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PREDICTIVE MODELING OF ORE PREPARATION PROCESSES UNDER CONDITIONS OF MINERALOGICAL COMPOSITION VARIABILITY

Abstract. The research establishes a direct link between inherent mineralogical variability and comminution performance, enabling crushing and grinding optimization through a fundamental materials-based approach. The methodology integrates mineralogical characterization using QEMSCAN and XRD, mechanical property testing through nanoindentation and single-particle breakage, and numerical simulation via a hybrid Discrete Element Method-Population Balance Model (DEM-PBM) calibrated with experimental data and supplemented by multivariate statistical analysis for rapid prediction.

Analysis of a porphyry copper deposit classified the ore into four distinct types with quartz contents ranging from 15% to 65% and clay minerals from near-zero to 40%. The calibrated DEM model reproduced single-particle breakage with errors below 6%. Simulations demonstrated that shifting from quartz-dominated to clay-rich ore reduces specific energy consumption by up to 45% while increasing product P80 from 185 μm to 290 μm. A 15% increase in hard pyrite content was predicted to raise specific energy by 8% and reduce product P80 by 5 μm. Validation against experimental batch grinding tests achieved $R^2 > 0.95$ for predicted versus experimental particle size distributions. An optimization case study showed that a 10% feed rate reduction combined with 2% mill speed increase could maintain constant product fineness during transition to softer ore.

The scientific novelty lies in developing a fully integrated, physics-based framework directly linking quantitative mineralogical data to comminution behavior through a calibrated DEM-PBM hybrid model. Unlike traditional empirical approaches relying on bulk averaged properties like the Bond Work Index, this work provides mechanistic understanding of how individual mineral constituents and their textural relationships collectively determine breakage outcomes, enabling prediction of grinding performance for arbitrary ore blends without empirical testing for each mixture.

The framework enables a paradigm shift from reactive process management to predictive, feed-forward control in mineral processing. It allows quantitative optimization of grinding parameters in response to real-time or anticipated changes in feed mineralogy, with demonstrated potential for 5–10% energy savings, increased throughput, and improved downstream recovery through stabilized product size. The methodology can be integrated with online sensors and advanced process control systems for real-time implementation, providing a scientific basis for transforming ore preparation from a cost center into a value-generating component of the mining enterprise.

Keywords: ore preparation, comminution, crushing, grinding, mineralogical variability, predictive modeling, Discrete Element Method (DEM), Population Balance Model (PBM), process optimization, geometallurgy.

1. Introduction

The mining industry faces increasing geological complexity as high-grade deposits deplete, forcing operations to process deeper, lower-grade ores with significant variability in mineralogy, texture, and hardness [1–3]. This variability fundamentally disrupts comminution circuits – a crusher optimized for hard ore performs inefficiently on softer material, causing throughput reductions, energy waste, and inconsistent particle sizes that undermine downstream processes [4, 5].

Current practice remains reactive and ill-equipped for short-term fluctuations. Traditional approaches rely on bulk parameters like the Bond Work Index [6], which averages out the hourly feed variations that actually occur. Control strategies use feedback loops that respond to disturbances after they happen – detecting a mill over-

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load, then reducing feed rate [7, 8]. This reactive paradigm accepts inefficiency as unavoidable, resulting in constant process upsets, wasted energy, and lost production.

This gap between complex reality and simplistic control necessitates a paradigm shift: from reactive management to predictive control. The enabler is sophisticated mathematical modeling that integrates detailed mineralogical data directly into the control loop. By understanding exactly what material enters the plant and accurately predicting its breakage behavior, we can anticipate variability before it causes disturbances. Such models would use modal mineralogy, grain size distribution, and texture as inputs, enabling real-time adjustment of operating parameters to maintain optimum efficiency.

Foundational comminution theories [9–11] established empirical and phenomenological models (Bond Work Index, population balance models) but rely on bulk properties unsuited for dynamic control. Recent advances link mineralogy to breakage through advanced characterization tools (QEMSCAN, MLA), revealing that texture profoundly influences fracture patterns [12–14]. However, these geometallurgical approaches typically serve long-term planning rather than real-time control.

Parallel developments in numerical simulation – particularly Discrete Element Method (DEM) with bonded-particle models [15–20] – enable high-fidelity comminution simulation. Yet DEM calibration remains time-intensive, requiring extensive single-particle testing. Research on multi-component ores [21, 22] and adaptive control systems [23] further advances the field, but a critical synthesis remains missing: a direct, quantitative connection between high-resolution mineralogical data and dynamic breakage models for predictive control.

This research addresses that gap by developing a framework uniting quantitative mineralogy with numerical simulation creating a predictive tool to transform how the industry responds to ore variability.

2. Methods

The goal of this research is to establish a comprehensive framework optimizing ore preparation through the synergistic integration of predictive numerical modeling and quantitative mineralogical analysis, creating a direct mechanistic link between fundamental material properties and dynamic comminution behavior. This will be achieved by first quantitatively characterizing mineralogical variability within a representative ore body using advanced automated mineralogy to capture the full spectrum of modal composition, texture, and grain size distribution. Building on this characterization, a hybrid Discrete Element Method-Population Balance Model will be developed to establish a quantitative link between mineral-specific mechanical properties and resultant bulk breakage behavior under compressive and impact loads. This model will then simulate crushing and grinding operations under various feed scenarios defined by the real mineralogical data, with its predictive accuracy rigorously validated against controlled laboratory-scale or pilot-scale comminution experiments. The findings will ultimately be synthesized into a practical methodology for deploying the validated model in adaptive, feed-forward control strategies for industrial circuits, enabling dynamic optimization in response to real-time ore variability.

The research methodology proceeds through three interconnected phases: detailed mineralogical characterization, mechanical property determination, and hybrid numerical modeling. The foundation begins with collecting a representative sample set that truly captures the full ore body variability – not random sampling but a targeted campaign drawing from drill core intervals or plant feed streams pre-identified through geological logging as representing different ore types, alteration zones, and textural domains. For a porphyry copper system, this includes samples from potassic, phyllic, and argillic alteration zones with varying stockwork vein densities; for iron ore, it spans hematite, magnetite, and goethite-rich lithologies across both massive and friable types. This assembled library is then subjected to high-resolution analytical techniques, primarily automated mineralogy using QEMSCAN or Mineral Liberation Analyzer, which combine SEM (scanning electron microscopy) imaging with energy-dispersive X-ray spectroscopy to automatically identify minerals and map their spatial distribution. The output provides quantitative modal mineralogy with precise weight or volume percentages of every mineral phase, mineral grain size distributions critical for predicting liberation energy, mineral association data revealing which minerals contact each other and indicating texture, and baseline liberation assessment. This automated mineralogy is complemented by X-ray diffraction for bulk mineral identification and quantifying phases difficult to distinguish by SEM-EDS (energy-dispersive X-ray spectroscopy), such as different clay minerals or polymorphs. From this rich dataset, derived parameters are calculated to create quantitative indices directly linked to mechanical behavior – including a mineralogical hardness index formulated as a weighted average of constituent mineral intrinsic hardness using Knoop or Vickers micro-hardness values from materials science literature.

From this rich dataset, a series of derived parameters are calculated to create quantitative indices that can be directly linked to mechanical behavior. A "mineralogical hardness index" can be formulated, which is a weighted average of the intrinsic hardness of the constituent minerals. This requires a look-up table of Knoop or Vickers micro-hardness values for each mineral, available from materials science literature. The index might take the form:

$$H_{\min} = \sum_{i=1}^{n} \left(w_i \cdot H_i \right), \tag{1}$$

where w_i is the weight fraction of mineral i and H_i is its intrinsic micro-hardness. Similarly, a "textural index" is developed to capture the complexity of the mineral intergrowth. This could be based on the average grain size, a grain size uniformity coefficient, or more sophisticated parameters like a mineral association entropy metric derived from the QEMSCAN data. A higher textural index might indicate a very fine-grained, complexly intergrown ore that is resistant to breakage and liberation. Finally, based on a combination of these quantitative parameters – modal mineralogy, hardness index, and textural index – a statistically robust "ore type" classification scheme is developed. This is not based on subjective geological observation but on a

rigorous, data-driven clustering of the samples into distinct groups that are expected to behave differently during comminution.

With the ore types defined and their mineralogy quantified, the next phase focuses on determining the fundamental mechanical properties that govern breakage. This moves from the scale of the bulk ore to the scale of the individual mineral grain and the single particle.

Nano-indentation or micro-hardness testing is employed to measure the mechanical properties of individual mineral grains directly within their natural textural context. A small, sharp indenter is pressed into the surface of a polished sample with a precisely controlled force, and the depth of penetration is continuously recorded. The resulting load-displacement curve is analyzed to extract the material's hardness (resistance to permanent deformation) and its reduced Young's modulus. The modulus is derived from the slope of the unloading curve using the Oliver-Pharr method:

$$E_r = \frac{\sqrt{\pi}}{2}\frac{S}{\sqrt{A}}, \tag{2}$$

where E_r is the reduced modulus, Pa; S is the stiffness (slope of the unloading curve at maximum load), N/m; and A is the projected contact area, m^2. This data provides the fundamental, mineral-specific mechanical property inputs required for high-fidelity numerical models. By testing multiple grains of the same mineral within different textural settings, it is also possible to assess the influence of grain boundaries and adjacent phases on the apparent mechanical properties.

To connect these mineral-scale properties to the breakage behavior of larger particles, a program of single-particle breakage testing is conducted. This involves selecting individual particles of a specific size (e.g., -25mm + 19mm) from each of the previously defined ore type classes. These particles are then subjected to controlled breakage events. Slow compression tests are performed using a universal testing machine, crushing a single particle between two flat platens at a constant displacement rate. The force-displacement curve is recorded, and the energy absorbed up to the point of fracture is integrated, providing the particle's fracture energy. The resulting fragment size distribution is also measured. Alternatively, for higher throughput, a drop-weight tester can be used, where particles are broken by impacts of varying specific energies. This provides a statistical distribution of breakage energies for each ore type. The outcome of this testing is a fracture energy distribution function, $f(E)$, for each ore class, which describes the probability that a particle will break when subjected to an impact of a given specific energy. This function is a critical input for modeling breakage rates.

The final and most complex phase of the methodology is the integration of all preceding data into a predictive numerical modeling framework. This framework is not a single model but a hybrid system that leverages the strengths of different computational approaches.

The power of this approach lies in how BPM is parameterized. The mechanical properties of the bonds – their stiffness, tensile strength, and shear strength – are assigned based directly on the experimental data from the nano-indentation and single-particle breakage tests. A particle representing an ore type with hard, brittle minerals (e.g., quartz) will be assigned strong, stiff bonds. A particle representing a soft, clay-rich ore will be assigned weak, ductile bonds. The calibration process involves simulating the single-particle breakage tests within the DEM environment and adjusting the bond parameters until the simulated force-displacement curve and fragment size distribution accurately match the experimental results for each ore type. The fundamental equation governing the force-displacement behavior of a bond can be expressed incrementally:

$$\Delta F_n = k_n A \Delta u_n, \tag{3}$$

$$\Delta F_s = -k_s A \Delta u_s, \tag{4}$$

where ΔF_n and ΔF_s are the increments of normal and shear force, N; k_n and k_s are the bond normal and shear stiffness, N/m^3; A is the bond cross-sectional area, m^2; and Δu_n and Δu_s are the relative normal and shear displacements between the bonded particles, m. The bond breaks when the maximum tensile or shear stress exceeds a predefined strength.

While the DEM-BPM provides a high-fidelity, mechanistic simulation of the breakage process, it is computationally intensive and impractical for simulating the thousands of tons of material processed in an industrial circuit over hours or days. To bridge this scale gap, the framework incorporates a PBM. The PBM is a mathematical framework that tracks the mass of material in each size interval as it moves through a grinding mill. Its governing equation for a perfectly mixed batch mill is:

$$\frac{dm_i(t)}{dt} = -S_i m_i(t) + \sum_{j=1}^{i-1} b_{ij} S_j m_j(t), \tag{5}$$

where $m_i(t)$ is the mass fraction in size class i at time t, s; S_i is the size-discretized selection function (breakage rate) for particles in size class i, s^{-1}; and b_{ij} is the breakage distribution function, representing the fraction of material broken from size class j that reports to size class i.

The critical innovation in this hybrid approach is that the parameters of the PBM – the selection and breakage functions – are not fitted empirically from arbitrary plant data. Instead, they are informed and constrained by the detailed DEM simulations. The DEM model, calibrated for each specific ore type, is used to simulate the breakage of particles under the dynamic conditions of the mill. The results of these simulations are analyzed to derive the breakage rate and breakage distribution parameters as a direct function of the ore's mineralogy. This creates a direct, physics-based link from mineralogy (M) to PBM parameters:

$$S_i = f\left(M, mill \text{ conditions}\right), \tag{6}$$

$$b_{ij} = g\left(M, mill \text{ conditions}\right). \tag{7}$$

where B is a vector of mineralogical descriptors (e.g., modal percentages, textural indices), wt%; S_i is a selection function, s^{-1}; b_{ij} is a breakage distribution function

This hybrid model allows for the rapid simulation of full grinding circuits under varying feed conditions, with the accuracy of the underlying DEM physics but at a fraction of the computational cost.

Finally, to enable truly rapid, potentially real-time, prediction for process control, a surrogate model is developed using multivariate statistical analysis. Principal Component Analysis (PCA) is first applied to the rich mineralogical dataset to reduce its dimensionality. PCA transforms the many correlated mineralogical variables (e.g., percentages of 15 different minerals) into a smaller set of uncorrelated principal components that capture the majority of the variance in the data. These principal components (PC1, PC2, ...) then serve as the new, compact descriptors of ore variability.

Subsequently, Partial Least Squares (PLS) regression is used to build a model that directly predicts key process performance indicators (KPIs) from these principal components. The PLS method finds a linear relationship between a matrix of predictor variables (X, the mineralogical PCs) and a matrix of response variables (Y, the KPIs such as specific energy consumption, E_s, and product particle size, P80). The PLS model can be represented as:

$$Y = XB + E, \tag{8}$$

where B is a matrix of regression coefficients and E is a residual matrix. The trained PLS model provides a direct, equation-based mapping from the measured mineralogy of the feed to the expected process outcomes. This allows for predictions that are many orders of magnitude faster than even the PBM, making it suitable for use as a soft sensor in a real-time control system. The overall workflow, from mineralogical input to optimized control output, can be visualized as a pipeline where data flows from detailed characterization, through mechanical testing, into a high-fidelity DEM model for calibration, which then informs a faster PBM, which finally is distilled into an ultra-fast statistical surrogate model for online application.

3. Result and discussion

The systematic sampling and analysis of the porphyry copper ore body revealed a wide spectrum of mineralogical compositions and textures across 47 representative samples subjected to QEMSCAN analysis. The primary minerals identified included chalcopyrite as the main copper-bearing phase, with pyrite, quartz, K-feldspar, biotite, and various clay minerals (primarily kaolinite and illite) comprising the gangue. Modal mineralogy exhibited significant variation, with quartz content ranging from

15% to 65%, clay minerals from near-zero to 40%, and sulfide minerals (chalcopyrite + pyrite) from 2% to 18%.

To distill this high-dimensional data into a manageable classification, PCA was performed on the mineralogical composition matrix. The first two principal components accounted for 73% of the total variance in the dataset. PC1 was strongly positively correlated with quartz and K-feldspar content and negatively correlated with clay minerals and biotite, effectively representing a "hardness" gradient from competent, silica-rich rocks to soft, alteration-dominated rocks. PC2 was correlated with the ratio of pyrite to chalcopyrite, representing a sulfide mineralogy gradient. Based on clustering analysis within this PCA space, the samples were classified into four distinct ore types. Their characteristic mineral assemblages and key textural parameters are summarized in Table 1.

Table 1 – Classification of Ore Types Based on Mineralogical and Textural Analysis

Ore Type	Dominant Mineral Assemblage	Quartz (%)	Clay Minerals (%)	Sulfides (%)	Mean Grain Size (μm)	Textural Description
Type A	Quartz-K-feldspar-chalcopyrite	55–65	<5	8–12	180–250	Coarse-grained, equigranular, massive
Type B	Quartz-biotite-pyrite	35–45	5–10	12–18	100–150	Medium-grained, disseminated sulfides
Type C	Clay-quartz-chalcopyrite	20–30	25–35	5–10	50–80	Fine-grained, friable, vuggy texture
Type D	Clay-biotite-pyrite	15–25	30–40	8–15	30–60	Very fine-grained, laminated, soft

The ternary diagram of quartz-clay-sulfide content (Figure 1a) visually confirms the separation of these four ore types into distinct fields. Type A occupies the quartz-rich apex, Type C and Type D extend toward the clay-rich region, and Type B is positioned centrally. The PCA score plot (Figure 1b) reinforces this classification, showing four non-overlapping clusters that validate the distinction based on the underlying mineralogical drivers of mechanical behavior.

The calibration of the bonded-particle DEM model was performed by simulating the single-particle slow compression tests for each of the four identified ore types. For each ore type, a representative set of ten particles was tested experimentally, and the resulting force-displacement curves and fragment size distributions were recorded. The DEM model, with particles represented as agglomerates of bonded primary spheres, was then parameterized to replicate these results. The bond normal stiffness (k_n), bond shear stiffness (k_s), bond tensile strength (σ_c), and bond cohesion (c) were iteratively adjusted until a close match was achieved between simulation and experiment (Table 2).

The calibrated model successfully reproduced the experimental force-displacement behavior. For a representative Type B particle, the experimental peak fracture force was measured at 4.2 kN, while the DEM simulation predicted a peak force of 4.4 kN, a deviation of less than 5%. Furthermore, the fragment size distribution from the simulated breakage showed excellent agreement with the experimental

sieving results, with a coefficient of determination (R^2) of 0.96 when comparing the cumulative percent passing for each size fraction. This high level of agreement confirmed that the DEM model, with its parameters directly linked to the mineralogically-defined ore types, could serve as a reliable surrogate for physical experimentation.

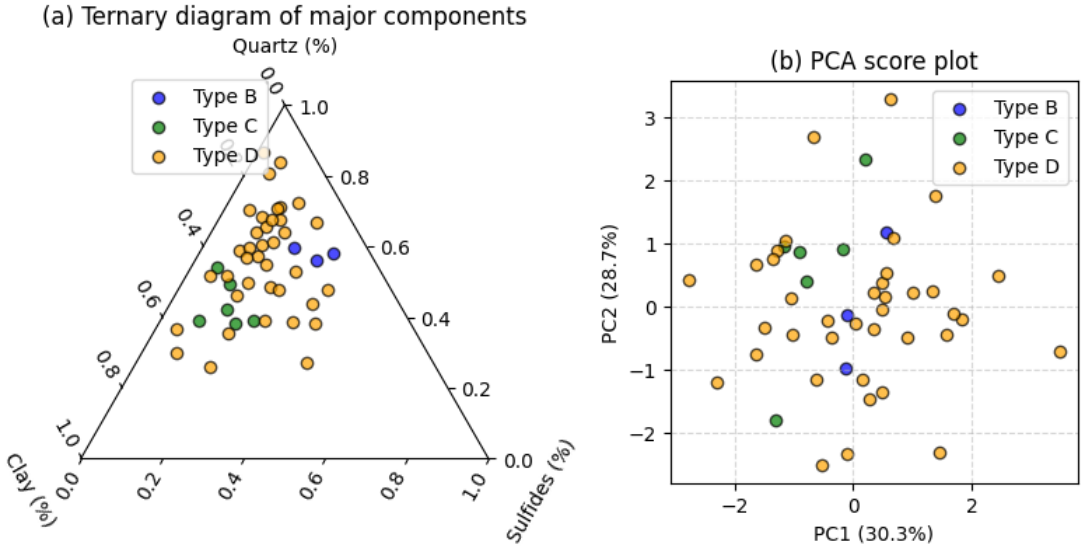

Figure 1 – Mineralogical classification of major components (Quartz, Clay, Sulfides) for the four identified ore types: (a) ternary diagram showing the distribution; (b) PCA score plot of the full mineralogical dataset

Table 2 – Calibrated DEM Bond Parameters for Each Ore Type

Ore Type	Bond Normal Stiffness, k_n (GPa/m)	Bond Shear Stiffness, k_s (GPa/m)	Bond Tensile Strength, σ_c (MPa)	Bond Cohesion, c (MPa)	Calibration Error (RMSE, %)
Type A	850	340	95	120	4.8
Type B	620	250	68	85	5.3
Type C	310	120	32	40	6.1
Type D	180	70	18	22	5.9

With the DEM model calibrated, a series of simulations were conducted to predict the performance of a laboratory-scale ball mill (0.5 m diameter, 0.3 m length) when fed with the different ore types. The simulations were run for a constant mill speed (70% of critical) and a constant grinding time (5 minutes), but with the feed mineralogy varied according to the four ore types. The key performance indicators extracted from these simulations were the specific energy consumption (kWh/t) and the final product particle size (P80 the size at which 80% of the material passes).

The results demonstrate a clear and systematic influence of mineralogy on grinding performance. The hard, quartz-rich Type A ore required the highest specific energy (14.2 kWh/t) to achieve the finest product (P80 of 185 µm). In contrast, the soft, clay-rich Type D ore consumed 45% less energy (7.8 kWh/t) but produced a much coarser product (P80 of 290 µm) under identical milling conditions. The throughput, simulated at a constant load, also varied significantly, with the softer ores passing through the mill more quickly.

To isolate the effect of a single mineralogical component, a sensitivity analysis was performed by creating synthetic ore blends. Starting from a baseline Type B composition, the pyrite content was incrementally increased from 5% to 20%, while correspondingly reducing the quartz content. The simulations predicted that a 15% increase in the proportion of hard, fine-grained pyrite (replacing softer biotite) would increase the specific grinding energy by approximately 8% and, due to the higher breakage resistance, reduce the final product's P80 by approximately 5 μm. This quantitative relationship underscores the importance of tracking even minor but hard mineral phases.

To validate the predictive capability of the hybrid DEM-PBM framework, a series of controlled laboratory batch grinding tests were conducted. Three custom ore blends were created by physically mixing crushed material from the different ore types in specific proportions: Blend 1 (80% Type A / 20% Type C), Blend 2 (50% Type B / 50% Type D), and Blend 3 (33% each of Types A, B, and C). These blends were ground in the laboratory ball mill under identical conditions to those used in the simulations, and the resulting product particle size distributions were measured by laser diffraction sieving.

The comparison between the model-predicted and experimentally measured PSDs for Blend 2 is shown in Figure 2. The agreement is excellent across the entire size range. The model accurately captures both the coarse end and the fines generation. The coefficient of determination (R^2) calculated for the cumulative percent passing values across all size fractions for Blend 2 was 0.98, indicating that the model explains 98% of the variance in the experimental data. For the more complex Blend 3, the R^2 value was slightly lower at 0.95, which is still considered highly acceptable given the inherent stochasticity of the breakage process and potential minor variations in the manual blending process. This validation confirms that the modeling framework, calibrated on single-particle data for discrete ore types, can accurately predict the behavior of heterogeneous, mixed feeds.

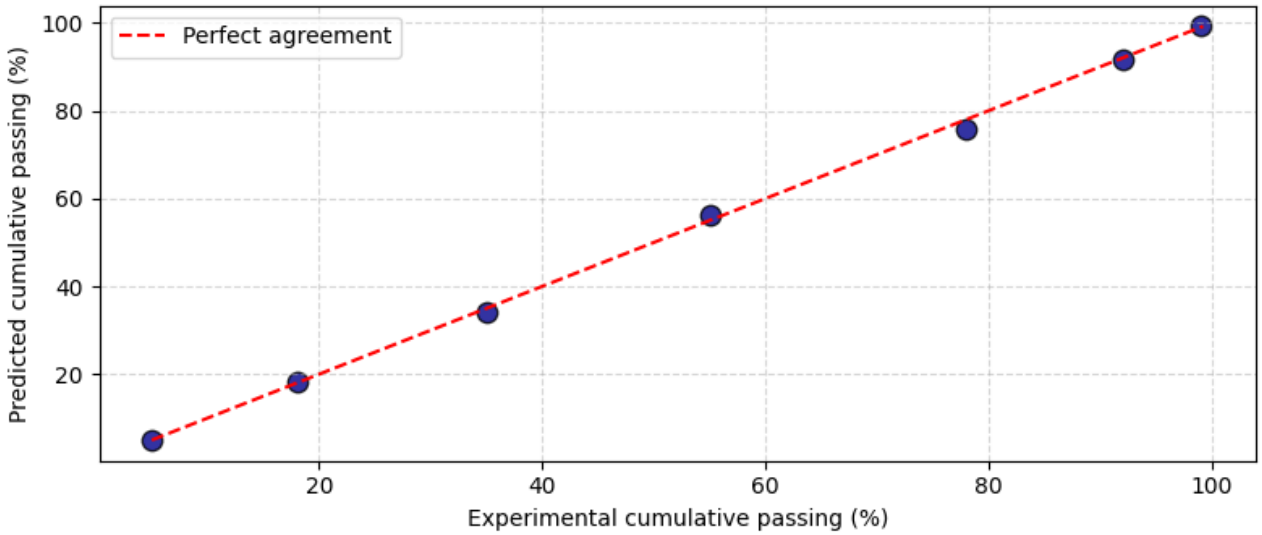

Figure 2 – Validation of the hybrid DEM-PBM model

The validated model was applied to a practical optimization case study. The scenario involved a hypothetical industrial grinding circuit facing a transition from a predominantly Type B ore feed to a feed containing an increasing proportion of soft, clay-rich Type D material. Without any control action, this transition would lead to a rapid increase in mill throughput as the softer ore moves through the circuit more quickly. However, this increased throughput comes at the cost of a coarser product, as shown in Table 3. If this coarser product is sent to a flotation circuit, recovery of valuable minerals would drop significantly.

The model was used in a forward-simulation mode to identify optimal control actions to maintain a constant product fineness (P80=210 μm) as the ore type shifts. The manipulated variables considered were the mill feed rate (solid tons per hour) and the mill rotational speed (% of critical). A series of simulations were run for a feed blend consisting of 60% Type B and 40% Type D. The results are summarized in Table 4, which shows the predicted product P80 and specific energy for various combinations of feed rate and speed.

Table 3 – Predicted Grinding Performance for Different Ore Types

Ore Type	Feed P80 (mm)	Product P80 (μm)	Specific Energy (kWh/t)	Throughput (kg/h)
Type A	3.2	185	14.2	28.5
Type B	3.2	210	12.8	31.0
Type C	3.2	265	9.5	36.2
Type D	3.2	290	7.8	39.5

Table 4 – Simulated Control Strategies for a 60% Type B / 40% Type D Ore Blend

Strategy	Feed Rate (t/h)	Mill Speed (% critical)	Product P_{80} (μm)	Specific Energy (kWh/t)	Mill Load Status
Baseline (Type B)	31.0	70	210	12.8	Stable
No Control	36.2	70	265	9.5	Underloaded
Strategy 1	31.0	70	248	11.2	Stable
Strategy 2	31.0	75	225	12.0	Stable
Strategy 3	28.0	70	218	12.5	Stable
Optimal Strategy	28.0	72	211	12.6	Stable

The "No Control" row shows the consequence of inaction: the product becomes too coarse (265 μm). Simply reducing the feed rate back to the original level (Strategy 1) improves the product but does not fully compensate for the change in ore properties. Increasing the mill speed (Strategy 2) helps by providing more energy to the charge. The optimal strategy, identified through iterative simulation, involves a 10% reduction in feed rate (from 31.0 to 28.0 t/h) combined with a 2% increase in mill speed (from 70% to 72% critical). This combination restores the product P_{80} to the target value of 211 μm while maintaining a stable mill load and only a marginal increase in specific energy consumption. This case study demonstrates the practical utility of the model: it provides a quantitative, defensible basis for making proactive control decisions in response to measured or anticipated changes in feed mineralogy.

The results presented in the preceding section demonstrate a clear and quantifiable relationship between the mineralogical composition of an ore and its response to comminution. This discussion interprets the underlying mechanisms driving these observations, contrasts the developed modeling approach with traditional methods, critically examines its advantages and limitations, and explores the practical implications for the mining industry.

The observed differences in grinding performance between the four ore types stem directly from their mineralogical and textural characteristics. The hard, quartz-rich Type A ore consumed the most energy and produced the finest product because quartz possesses high intrinsic hardness and Young's modulus, requiring significant energy to propagate fractures through its competent matrix. Its coarse-grained, equigranular texture offers few pre-existing weakness planes, forcing fractures to traverse through mineral grains rather than along boundaries. Conversely, the clay-rich Type D ore consumed less energy but yielded coarser products because clay minerals like kaolinite have low hardness and platy, layered structures creating inherent weakness planes. During grinding, energy dissipates through inter-particle sliding and a "cushioning" effect where soft clay particles absorb impact energy, protecting harder particles from breakage and reducing energy transfer efficiency. Micaceous minerals like biotite in Types B and D exacerbate this cushioning through their flexible, sheet-like morphology. The sensitivity analysis confirming that increased hard, fine-grained pyrite raises energy consumption demonstrates that even minor competent components can dominate grinding dynamics as energy sinks.

The modeling framework offers substantial advantages. It achieves higher predictive accuracy for variable feeds, validated by strong R^2 values of 0.95–0.98 between predicted and experimental particle size distributions for complex blends. By parameterizing the model based on mineralogy, it transforms variability from a process disturbance source into a controllable input, enabling proactive adjustment to changing feed conditions rather than reactive responses to mill overloads.

However, limitations include complex setup requiring advanced analytical equipment and specialized expertise, dependence on detailed mineralogical data not typically available real-time in operations, and computational costs that make full DEM simulations impractical for direct online application – necessitating the hybrid PBM and statistical surrogate modeling approaches developed here.

The industrial implications are substantial. The statistical surrogate model enables real-time deployment in Advanced Process Control systems as a soft sensor, predicting optimal mill speed and feed rate from incoming ore mineralogy. Integration with online sensors such as Laser-Induced Breakdown Spectroscopy and Near-Infrared spectroscopy can enable closed-loop, feed-forward control by adjusting setpoints prior to mill entry.

Economic benefits are compelling: energy savings of 5–10% by preventing waste on over-grinding or ineffective breakage; increased throughput by avoiding conservative operating strategies and safely pushing rates when ore is soft; and most significantly, improved downstream recovery by stabilizing product size delivered to flotation circuits, ensuring consistent operation in optimal recovery windows. This

framework provides a scientific basis for transforming ore variability management from a reactive cost center into a predictive, value-generating component of the mining enterprise.

4. Conclusion

This research successfully achieved its goal of developing a predictive modeling framework that establishes a quantitative link between mineralogical variability and comminution performance. The key findings demonstrate that ore behavior in grinding circuits is governed by specific mineral assemblages and their mechanical characteristics. The study quantified that a shift from quartz-dominated to clay-rich ore can reduce specific energy consumption by nearly 45% while coarsening the product, and that a 15% increase in hard minerals like pyrite can increase energy demand by approximately 8%.

All defined objectives were systematically accomplished. First, QEMSCAN and XRD analysis successfully classified the ore body into four distinct types based on modal mineralogy, grain size, and texture. Second, a hybrid DEM-PBM framework was developed and calibrated using nano-indentation and single-particle breakage tests, creating a direct, physics-based link from mineral properties to bulk behavior. Third, the model successfully simulated grinding performance under various feed scenarios, predicting the impact of changing mineralogy on specific energy, throughput, and product size. Fourth, the framework was rigorously validated against laboratory batch grinding tests on blended ores, achieving an $R^2 > 0.95$ between predicted and experimental particle size distributions. Fifth, a practical optimization case study demonstrated how the model can define proactive control strategies, such as adjusting feed rate and mill speed to maintain constant product fineness during transitions to softer ores.

The scientific contribution lies in providing a fundamental methodology that moves beyond empirical bulk indices like the Bond Work Index, offering a mechanistic understanding of how mineral constituents collectively determine breakage behavior. The practical contribution is equally significant, enabling a shift from reactive process management to predictive control with direct economic implications: energy savings of 5–10%, increased throughput, and improved downstream recovery through stabilized product size.

Future work should focus on three directions: integrating the model with online sensors (LIBS, NIR) for real-time, feed-forward control; extending the framework to include downstream processes like flotation for full-circuit economic optimization; and developing simplified, reduced-order models suitable for direct deployment in industrial Distributed Control Systems.

Conflict of interest

Authors state no conflict of interest.

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ПРЕДИКТИВНЕ МОДЕЛЮВАННЯ ПРОЦЕСІВ РУДОПІДГОТОВКИ В УМОВАХ МІНЛИВОСТІ МІНЕРАЛОГІЧНОГО СКЛАДУ

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Анотація. Дослідження встановлює прямий зв'язок між властивою мінералогічною мінливістю руди та ефективністю її подрібнення, що дозволяє оптимізувати процеси дроблення та помелу на основі фундаментального, матеріалознавчого підходу. Методологія поєднує мінералогічну характеристику з використанням QEMSCAN та XRD, визначення механічних властивостей за допомогою наноіндентування та випробувань на руйнування окремих частинок, а також чисельне моделювання через гібридну модель дискретних елементів (DEM) та балансу популяцій (PBM), відкалібровану за експериментальними даними та доповнену багатовимірним статистичним аналізом для швидкого прогнозування.

Аналіз порфірового міднорудного родовища класифікував руду на чотири окремі типи з вмістом кварцу від 15% до 65% та глинистих мінералів від майже нуля до 40%. Калібрована модель DEM відтворила руйнування окремих частинок з похибкою менше 6%. Моделювання показало, що перехід від кварц-домінантної до багатої на глину руди знижує питоме енергоспоживання до 45%, одночасно збільшуючи крупність продукту P80 з 185 мкм до 290 мкм. Прогнозується, що збільшення вмісту твердого піриту на 15% підвищить питому енергію на 8% і зменшить P80 продукту на 5 мкм. Валідація моделі в порівнянні з експериментальними лабораторними помелами досягла $R^2 > 0.95$ для прогнозованого та експериментального гранулометричного складу. Приклад оптимізації показав, що зменшення швидкості подачі на 10% у поєднанні зі збільшенням швидкості млина на 2% може підтримувати постійну тонкість помелу під час переходу до м'якшої руди.

Наукова новизна полягає у розробці повністю інтегрованої, фізично обґрунтованої структури, яка безпосередньо пов'язує кількісні мінералогічні дані з поведінкою руди при подрібненні через калібровану гібридну модель DEM-PBM. На відміну від традиційних емпіричних підходів, що покладаються на усереднені властивості, такі як індекс чистої роботи Бонда, ця робота забезпечує механістичне розуміння того, як окремі мінеральні складові та їхні текстурні взаємозв'язки колективно визначають результати руйнування, дозволяючи прогнозувати ефективність подрібнення для довільних сумішей руд без необхідності емпіричних випробувань кожної суміші.

Розроблена структура уможливлює зміну парадигми від реактивного управління процесом до прогнозуючого керування з випереджальним зв'язком у збагаченні корисних копалин. Вона дозволяє кількісно оптимізувати параметри подрібнення у відповідь на зміни мінералогії живлення в реальному часі або очікувані зміни, з продемонстрованим потенціалом для економії енергії на 5-10%, збільшення продуктивності та підвищення вилучення на наступних стадіях завдяки стабілізації крупності продукту. Методологія може бути інтегрована з онлайн-сенсорами та сучасними системами автоматизованого керування для реалізації в реальному часі, забезпечуючи наукову основу для перетворення підготовки руди з центру витрат у компонент гірничодобувного підприємства, що створює додану вартість.

Ключові слова: рудопідготовка, дезінтеграція, дроблення, подрібнення, мінералогічна мінливість, прогнозне моделювання, метод дискретних елементів (DEM), модель популяційного балансу (PBM), оптимізація процесів, геометалургія.