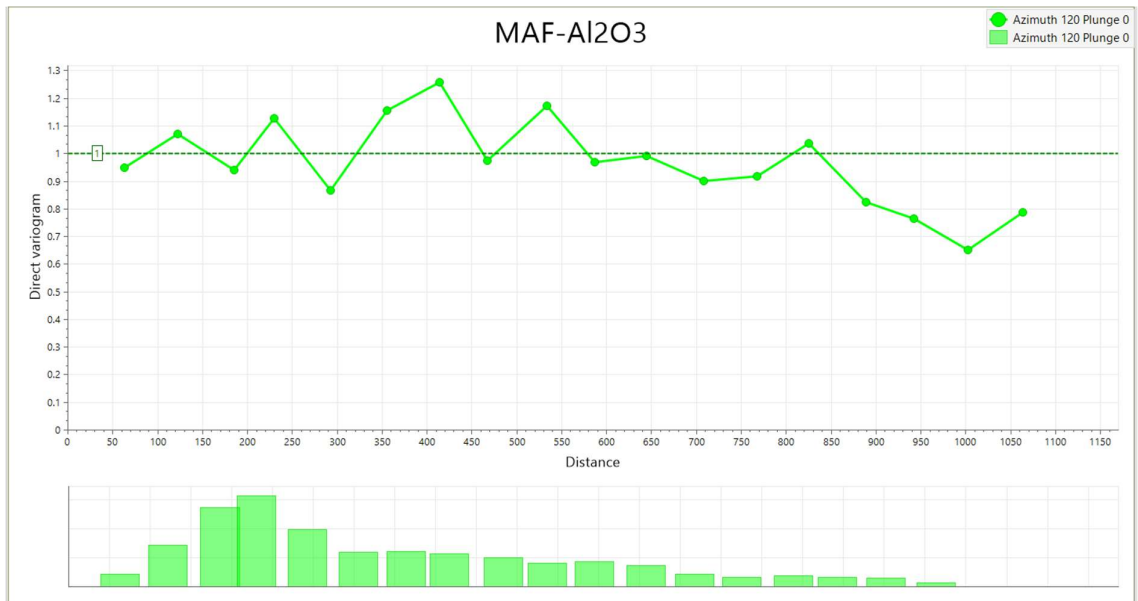




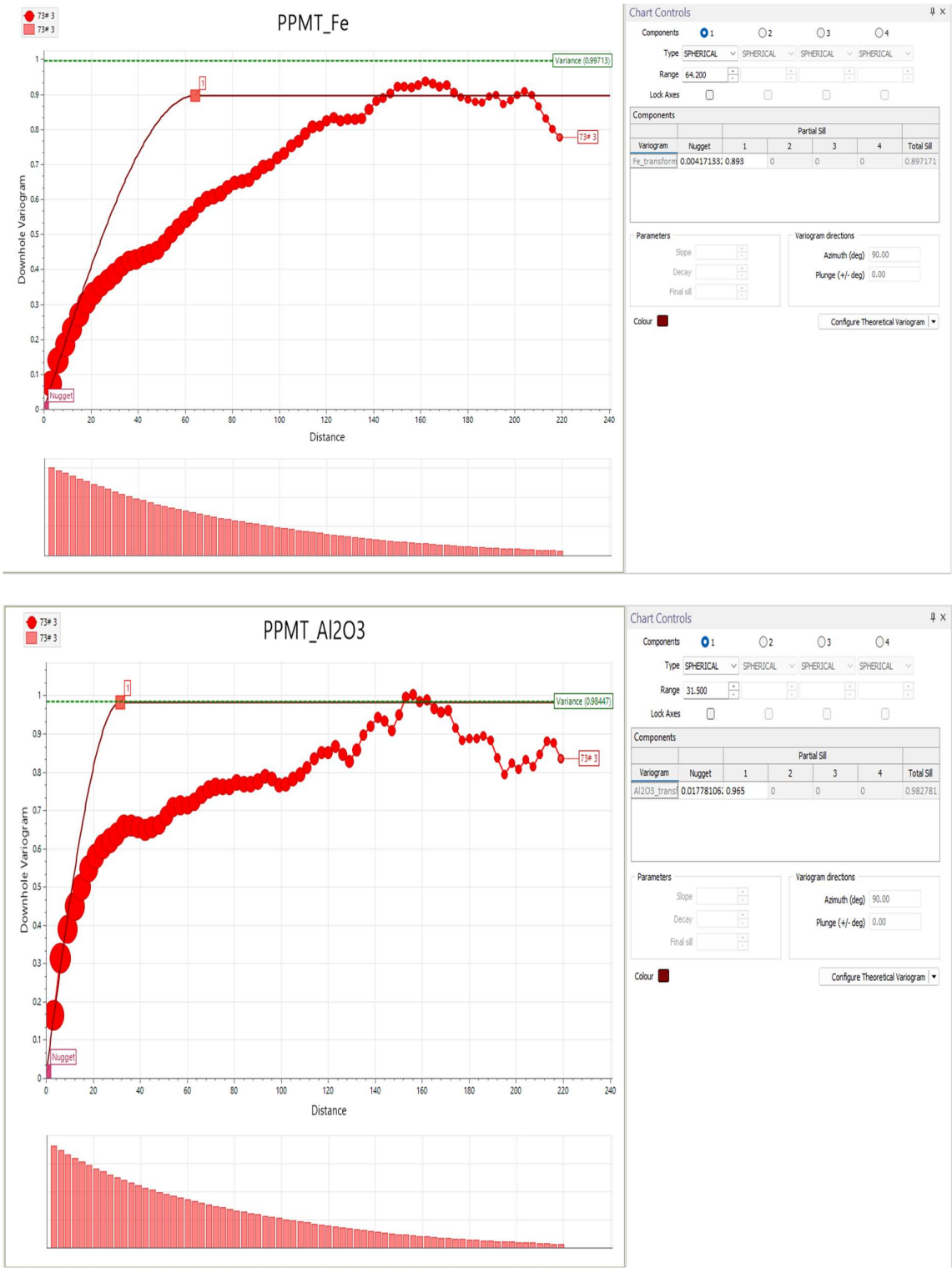


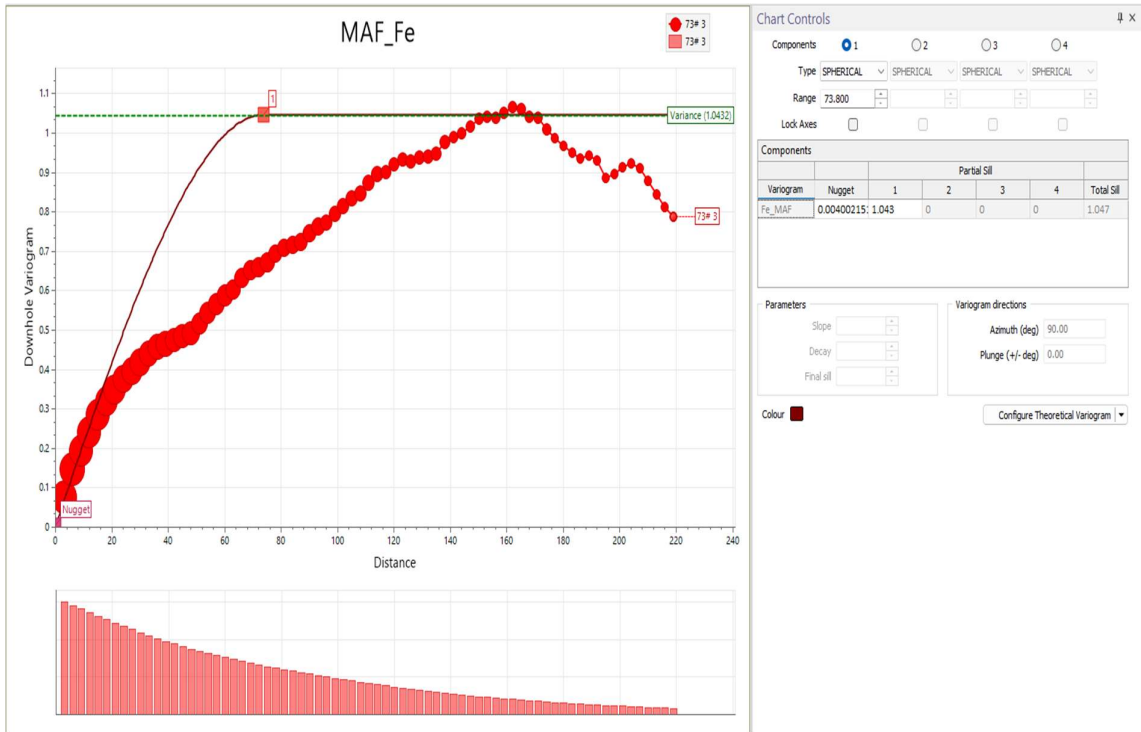






Appendix 3.3: Downhole variogram showing nugget effect of PPMT-Fe, PPMT-Al₂O₃, MAF-Fe, and MAF-Al₂O₃





Appendix 3.4: Variogram model of each transformed variable, including major axis (in blue line), semi-major axis (in green line), and minor axis (in red line).



