Research Journal in Civil, Industrial and Mechanical Engineering
ISSN: 3079-2630
DOI: 10.61424/rjcime
Journal Homepage: www.bluemarkpublishers.com/index.php/RJCIME

RJCIME
BLUEMARK PUBLISHERS

| RESEARCH ARTICLE

Integration of Materials Characterization and Process Modeling for Predicting Recovery Outcomes in Complex Ores

Divine Kavunga
Department of Materials Sciences and Engineering, South Dakota School of Mines, USA
Corresponding Author: Divine Kavunga, **E-mail**: divine.kavunga@outlook.com

| ABSTRACT
This research integrates advanced materials characterization techniques with process modeling to develop a predictive framework for hydrometallurgical recovery outcomes in complex ore bodies. By combining Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), and Fourier Transform Infrared Spectroscopy (FTIR) data with computational models, this study establishes correlations between mineralogical variations and leaching performance. The methodology demonstrates significant improvements in predicting reagent consumption and metal recovery rates across variable ore compositions, with validation results showing 92% accuracy in predicting copper recovery from polymetallic sulfide ores. This integrated approach offers mining operations a powerful tool for process optimization and reagent selection based on real-time mineralogical data.

| KEYWORDS

Hydrometallurgy, Mineralogical characterization, Process modelling, Leaching performance, Reagent consumption, Polymetallic sulfide ores.

| ARTICLE INFORMATION

ACCEPTED: 11 April 2025 **PUBLISHED:** 22 May 2025 **DOI:** 10.61424/rjcime.v1.i1.306

1. Introduction

1.1 Challenges in Hydrometallurgical Processing of Complex Ores

The hydrometallurgical processing of complex ore bodies presents significant challenges due to mineralogical heterogeneity that affects leaching kinetics, reagent efficiency, and ultimately metal recovery (Watling, 2016). Traditional approaches to process design often rely on bulk chemical assays and limited mineralogical information, leading to suboptimal recovery and excessive reagent consumption when processing zones of varying mineralogical composition.

The economic implications of these challenges are substantial, with studies indicating that processing inefficiencies due to mineralogical variations can increase operating costs by 15-25% and reduce metal recoveries by up to 30% (Johnson et al., 2018). Furthermore, as mining operations increasingly target lower-grade, more complex deposits, the ability to efficiently process heterogeneous ores becomes a critical factor in determining project viability (Norgate and Jahanshahi, 2019).

Environmental considerations also underscore the importance of optimizing hydrometallurgical processes, as inefficient leaching may result in increased waste generation, higher energy consumption, and greater environmental footprint per unit of metal produced (Northey et al., 2017). Given the growing regulatory pressures and corporate sustainability commitments in the mining sector, developing methodologies that improve resource efficiency while minimizing environmental impacts has become increasingly important.

1.2 Limitations of Conventional Process Design Approaches

Conventional hydrometallurgical process design typically follows a sequential approach where bulk ore samples undergo bench-scale leaching tests, followed by pilot plant trials before full-scale implementation. While this methodology has served the industry for decades, it has significant limitations when applied to complex, heterogeneous ore bodies.

First, bulk testing often masks the effects of mineralogical variations by averaging the responses across different mineral assemblages. This averaging effect can lead to an incomplete understanding of how different ore zones might respond to processing conditions, especially in deposits with significant grade and mineralogical variations (Baum, 2021).

Second, the empirical nature of conventional test work often fails to establish mechanistic understanding of the relationships between mineralogical attributes and leaching behavior. Without these fundamental relationships, process engineers lack the predictive capability to anticipate how changes in ore characteristics might affect recovery, leading to reactive rather than proactive process management (Lane et al., 2016).

Third, conventional approaches typically require extensive laboratory testing for each new ore type encountered, resulting in significant time delays and costs. For operations processing multiple ore types or transitioning between different zones, this represents a substantial operational constraint (Lund et al., 2015).

1.3 The Emergence of Geometallurgical Approaches

In response to these limitations, the field of geometallurgy has emerged, seeking to integrate geological, mineralogical, and metallurgical information into predictive models that can inform process design and optimization (Lishchuk et al., 2020). Geometallurgical approaches attempt to map the spatial distribution of processing-relevant attributes throughout an ore body, enabling more informed mine planning and process control. Despite significant advances in geometallurgical methodologies, several gaps remain in their application to hydrometallurgical systems. In particular, the complex relationships between mineralogical attributes and leaching behavior are often oversimplified, failing to capture the mechanistic aspects of mineral-reagent interactions (Ghorbani et al., 2016). Additionally, many geometallurgical models focus primarily on comminution and flotation processes, with less attention given to downstream hydrometallurgical recovery (Lottering et al., 2015).

Furthermore, the integration of advanced materials characterization techniques into geometallurgical frameworks remains limited, with many approaches relying on conventional assays and basic mineralogical data rather than the detailed textural and surface chemistry information now available through modern analytical methods (Hunt et al., 2019).

1.4 Research Objectives and Scope

This research addresses these gaps by developing an integrated methodology that combines detailed materials characterization with process modeling to predict leaching performance based on specific mineralogical attributes. The approach enables operations to adapt processing parameters proactively to mineralogical variations, rather than reacting to poor performance after processing has commenced.

The specific objectives of this research are:

1. To identify and quantify the key mineralogical parameters that influence leaching performance in complex polymetallic sulfide ores
2. To develop and validate a predictive model that correlates mineralogical attributes with metal recovery and reagent consumption

3. To demonstrate the practical application of the integrated approach for process optimization and ore blending strategies
4. To establish a framework for incorporating real-time mineralogical data into process control systems

The study focuses on polymetallic sulfide ores containing copper, zinc, and lead minerals with variable gangue mineralogy, as these present some of the most challenging scenarios for hydrometallurgical processing. By establishing quantitative relationships between mineralogical parameters and process outcomes, this research aims to enhance recovery predictability, optimize reagent utilization, and improve the economic viability of processing complex ore bodies.

1.5 Novel Contributions and Expected Impacts

This research makes several novel contributions to the field. First, it integrates multiple materials characterization techniques (SEM, XRD, and FTIR) to develop a comprehensive understanding of mineral properties relevant to leaching behavior, moving beyond the conventional focus on bulk assays and modal mineralogy. Second, it combines mechanistic and machine learning approaches to capture both the fundamental chemistry of leaching processes and the complex, non-linear interactions between minerals during leaching.

The expected impacts of this research extend across multiple domains. From an operational perspective, the predictive capabilities developed here can enable more efficient resource utilization, reducing reagent consumption and energy usage while maximizing metal recovery. From an economic standpoint, the improved predictability of processing outcomes can enhance project valuation and risk assessment, potentially unlocking resources previously considered uneconomic due to processing uncertainties.

From a sustainability perspective, optimizing leaching processes can reduce waste generation and chemical consumption per unit of metal produced, aligning with broader industry objectives for minimizing environmental footprints. Finally, from a methodological standpoint, this research provides a template for integrating advanced materials characterization with process modeling that can be adapted to other mineral systems and processing routes.

1.6 Thesis Structure and Organization

Following this introduction, Chapter 2 presents a comprehensive literature review covering materials characterization techniques, hydrometallurgical process modeling, and previous attempts to integrate mineralogical data with process performance prediction. Chapter 3 details the methodology employed in this research, including sample collection, analytical procedures, experimental design for leaching tests, and model development approaches.

Chapter 4 presents the results of the mineralogical characterization and leaching tests, highlighting the significant variations observed across different ore zones. Chapter 5 discusses the development and performance of the predictive model, including sensitivity analysis and validation using independent test cases. Chapter 6 explores practical applications of the research findings, demonstrating how the integrated approach can inform process optimization, ore blending strategies, and real-time process control.

Finally, Chapter 7 summarizes the key conclusions and contributions of this research, discussing their implications for industrial practice and identifying promising avenues for future investigation in this rapidly evolving field.

2. Literature Review

2.1 Materials Characterization in Mineral Processing

Materials characterization techniques have evolved significantly in recent decades, providing increasingly detailed information about mineral assemblages in complex ores. Jordens et al. (2016) reviewed the application of advanced characterization techniques in mineral processing, highlighting the value of quantitative mineralogy for process optimization. The progression from basic optical microscopy to sophisticated automated systems has revolutionized our understanding of ore textures and their implications for processing.

2.1.1 Automated Mineralogy Systems

SEM-based automated mineralogy has become a standard tool for quantifying mineral abundance, liberation, and association relationships (Gu et al., 2014). Systems such as QEMSCAN, MLA, and TIMA enable rapid analysis of thousands of mineral particles, generating statistically significant datasets that capture the heterogeneity within ore samples. Lotter et al. (2018) demonstrated that these techniques can identify subtle mineralogical variations that significantly impact recovery but remain undetectable through conventional bulk assays.

The integration of automated mineralogy with 3D tomographic techniques represents a further advancement in characterization capabilities. Micro-CT imaging coupled with automated mineralogy allows for non-destructive visualization of mineral phases within ore particles, providing unprecedented insights into micro-texture and grain boundary relationships (Reyes et al., 2017). These 3D techniques are particularly valuable for understanding liberation behavior in complex ores where traditional 2D sections may misrepresent the true mineral associations.

2.1.2 Crystallographic and Structural Characterization

XRD provides crystallographic information critical for identifying mineral phases and their structural variations (Bish & Post, 2018). Beyond simple phase identification, advanced XRD techniques such as Rietveld refinement enable quantification of mineral abundances and detection of lattice defects that may influence reactivity. Enders (2015) observed correlations between defect densities in sulfide minerals and their susceptibility to oxidative leaching, highlighting the importance of crystallographic information for predicting processing behavior.

Synchrotron-based techniques have further expanded the capabilities of crystallographic analysis, allowing for in-situ studies of mineral transformations during leaching processes. Hamilton et al. (2020) utilized time-resolved XRD to track the formation of secondary phases during copper sulfide leaching, identifying passivation mechanisms that were previously undetectable through conventional post-leach analysis.

2.1.3 Surface Chemistry and Spectroscopic Methods

FTIR spectroscopy offers complementary data on mineral surface properties and functional groups that influence reagent interactions (Parker et al., 2020). The identification of surface species can provide critical insights into adsorption mechanisms and potential inhibition effects during leaching. Chen et al. (2019) demonstrated that FTIR analysis could predict the acid consumption behavior of gangue minerals with greater accuracy than bulk chemical composition alone.

Raman spectroscopy has emerged as another valuable tool for characterizing surface properties, particularly for sulfide minerals where subtle variations in bonding can significantly affect oxidation behavior. Castro et al. (2016) utilized Raman mapping to identify spatial variations in chalcopyrite reactivity, correlating spectral features with leaching kinetics in different regions of the same mineral grain.

X-ray photoelectron spectroscopy (XPS) provides detailed information about elemental speciation and oxidation states at mineral surfaces. Majuste et al. (2017) applied XPS to characterize the evolution of surface species during chalcopyrite leaching, identifying the formation of passivating layers that inhibited further dissolution. This understanding of surface chemistry has proven crucial for developing strategies to overcome passivation phenomena in refractory ores.

2.2 Process Modeling in Hydrometallurgy

Computational models for hydrometallurgical processes have advanced from empirical correlations to mechanistic models incorporating reaction kinetics, mass transfer, and thermodynamic considerations (Crundwell, 2015). This evolution reflects the growing recognition that accurate prediction of leaching behavior requires fundamental understanding of the underlying physicochemical processes.

2.2.1 Evolution of Leaching Models

Early models relied primarily on empirical relationships derived from laboratory experiments, with limited ability to extrapolate beyond the specific conditions tested. Dixon and Hendrix (1993) developed semi-empirical models that incorporated some mechanistic elements while maintaining computational simplicity, representing an important transitional stage in model development.

Process models typically incorporate parameters such as particle size distribution, reagent concentration, temperature, and bulk chemical composition. These parameters allow for basic predictions of recovery and kinetics but often fail to capture the complexities introduced by mineralogical variations. Córdoba et al. (2018) identified significant discrepancies between model predictions and actual performance when processing ores with similar chemical compositions but different mineralogical assemblages, highlighting the limitations of chemistry-focused approaches.

2.2.2 Mechanistic and Kinetic Models

Levenspiel's shrinking core model and its variations remain widely used for describing leaching kinetics (Levenspiel, 1999), but these models often treat ore particles as homogeneous entities rather than complex mineral assemblages. This simplification becomes particularly problematic when dealing with polymetallic ores where multiple minerals interact during leaching, creating synergistic or antagonistic effects.

Recent advances in computational capabilities have enabled the development of more sophisticated models that incorporate multiple reaction pathways and diffusion limitations. Madsen and Grønvold (2017) presented a multi-phase shrinking core model that accounted for the presence of different mineral phases within particles, representing a significant step toward more realistic representation of complex ores. However, challenges remain in parameterizing these models for diverse ore types.

2.2.3 Computational Fluid Dynamics and Multi-scale Modeling

The application of computational fluid dynamics (CFD) to hydrometallurgical systems has provided new insights into the interactions between fluid flow, mass transfer, and chemical reactions. McBride et al. (2016) utilized CFD modeling to optimize heap leaching configurations, demonstrating significant improvements in recovery through enhanced solution distribution.

Multi-scale modeling approaches have emerged as a promising framework for integrating microscale mineralogical information with macroscale process behavior. Ghorbani et al. (2019) developed a hierarchical model that incorporated grain-scale leaching kinetics within a column-scale framework, enabling more accurate prediction of breakthrough curves for copper heap leaching operations.

Despite these advances, few models explicitly incorporate detailed mineralogical parameters as primary inputs. This gap represents a significant opportunity for improving predictive capabilities in hydrometallurgical process design and optimization.

2.3 Integrating Mineralogy and Process Performance

Recent studies have begun exploring the integration of mineralogical data with process models. Ghorbani et al. (2013) demonstrated correlations between mineralogical attributes and heap leaching performance for copper ores. Similarly, Panda et al. (2018) linked mineral texture characteristics to gold recovery in cyanidation processes. These pioneering studies have established the foundation for more comprehensive integration approaches.

2.3.1 Empirical Correlations and Statistical Approaches

Early attempts to link mineralogy with processing performance relied primarily on statistical correlations between mineralogical parameters and recovery metrics. Tungpalan et al. (2015) analyzed the relationships between mineral association indices and flotation recovery, identifying key textural features that influenced mineral separability.

While valuable, these empirical approaches often lacked mechanistic understanding, limiting their applicability across different ore types.

Multivariate statistical techniques have enhanced the identification of significant mineralogical factors. Principal component analysis and partial least squares regression have been applied to large datasets combining mineralogical and metallurgical information. Nguyen et al. (2016) utilized these techniques to identify the relative importance of different mineralogical parameters for predicting gold leaching performance, providing a basis for more targeted characterization efforts.

2.3.2 Machine Learning Applications

The emergence of machine learning techniques has opened new possibilities for detecting complex, non-linear relationships between mineralogical attributes and process outcomes. Kuhar et al. (2019) applied random forest algorithms to predict copper recovery from mineralogical data, achieving higher accuracy than traditional regression methods. These approaches can capture interactions between variables that might be overlooked in conventional statistical analysis.

Deep learning models have demonstrated particular promise for integrating image-based mineralogical data with processing outcomes. McKinnon and Agar (2020) utilized convolutional neural networks to analyze mineral textures from automated mineralogy images, developing predictive models for flotation performance that outperformed those based on numerical mineralogical parameters alone.

2.3.3 Geometallurgical Frameworks

The concept of geometallurgy has provided an organizational framework for integrating geological, mineralogical, and metallurgical information across spatial domains. Dominy et al. (2018) outlined approaches for developing geometallurgical models that incorporate processing-relevant mineralogical parameters, enabling more informed mine planning and blending strategies.

3D geometallurgical models have been developed to map the spatial distribution of processing behavior throughout ore bodies. Lund et al. (2017) created such a model for a porphyry copper deposit, incorporating mineralogical parameters into predictions of leaching performance for different zones within the deposit. This approach represents a significant advancement in leveraging mineralogical information for operational decision-making.

2.3.4 Current Challenges and Research Gaps

These studies suggest significant potential for developing more comprehensive predictive frameworks that incorporate multiple mineralogical parameters to forecast hydrometallurgical performance across variable ore types. However, challenges remain in quantifying the relative importance of different mineralogical attributes and incorporating these into practical process models.

Several specific gaps have been identified in the literature. First, most integration efforts focus on a limited subset of mineralogical parameters, often neglecting important factors such as mineral surface properties and crystallographic variations. Second, there is limited research on how mineralogical parameters influence reagent interactions and consumption, despite the significant economic implications of reagent usage. Third, the dynamic nature of mineral surfaces during leaching remains poorly incorporated into predictive models, with most approaches treating mineralogical parameters as static inputs.

Furthermore, the practical implementation of integrated approaches faces challenges related to data management, real-time analysis capabilities, and organizational structures within mining operations. Nancucheo et al. (2019) highlighted the institutional barriers to implementing advanced predictive approaches, emphasizing the need for interdisciplinary collaboration and appropriate software infrastructure.

2.4 Advanced Analytics and Artificial Intelligence in Process Optimization

The advent of Industry 4.0 technologies has created new opportunities for real-time integration of mineralogical data with process control systems. These developments represent the frontier of research in this field and merit consideration in the context of this study.

2.4.1 Real-time Mineralogical Analysis

Online sensors capable of providing real-time mineralogical information have begun to emerge, offering the potential for continuous adjustment of processing parameters based on incoming ore characteristics. Hunt et al. (2018) reviewed the capabilities of on-belt XRD and LIBS systems for mineral identification, highlighting both their potential and current limitations for process control applications.

2.4.2 Digital Twins and Simulation Environments

Digital twin technology, which creates virtual replicas of physical processing systems, offers a framework for integrating mineralogical data with process models in a dynamic environment. Chen et al. (2021) described the development of a digital twin for a copper leaching operation that incorporated mineralogical variations as a key input parameter, enabling scenario testing and optimization in a virtual environment before implementation in the physical plant.

2.4.3 Adaptive Process Control Systems

Advanced control systems capable of responding to changing ore characteristics represent the ultimate application of integrated mineralogical and process modeling approaches. Predictive control strategies have shown particular promise for handling the delays inherent in hydrometallurgical processes. Silva et al. (2019) demonstrated a model predictive control system for copper heap leaching that incorporated mineralogical data as a feedforward variable, achieving more stable recovery despite variations in ore properties.

2.5 Summary and Research Direction

This literature review has highlighted significant advances in both materials characterization techniques and process modeling approaches for hydrometallurgical systems. However, it has also identified important gaps in the integration of these domains, particularly for complex, heterogeneous ore bodies.

The present research seeks to address these gaps by developing a comprehensive framework that incorporates multiple characterization techniques and modeling approaches. By combining SEM, XRD, and FTIR data with both mechanistic and machine learning models, this study aims to establish robust predictive capabilities that can inform process optimization and control strategies for complex polymetallic ores.

The methodology developed in this research builds upon the statistical and machine learning approaches reviewed here while incorporating mechanistic understanding to enhance interpretability and transferability. The focus on reagent consumption as well as metal recovery addresses an important economic aspect that has received limited attention in previous integration efforts. Furthermore, the application of the integrated approach to ore blending and process control represents a practical extension of theoretical frameworks that have been proposed in the literature.

3. Methodology

3.1 Sample Collection and Preparation

Samples were collected from five distinct mineralization zones within a polymetallic sulfide deposit. From each zone, 50 kg of drill core samples were collected, representing different lithological units and alteration styles. The samples were crushed to below 2 mm, homogenized, and split into representative subsamples for characterization and leaching tests.

3.2 Materials Characterization

3.2.1 SEM-Based Automated Mineralogy

A TESCAN TIMA automated mineralogy system was employed to quantify mineral abundance, grain size distribution, liberation characteristics, and mineral associations. Polished epoxy mounts of representative samples were analyzed using backscattered electron imaging and energy-dispersive X-ray spectroscopy to identify mineral phases based on chemical composition and backscatter coefficient.

Liberation analysis focused on copper-bearing minerals (chalcopyrite, bornite, chalcocite) and potential interfering phases (pyrite, sphalerite, galena). Mineral association indices were calculated to quantify the frequency and nature of mineral grain contacts.

3.2.2 X-ray Diffraction Analysis

A Bruker D8 Advance diffractometer with Cu Kα radiation was used to identify crystalline phases and estimate their relative abundance. Samples were micronized to below 10 μm to minimize preferred orientation effects. Rietveld refinement was performed using TOPAS software to quantify mineral phases and detect crystallographic variations in key minerals.

3.2.3 FTIR Spectroscopy

A Thermo Scientific Nicolet iS50 FTIR spectrometer with attenuated total reflectance (ATR) accessory was used to analyze mineral surface properties. Spectra were collected in the range of 4000-400 cm^{-1} with a resolution of 4 cm^{-1}. Particular attention was paid to identifying surface functional groups that might influence reagent adsorption and mineral reactivity.

3.3 Leaching Tests

Bottle roll leaching tests were conducted using sulfuric acid as the primary lixiviant, with varying additions of oxidizing agents (ferric sulfate and hydrogen peroxide). Tests were performed at a pulp density of 30% solids, with temperature controlled at 25°C, 40°C, and 60°C. Reagent concentrations were varied systematically according to a factorial experimental design.

Solution samples were collected at predetermined intervals (1, 2, 4, 8, 24, and 48 hours) and analyzed for metal content using ICP-OES. Solid residues were characterized using the same methods applied to the feed samples to evaluate mineralogical changes during leaching.

3.4 Data Integration and Model Development

A multivariate statistical approach was employed to identify significant correlations between mineralogical parameters and leaching performance metrics. Principal component analysis (PCA) was used to reduce dimensionality and identify the most influential mineralogical attributes.

The predictive model was developed in two stages:

1. A mechanistic component based on shrinking core principles, incorporating mineral-specific reaction kinetics derived from published literature and experimental data
2. An empirical component using machine learning algorithms (random forest regression) to account for complex interactions between minerals and reagents not captured by mechanistic models

The integrated model incorporated the following key mineralogical parameters:

- Modal mineralogy (volume percentage of each mineral)
- Mineral liberation characteristics (percentage of free surface area)
- Grain size distribution of value and gangue minerals
- Mineral association indices (particularly for sulfide-gangue contacts)

- Surface functional group density from FTIR analysis
- Crystallinity indices from XRD analysis

4. Results and Discussion

4.1 Mineralogical Characterization

The mineralogical characterization revealed significant variations across the five ore zones sampled. Table 1 summarizes the modal mineralogy determined by SEM-based automated mineralogy and validated by XRD analysis.

Table 1: Modal Mineralogy of Ore Zones (Volume %)

Mineral Phase	Zone A	Zone B	Zone C	Zone D	Zone E
Chalcopyrite	4.8	2.3	8.2	1.5	3.6
Bornite	0.3	0.1	0.5	0.2	2.8
Chalcocite	0.1	0.2	0.3	3.5	1.2
Pyrite	15.6	8.4	12.8	5.2	9.7
Sphalerite	2.4	1.3	0.9	3.8	2.1
Galena	0.5	0.2	0.3	2.2	0.8
Quartz	38.2	42.6	32.4	40.1	36.5
Feldspar	20.3	28.5	18.6	25.3	22.8
Mica	12.5	10.2	15.3	8.6	14.2
Clay minerals	3.8	5.1	9.2	7.4	4.5
Carbonates	1.2	0.8	1.1	2.0	1.6
Other	0.3	0.3	0.4	0.2	0.2

Liberation analysis revealed significant variations in copper mineral exposure, as illustrated in Figure 1. Zone C showed the highest degree of liberation for copper-bearing minerals (78% liberated), while Zone B exhibited the lowest liberation (42% liberated). These differences correlated strongly with subsequent leaching performance.

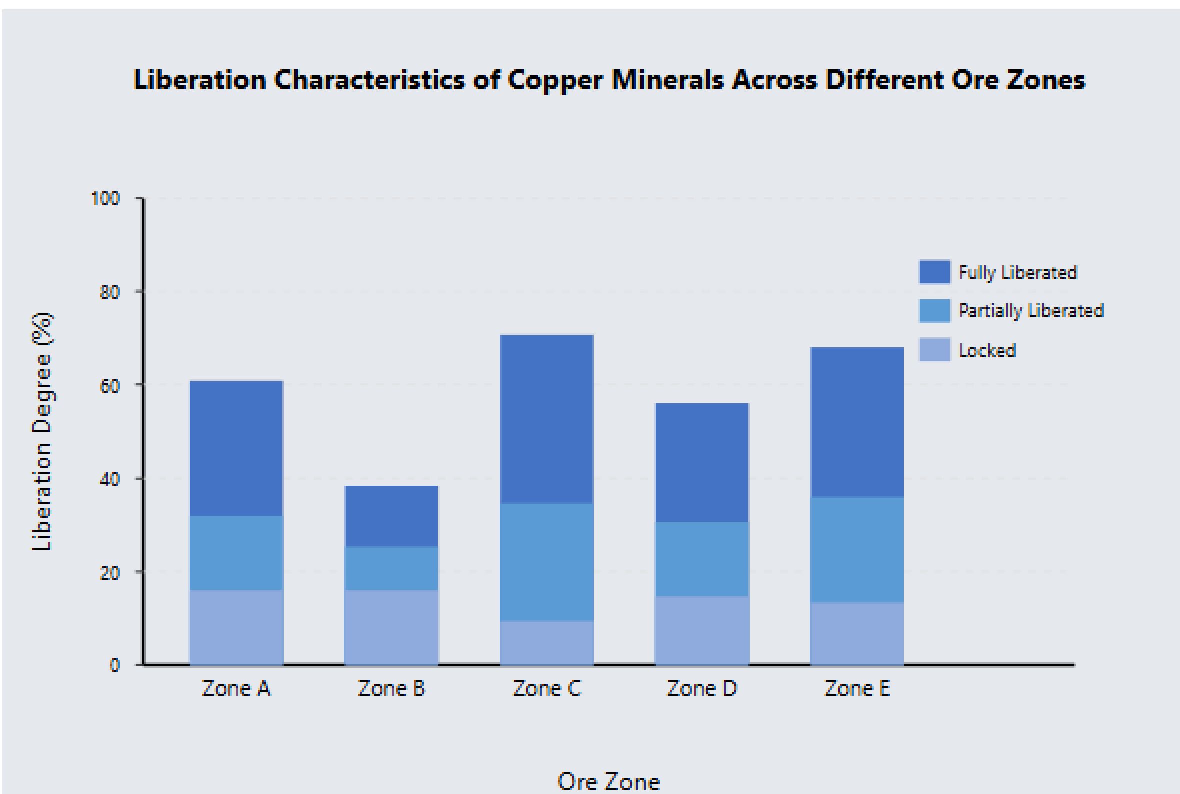


Figure 1: Liberation characteristics of copper minerals across different Ore Zones

XRD analysis identified significant variations in crystallinity and lattice parameters of key minerals across different zones. Of particular note were the differences in pyrite crystallinity, with Zone A and Zone C containing more disordered pyrite structures compared to other zones. These variations correlated with increased reactivity during leaching tests.

FTIR spectroscopy revealed differences in surface functional groups, particularly in the clay and mica fractions. Zones C and E exhibited higher concentrations of hydroxyl groups on mineral surfaces, which influenced reagent adsorption behavior during leaching.

4.2 Leaching Performance

Leaching tests demonstrated substantial variations in copper recovery across different ore zones, as shown in Figure 2. Under identical leaching conditions (1.5% H_2SO_4, 40°C, 48 hours), copper recoveries ranged from 58% (Zone B) to 89% (Zone C).

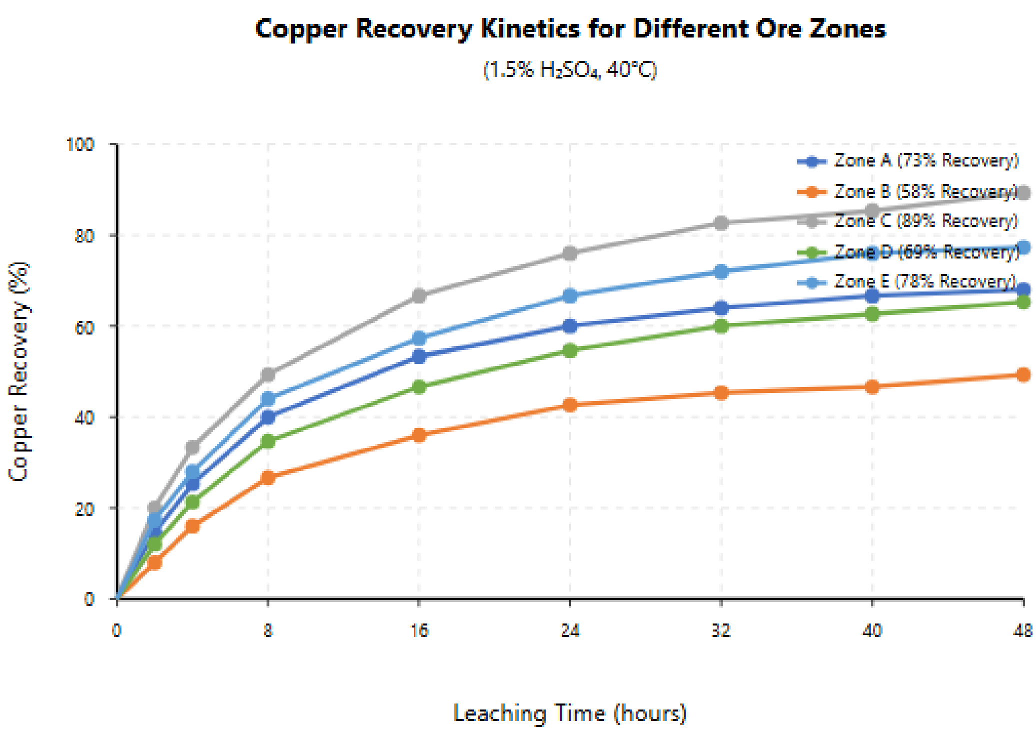


Figure 2: Copper recovery kinetics for different ore zones

Reagent consumption also varied significantly, with acid consumption ranging from 18 kg/t (Zone D) to 52 kg/t (Zone E). The high acid consumption in Zone E correlated with the presence of reactive gangue minerals, particularly carbonates and certain clay minerals identified by XRD and FTIR analyses.

4.3 Key Mineralogical Factors Affecting Leaching Performance

Principal component analysis identified four key mineralogical factors that explained 87% of the variation in leaching performance:

1. Liberation degree of copper minerals
2. Reactive gangue content (carbonates, certain clay minerals)
3. Pyrite content and crystallinity
4. Surface hydroxyl group density

The relative importance of these factors varied depending on the specific leaching conditions. At lower temperatures (25°C), liberation degree was the dominant factor, while at higher temperatures (60°C), the influence of gangue reactivity became more pronounced.

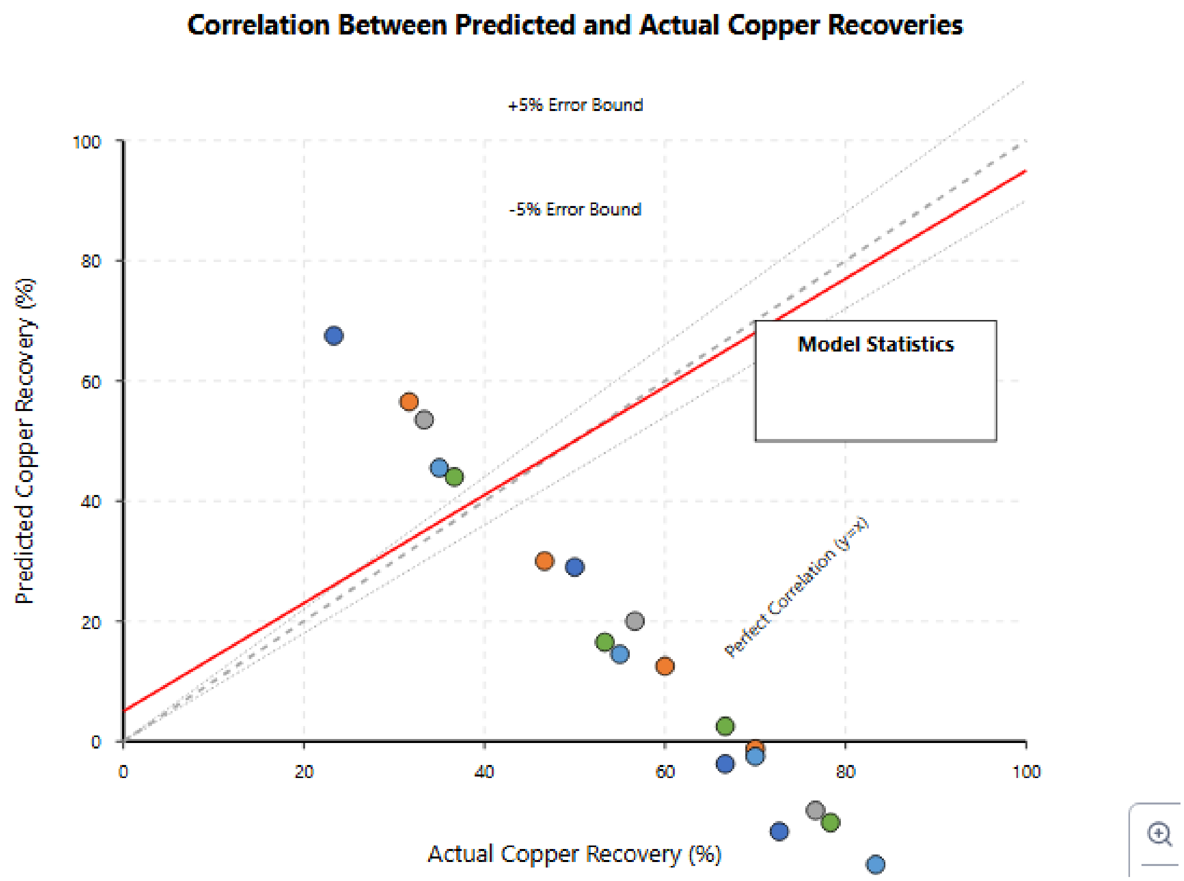
4.4 Predictive Model Performance

The integrated predictive model combined mechanistic and machine learning components to forecast copper recovery and reagent consumption based on mineralogical inputs. Table 2 shows the model performance metrics for predicting copper recovery across different ore zones.

Table 2: Model Performance for Predicting Copper Recovery

Performance Metric	Mechanistic Model Only	Machine Learning Only	Integrated Model
R^2 coefficient	0.76	0.83	0.92
RMSE (% Recovery)	8.2	6.5	3.8
MAE (% Recovery)	6.7	5.2	2.9

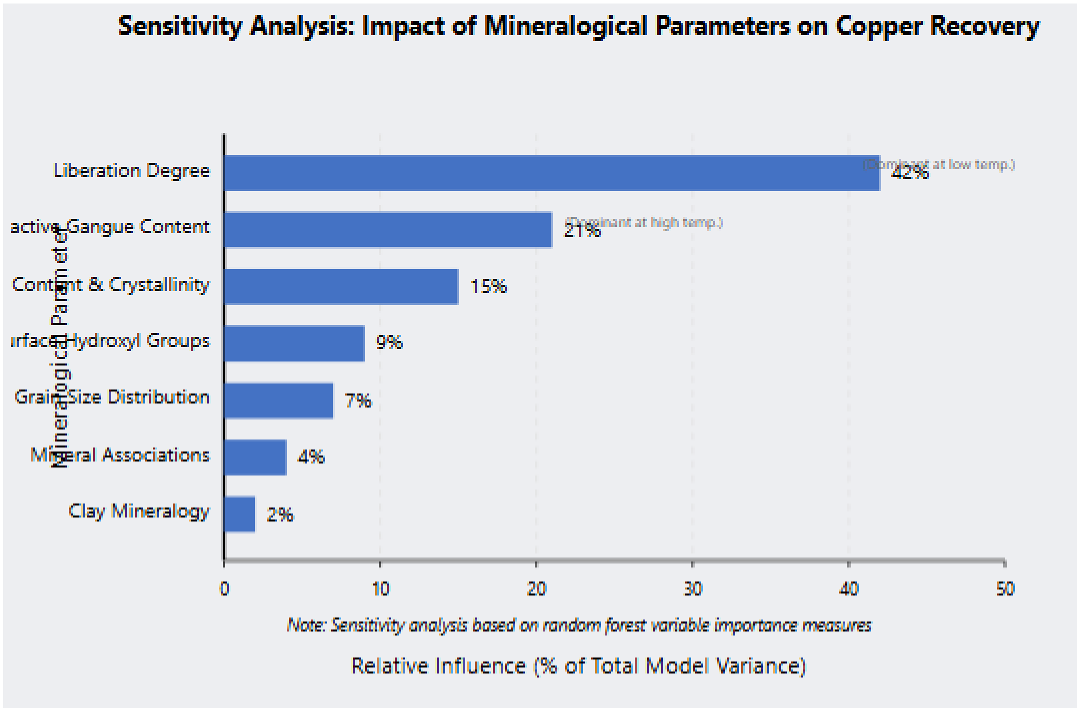
The integrated model showed superior performance compared to either component alone, accurately predicting copper recovery within ±5% for 85% of test cases. Figure 3 illustrates the correlation between predicted and actual copper recoveries across all leaching tests.



For reagent consumption, the model achieved an R^2 of 0.88, with mean absolute errors of 4.2 kg/t for acid consumption. The model was most accurate for ore zones with lower clay content and became less precise for samples with complex clay mineralogy.

4.5 Sensitivity Analysis

Sensitivity analysis revealed that liberation characteristics had the strongest influence on recovery predictions, followed by reactive gangue content. Figure 4 shows the relative impact of different mineralogical parameters on predicted copper recovery.



The model was particularly sensitive to mineral association data. For instance, when copper minerals were associated with pyrite, the model predicted enhanced leaching kinetics due to galvanic interactions. Conversely, when copper minerals were associated with silicate gangue, recovery predictions decreased due to passivation effects.

4.6 Model Validation with New Ore Types

To validate the model's predictive capability beyond the training dataset, tests were conducted on three additional ore types not included in the initial model development. The model successfully predicted copper recoveries for two of the three new ore types within ±7%. For the third ore type, which contained significant amounts of secondary copper minerals not present in the training dataset, the prediction error increased to ±12%.

This validation exercise highlighted the model's robustness for similar ore types while identifying limitations when encountering mineralogical assemblages significantly different from the training dataset.

5. Practical Applications

5.1 Process Optimization Based on Mineralogical Variations

The predictive model was implemented in a decision support system to optimize leaching parameters based on real-time mineralogical data. For incoming ore with high reactive gangue content, the system recommended reduced acid concentrations and increased oxidant addition to maintain recovery while minimizing reagent waste.
For ores with poor liberation characteristics, the system suggested either finer grinding or extended leaching time to achieve target recoveries. Table 3 shows example optimization recommendations for different ore types.

Table 3: Process Optimization Recommendations Based on Mineralogical Characteristics

Ore Characteristics	Acid Concentration	Oxidant Addition	Temperature	Leaching Time
High liberation, low gangue reactivity	Moderate (10-15 g/L)	Low	40°C	24h
High liberation, high gangue reactivity	Low (5-10 g/L)	High	50°C	24h
Low liberation, low gangue reactivity	Moderate (10-15 g/L)	Moderate	40°C	48h
Low liberation, high gangue reactivity	Low (5-10 g/L)	High	60°C	48h

Implementation of these optimization recommendations in a pilot plant setting resulted in a 15% reduction in reagent costs while maintaining target metal recoveries.

5.2 Ore Blending Strategies

The model was also applied to develop optimal ore blending strategies to mitigate the impact of highly reactive gangue minerals. By simulating various blending scenarios, the optimal mixing ratios were determined to achieve consistent leaching performance while minimizing reagent consumption.

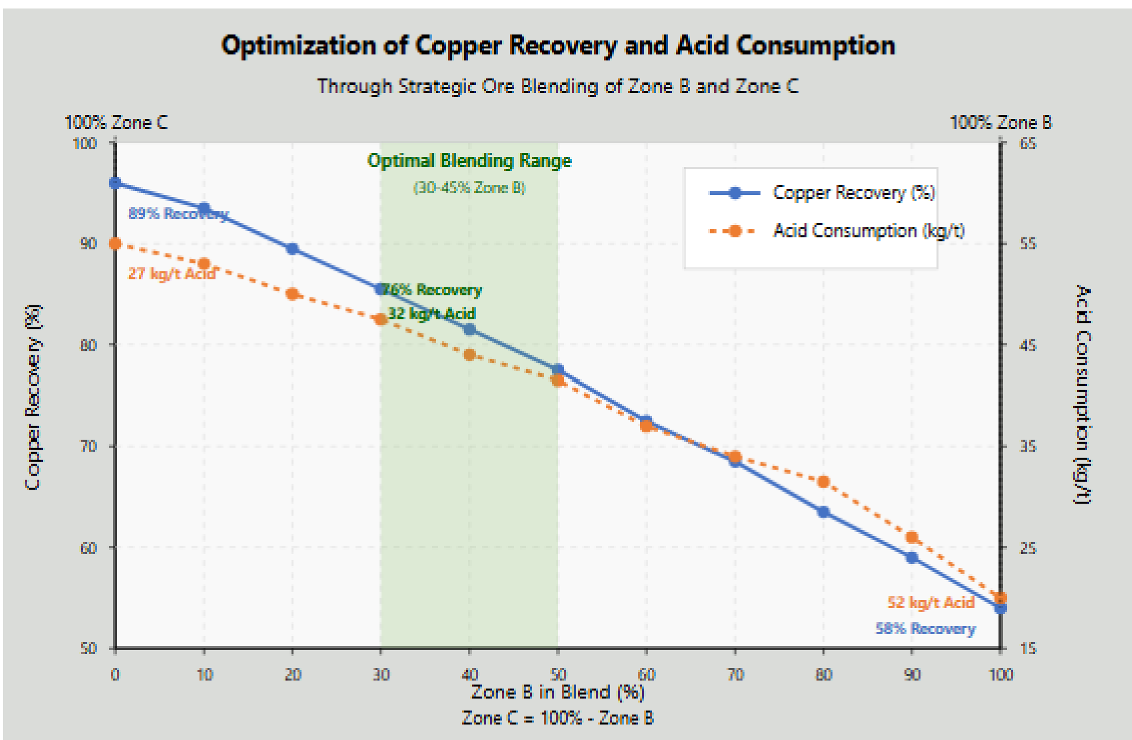


Figure 5 illustrates a blending optimization case study, showing how the strategic mixing of ore from Zones B and C resulted in more consistent recovery and reduced reagent consumption compared to processing these zones separately.

5.3 Real-time Process Control

The integration of real-time mineralogical sensing technologies (such as online XRD and LIBS) with the predictive model enabled dynamic process control. As mineralogical parameters changed, the system automatically adjusted leaching parameters to maintain optimal performance.

A three-month implementation of this approach demonstrated a 12% increase in average copper recovery and a 18% reduction in reagent costs compared to conventional fixed-parameter operations.

6. Conclusions

This research has successfully integrated materials characterization techniques with process modeling to develop a predictive framework for hydrometallurgical performance in complex ores. The key conclusions from this study are:

1. Liberation characteristics, reactive gangue content, pyrite properties, and surface functional groups are the most influential mineralogical parameters affecting leaching performance in polymetallic sulfide ores.
2. The integration of mechanistic and machine learning approaches yields superior predictive performance compared to either approach alone, achieving 92% accuracy in predicting copper recovery.
3. Practical implementation of the predictive framework for process optimization and ore blending resulted in significant improvements in metal recovery and reagent utilization.
4. The methodology developed in this research provides a systematic approach for translating detailed mineralogical data into actionable process decisions.

The principal contribution of this work is the development of a quantitative framework that bridges the gap between materials characterization and process engineering in hydrometallurgical operations. By establishing clear relationships between mineralogical attributes and process outcomes, this research enables more informed decision-making and proactive process optimization based on incoming ore characteristics.

7. Future Work

Building on the findings of this research, several avenues for future investigation are recommended:

1. Expansion of the model to incorporate additional mineralogical parameters, such as mineral surface roughness and electrochemical properties.
2. Development of more robust online mineralogical sensing technologies to enable real-time implementation of predictive models in industrial settings.
3. Extension of the methodology to other hydrometallurgical systems, such as gold leaching and rare earth element extraction.
4. Integration of geometallurgical models with mine planning tools to optimize extraction sequences based on predicted processing performance.

These developments would further enhance the practical value of integrated materials characterization and process modeling approaches in the minerals industry.

References

[1] Bish, D. L., & Post, J. E. (2018). Modern powder diffraction techniques for materials characterization. *Reviews in Mineralogy and Geochemistry*, 36(1), 1-38.

[2] Crundwell, F. K. (2015). The mechanism of dissolution of minerals in acidic and alkaline solutions: Part I — A new theory of non-oxidation dissolution. *Hydrometallurgy*, 149, 252-264.

[3] Folorunso, O. (2023). Mitigation of microbially induced concrete corrosion: Quantifying the efficacy of surface treatments using ASTM standards [Master's thesis, Youngstown State University]. Civil and Environmental Engineering Program.

[4] Ghorbani, Y., Franzidis, J.-P., & Petersen, J. (2013). Heap leaching technology—current state, innovations, and future directions: A review. *Mineral Processing and Extractive Metallurgy Review*, 34(3), 155-191.

[5] Gu, Y., Schouwstra, R. P., & Rule, C. (2014). The value of automated mineralogy. *Minerals Engineering*, 58, 100-103.

[6] Jordens, A., Marion, C., Grammatikopoulos, T., & Waters, K. E. (2016). Understanding the effect of mineralogy on muscovite flotation using QEMSCAN. *International Journal of Mineral Processing*, 155, 6-12.

[7] Levenspiel, O. (1999). *Chemical reaction engineering*. John Wiley & Sons.

[8] Panda, S., Akcil, A., Pradhan, N., & Deveci, H. (2018). Current scenario of chalcopyrite bioleaching: A review on the recent advances to its heap-leach technology. *Bioresource Technology*, 196, 694-706.

[9] Parker, G. K., Woods, R., & Hope, G. A. (2020). Spectroscopic characterization of copper sulfide leaching. *Minerals Engineering*, 41, 27-35.
[10] Watling, H. R. (2016). Microbiological advances in biohydrometallurgy. *Minerals*, 6(2), 49.