High-Throughput Bauxite Characterization and Process Monitoring via Automated QXRD Integrated with Cluster Analysis and PLSR Modelling

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https://doi.org/10.71659/icsoba2025-bx010

Abstract

The aluminium industry faces growing challenges due to declining bauxite grades, compositional variability, and the demand for sustainable refining. This study demonstrates a fully automated, high-throughput XRD workflow using Malvern Panalytical's Aeris (Minerals Edition) compact diffractometer for mineralogical and process-oriented characterization of bauxite and red mud, integrating Rietveld refinement, cluster analysis, and Partial Least Squares Regression (PLSR). Besides enabling mineralogical discrimination between lateritic bauxite, karstic-diasporic types, and red mud- critical for Bayer feed quality assessment, residue valorisation, and environmental risk mitigation- the method also identified five distinct subtypes within the lateritic group. These were defined by diagnostic mineralogical profiles (e.g., gibbsite-rich, kaolinite-dominant, high-iron, boehmitic), each linked to specific digestion strategies. Amorphous content was quantified using a corrected external standard approach, and kaolinite crystallinity (via FWHM of the 001 reflection) was evaluated as an indicator of silica reactivity.

PLSR models trained on full-pattern XRD data demonstrated excellent predictive power for Total Extractable Alumina, Total Al_2O_3, Reactive Silica, and LOI, with R^2 values ranging from 0.989 to 0.999, minimal bias, and strong agreement with reference data across all parameters. This integrated approach enables simultaneous extraction of mineralogical and compositional parameters within minutes, providing a robust decision-support tool for ore classification, blending, and Bayer process optimization – especially for complex and low-grade bauxites.

Keywords: Quantitative XRD, Bayer process parameters, kaolinite crystallinity, amorphous content, HighScore Plus.

1. Introduction

Bauxite, the principal ore of aluminium, is geologically diverse and mineralogically complex. It primarily contains aluminium hydroxide minerals – gibbsite [$Al(OH)_3$], boehmite [γ-AlO(OH)], and diaspore [α-AlO(OH)] – alongside iron oxides (goethite, hematite), silica (mainly as kaolinite and quartz), and titanium-bearing phases such as anatase and rutile [1]. This variability critically influences grade classification and processing performance, directly affecting digestion efficiency, caustic soda consumption, desilication product (DSP) formation, and red mud generation during the Bayer process [2].

As global aluminium demand grows – driven by its lightweight, corrosion-resistant properties and broad industrial use – bauxite mining and alumina refining face increasing pressure to enhance efficiency, reduce waste, and meet environmental regulations. These challenges are compounded by declining ore grades, greater feed variability, and the need for improved residue management.

Conventional grade control methods like X-ray fluorescence (XRF) provide elemental data but limited insight into mineralogical phases that govern reactivity. The form of alumina phases and the presence of reactive silicates such as kaolinite strongly influence the choice of digestion temperature (which depends on the dominant aluminium-bearing mineral in the bauxite), caustic loss, and red mud characteristics. Bauxites with high reactive silica (> 8.0 wt%) are often uneconomical due to excessive soda loss and DSP formation [3].

To overcome these limitations, X-ray diffraction (XRD), especially with Rietveld refinement and multivariate analysis, has become vital for bauxite quality assessment. XRD enables the identification and quantification of both crystalline phases (via the Rietveld method) and amorphous content (via calibration), allowing accurate estimation of process-critical parameters such as the Total Extractable Alumina (TEA) and reactive silica. The mineralogical composition also guides digestion strategy; for example, gibbsite-rich bauxites are typically digested at 150 °C, while those containing significant boehmite require higher temperatures, generally 225 °C.

Recent advances in detector technology, low-power instruments, and high-throughput handling have improved the speed, precision, and sustainability of XRD, making it suitable for both mine-site screening and in-plant control. Comprehensive mineralogical profiling also aids in identifying by-products such as iron, titanium, and gallium. This article discusses bauxite's mineralogical complexity, its impact on the Bayer process, and the increasing role of XRD in enabling efficient, sustainable alumina production.

2. Materials and Methods

This study refines a methodology originally established in 2012 [4], which demonstrated the use of rapid X-ray diffraction (XRD) and cluster analysis for fast mineralogical grade control of bauxite based on Rietveld quantification [5] and calculated process parameters including the TEA and reactive silica. Building on this foundation, we incorporated advancements in quantitative XRD (QXRD), Rietveld refinement strategies, and multivariate statistical tools to enhance scalability and accuracy. The updated workflow was applied to a dataset of 40 industrial samples and 10 certified reference materials from NIST and ALCAN. As industrial bauxites are commonly blended ores tailored to meet specific grade specifications, the use of certified standards with well-defined mineralogy is critical – they act as anchors for model calibration and validation, ensuring reliable quantification across diverse compositions. All samples were prepared using automated milling and pressing to ensure consistency and reproducibility. Notably, gibbsite quantification may be affected by preferred orientation due to its platy morphology, potentially leading to overestimation. While careful sample preparation helps minimize this effect, minor bias may persist.

In addition, the abovementioned samples, a larger dataset of 110 bauxite mining samples, with complementary chemical reference data, was used to explore the potential of Partial Least Squares Regression (PLSR) calibration in HighScore Plus for predicting key compositional parameters.

2.1 System Features and XRD Measurements

XRD measurements were performed using the Aeris Minerals Edition compact diffractometer (Malvern Panalytical), equipped with a Co-anode tube (40 kV, 15 mA), 145 mm goniometer, and Bragg–Brentano geometry. A high-capacity sample changer (HCSC, 67 positions) enabled high-throughput analysis. Detection was carried out using the 1Der energy-resolving detector, which provides automatic control of the energy window, allowing fluorescence-free, high-resolution data acquisition without the need for Kβ filters. This is particularly advantageous for compositionally complex samples like bauxite that commonly contain amorphous and/or disordered phases. While Co radiation was used in this study, the system also supports the use of

Cu radiation on Fe-rich materials without requiring fluorescence suppression optics, enabling a unified XRD setup from bauxite to aluminium analysis, consistent with literature practices. The XRD scans were collected from 9° to 70° 2θ with 0.027° steps and 32.5 s per step (~10 min per sample), producing net peak intensities >10,000 counts and an average signal-to-noise ratio (SNR) of ~1880—well above thresholds required for confident phase identification and quantification.

2.2 Cluster Analysis and Rietveld Refinement Methods

To support mineralogical characterization across a large and compositionally diverse dataset, hierarchical cluster analysis was performed on 50 XRD scans, comprising 40 industrial bauxite samples and 10 certified reference materials (CRMs) from NIST and ALCAN. The analysis was conducted using HighScore Plus version 5.3, integrated with the ICDD PDF-5 database [6, 7]. The software's cluster analysis module calculates correlation distances between scans, applies agglomerative hierarchical clustering, and visualizes groupings via dendrograms. This enables automated grouping of compositionally similar samples, selection of representative patterns for Rietveld refinement, and the detection of compositional outliers.

Industrial bauxites, typically blended ores engineered to meet target grade specifications, often show inherent compositional variability. In contrast, certified standards are well-characterized, homogeneous materials. Including CRMs in the cluster analysis provides a dual benefit: it anchors the compositional space for meaningful grouping and enables validation of the Rietveld quantification model by comparing calculated mineral contents to known reference values.

2.3 Partial Least Squares Regression Calibration

Partial Least Squares Regression (PLSR), developed by Wold [8], is a multivariate statistical method that predicts properties directly from complex raw data. It establishes a relationship between a known property (Y) and a multivariable data matrix (X) that captures both systematic (e.g., compositional) and non-systematic (e.g. grain size, impurities) variations. In XRD, PLSR uses a full-pattern approach, analysing the entire diffractogram independent of peak shape to identify predictive trends. HighScore Plus implements the SIMPLS algorithm with semi-automated model evaluation and optimization. Two scaling options are available, “centre” (mean subtraction) and “standardize” (mean subtraction and division by standard deviation), to efficiently reveal hidden correlations and identify key factors contributing to group discrimination within the dataset. Model accuracy is commonly assessed using cross-validation, where each sample is predicted after being left out of the calibration set, yielding a root mean square error of prediction (RMSEP). Nonetheless, external validation with independent samples remains the most robust method to evaluate model performance [9]. In this study, PLSR was employed to estimate Bayer process critical parameters such as the TEA and Loss on Ignition (LOI) from the XRD patterns.

2.4 Crystallinity Assessment by XRD

To evaluate kaolinite crystallinity and its potential influence on Bayer process performance, X-ray diffraction (XRD) was used following the method of Amigó et al. [10], as reviewed by Aparicio and Galán [11]. Crystallinity was assessed by measuring the Full Width at Half Maximum (FWHM) of the 001 reflection near 14.3° 2θ (CoKα radiation), with narrow peaks (FWHM < ~ 0.3°) indicating well-ordered structures and broader peaks (FWHM > ~ 0.4°) reflecting structural disorder due to stacking faults and interlayer disruption. A total of 50 reference and industrial bauxite samples were analyzed. For each sample, key peak parameters-including 2θ position, FWHM, peak area, height, background level, and signal-to-noise ratio (SNR)- were extracted for comparative analysis.

This assessment demonstrated that the kaolinite crystallinity within the dataset varied widely (Table 1). Well-ordered kaolinite (e.g., NIST-69b) showed sharp 001 reflections with high SNR, while structurally disordered samples (e.g., Alcan-BXT-05) exhibited broad, low-intensity peaks (FWHM > 1.0°). These differences are functionally relevant, as lower kaolinite crystallinity correlates with higher reactivity during Bayer digestion, resulting in increased silica dissolution, DSP formation, and soda consumption. While peak broadening is primarily linked to crystallographic disorder, potential overlap with associated phases such as halloysite, amorphous silica, or chlorite should be considered when interpreting results.

2.5 Quantification of Amorphous Content by XRD

XRD detects only crystalline phases, so undetected amorphous content leads to overestimation of crystalline phases in Rietveld refinement unless corrected. Given the growing recognition of amorphous phases in bauxite and red mud as key process variables, their accurate quantification is essential. To evaluate the consistency and reliability of quantifying amorphous content, three 100 % crystalline standards, α-Al_2O_3 (corundum), ZnO (zincite), and TiO_2 (rutile) were tested using internal and external standard methods. The internal method involved mixing 20 wt% of each standard with the sample, while the external method used separately measured standards to calculate a K-factor. As shown in Table 1, all internal standard results showed higher amorphous content than external estimates due to matrix absorption effects not accounted for in the default external method. While more accurate, the internal standard method is impractical for routine use due to its cost and complex preparation. To improve the reliability of the external method, a custom mass absorption coefficient (MAC, 52.7 cm^2/g), calculated as the weighted average of the MAC values of all constituent oxides in the bauxite sample, was applied to correct for matrix absorption effects. Amorphous content in bauxite samples was then quantified using this corrected external approach with an α-Al_2O_3 pressed pellet prepared and measured under the same conditions as samples, ensuring fair comparison.

Table 1. Amorphous content in bauxite determined using internal and external standard methods with three crystalline references.

	Internal standard	External Standard	External standard with custom MAC* = 52.7
Al_2O_3	33	25.2	27.9
ZnO	30	23.1	25.9
TiO_2	26.4	19.9	22.8

* Mass Absorption Coefficient.

3. Results and Discussion

3.1 Mineralogical Characteristics of Various Bauxite Types and Residue by QXRD

The extended cluster analysis (Figure 1) grouped the 50 studied samples – 40 industrial bauxites and 10 CRMs – into five compositionally distinct clusters and one outlier. These groupings, supported by QXRD-derived mineralogical profiles and Bayer process parameters, form the basis for assessing refining performance. To improve the reliability of trace phase reporting, Phase Guard filtering was applied in HighScore Plus. Phases with a SNR < 7 at their primary peak were set to zero, minimizing the risk of false positives caused by background noise or spectral compensation artifacts – a common issue in low-abundance phase detection in QXRD. Summary statistics for major mineral phases and key process parameters are provided in Table 2 and visualized in Figure 2. Variations in kaolinite crystallinity across clusters are illustrated in the box-and-whisker plots (Figure 3).

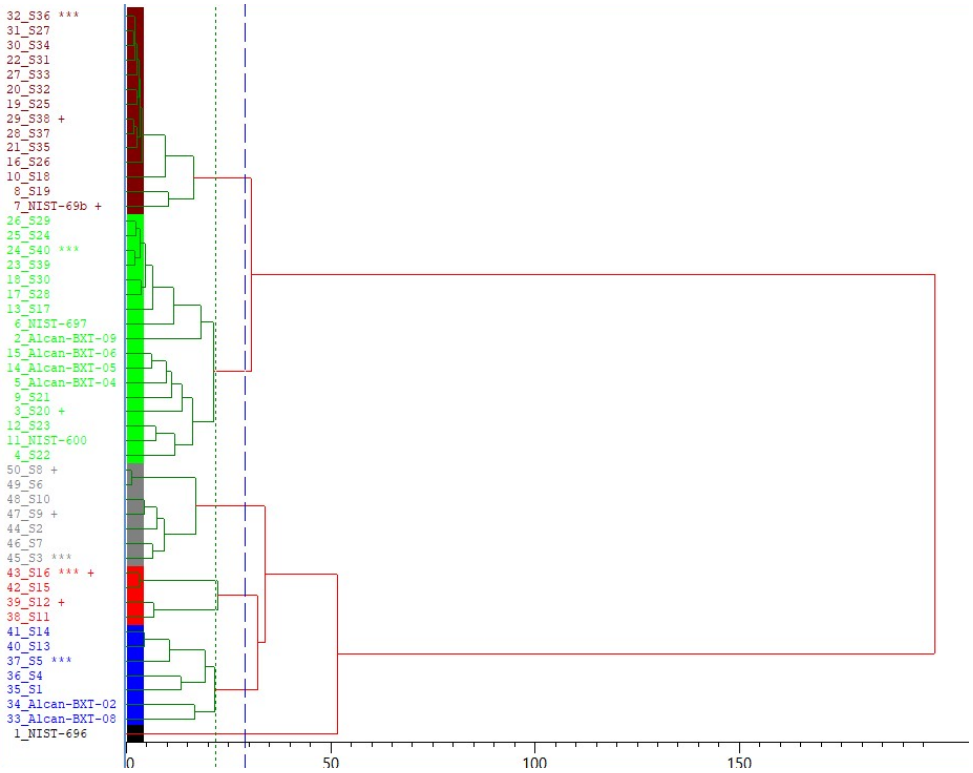


Figure 1. Dendrogram illustrating the results of extended cluster analysis performed on the XRD patterns of the 50 studied samples in HighScore Plus. The X-axis denotes the dissimilarity values of the tie bars, reflecting the degree of difference between clusters. The most representative scan within each cluster is marked with *.**

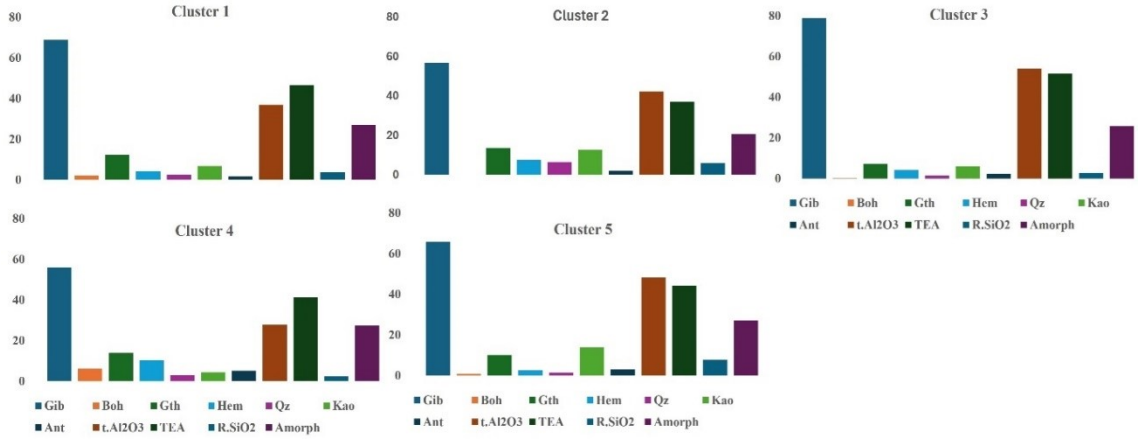


Figure 2. Histograms illustrating mean composition of different mineral phases and process parameters for the 5 identified clusters. Abbreviations are defined in Table 2.

3.1.1 Bauxite Types based on Cluster Analysis

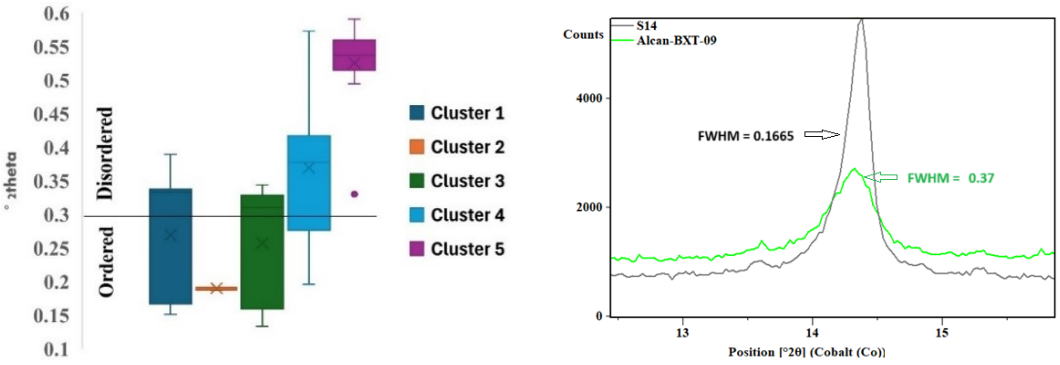
Bauxite suitable for low-temperature digestion - Clusters 1 and 3 represent high-grade, gibbsite-rich bauxites with low impurity levels. Cluster 3 (grey) contains the highest gibbsite concentrations (mean 78.7 wt%), minimal iron oxides, and moderate kaolinite with ordered structure, as confirmed by low FWHM values (Figure 3a). These characteristics point to excellent

digestibility at low temperatures (150 °C), high alumina recovery (TEA ≈ 51.5 wt%), and reduced DSP formation due to low reactive silica content (< 3.0 wt%). Cluster 1 (blue), while also gibbsite-dominant (68.8 wt%), shows slightly higher kaolinite and iron content, indicating comparable but slightly more variable performance. The presence of certified standards (Alcan-BXT-02, -08) within this cluster reinforces its industrial representativeness.

Bauxites requiring moderate to high-temperature digestion - Clusters 2 and 5 present more variable mineralogical compositions that influence digestion strategy. Cluster 2 (red) includes samples with moderate gibbsite (56.9 wt%), elevated kaolinite (12.8 wt%) – predominantly well-ordered – and significant hematite and goethite. These features suggest intermediate reactivity and the potential for higher soda consumption and DSP formation, particularly if kaolinite exceeds 12.0 wt%. Nonetheless, relatively low amorphous content (20.8 wt%) and high structural order favor predictable performance under controlled digestion conditions. Cluster 5 (purple) is defined by very high kaolinite content (mean 13.9 wt%) and consistently high amorphous fractions (~ 27.2–29.6 wt%). Crystallinity assessments (Figure 3a) confirm that kaolinite in this group is largely disordered, implying enhanced reactivity and increased silica solubility during digestion. While some samples (e.g., S27 to S38) show high gibbsite levels (> 70.0 wt%), the reactive silica burden and potential for DSP formation are also high ($R.SiO_2$ ≈ 7.8 wt%), requiring careful process control or blending strategies.

Challenging high-iron, high-temperature digestible bauxites - Cluster 4 (green) encompasses mineralogically complex bauxites with broad variability in gibbsite (39.0–72.0 wt%) and significant iron-bearing phases (goethite + hematite > 20.0 wt% in most samples). This group also contains the highest diversity in amorphous content (23.0–30.0 wt%) and frequent presence of disordered kaolinite. Certified boehmite-rich standards such as Alcan-BXT-09 and NIST-697 anchor this cluster, confirming its alignment with high-temperature digestion regimes (225 °C). These samples may require higher caustic dosages and generate more DSP, but also present potential for secondary iron or titanium valorisation.

High-grade reference outlier - NIST-696, identified as a compositional outlier (Cluster 0, black), contains 79.8 wt% gibbsite with minimal impurities and a stoichiometric alumina content (total Al_2O_3 = 54.6 wt%) in close agreement with its certified value (54.5 wt%). This sample serves as a high-grade benchmark for model validation and system calibration.



a) b)

Figure 3. a) Box-and-whisker plots of the FWHM of the primary kaolinite peak across sample clusters. FWHM > 0.3° indicates structural disorder; FWHM ≤ 0.3° reflects higher crystallinity. b) Peak broadening comparison in two samples illustrating crystallinity differences.

Table 2. Average QXRD results (wt.%) of major mineral phases for 50 studied bauxite samples. Process parameters including total alumina (t.Al_2O_3), total extractable alumina (TEA), and reactive silica (R.SiO_2) were derived from the phase composition using stoichiometric calculations. Amorphous content (Amorph) is also reported for each sample.

		Gib	Boh	Gth	Hem	Qz	Kao	Ant	t.Al_2O_3	TEA	R.SiO_2	Amorph
Cluster 1	mean	68.8	2.0	12.3	4.3	2.5	6.8	1.6	37.0	46.6	3.8	27.0
	SD	3.2	2.7	5.9	2.7	2.7	5.8	2.5	20.8	1.9	2.3	1.6
Cluster 2	mean	56.9	0.0	13.8	7.5	6.6	12.8	2.1	42.3	37.2	6.0	20.8
	SD	3.5	0.0	4.7	2.9	1.0	3.1	1.0	1.0	2.3	1.5	0.8
Cluster 3	mean	78.7	0.0	7.2	4.1	1.3	6.0	2.3	53.9	51.5	2.8	25.7
	SD	6.0	0.0	3.8	3.3	0.9	5.5	1.9	2.8	3.9	2.6	1.9
Cluster 4	mean	56.0	6.1	13.8	10.3	2.9	4.4	5.2	27.7	41.2	2.4	27.3
	SD	11.1	6.9	5.4	4.9	6.5	4.4	4.8	18.9	5.4	1.9	1.9
Cluster 5	mean	65.7	0.8	10.1	2.5	1.5	13.9	3.1	48.1	44.2	7.8	27.2
	SD	8.5	2.6	3.0	3.7	1.2	6.7	6.9	13.7	3.0	2.9	2.6
Outlier		79.8	0.05	8.02	2.4	1.13	0.09	6.0	2.13	52.2	2.81	25.6

Abbreviations: Gib – gibbsite; Boh – boehmite; Gth – goethite; Hem – hematite; Qz – quartz; Kao – kaolinite; Ant – anatase.

3.1.2 Diasporic Karstic Type Bauxite

Comparative mineralogical assessment is essential across different bauxite types – lateritic, karstic, and Tikhvin-type – since each represents distinct challenges in Bayer refining and residue management. Reliable phase quantification, as demonstrated here, is critical for tailoring digestion strategies, optimizing caustic consumption, and identifying opportunities for residue reuse. Figure 5 presents the Rietveld refinement of a diasporic karstic-type bauxite sample, showing a good fit (Rwp = 1.91) highlighting the reliability of quantification results. Diaspore dominates the composition (69.4 wt%), with significant hematite (9.9 wt%) and calcite (9.2 wt%), and minor phases including goethite, quartz, mica, kaolinite, and rutile. The high diaspore content indicates a requirement for high-temperature digestion, while the low quartz and moderate kaolinite levels suggest that reactive silica is likely manageable. Additionally, the presence of calcite may affect slurry behavior, contribute to pH buffering, and influence residue composition – potentially promoting the formation of Ca-bearing DSP phases.

Due to its low reactivity and complex composition, this type of bauxites (diasporic karstic) is often considered more suitable for construction and building materials, such as cement, pozzolanic binders, or geopolymers, than for economic alumina extraction via the Bayer process.

3.1.3 Red Mud

The composition of red mud is largely determined by the type of bauxite ore and the processing route. Residues from the Bayer process typically exhibit the highest concentrations of Fe_2O_3 and Al_2O_3. Accurate mineralogical characterization, particularly through quantitative X-ray diffraction (QXRD), is essential for assessing mud reuse potential and managing environmental risks.

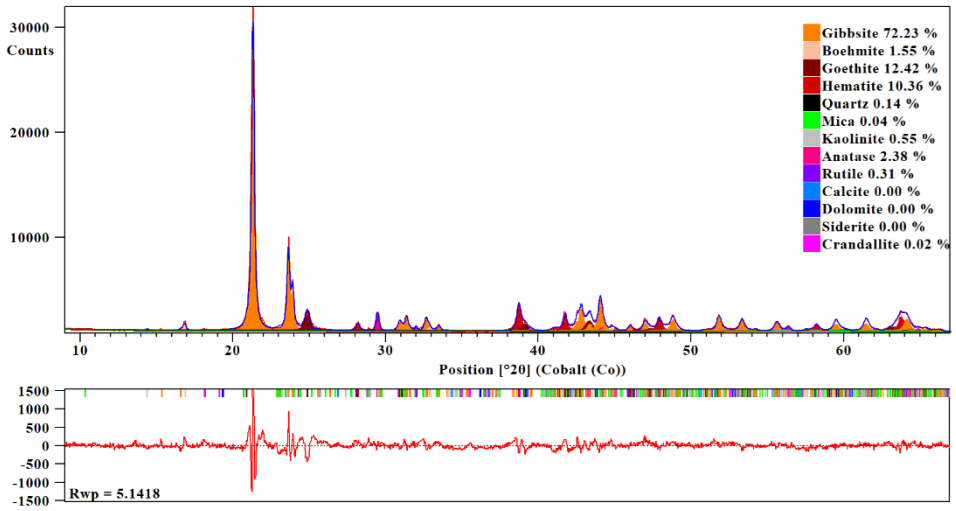


Figure 4. Quantitative XRD analysis conducted on a bauxite sample (Alcan-BXT-09), presenting the measured (pattern in red) and calculated patterns (pattern in blue) along with the difference plot (below) and the corresponding residual-weighted pattern (Rwp).

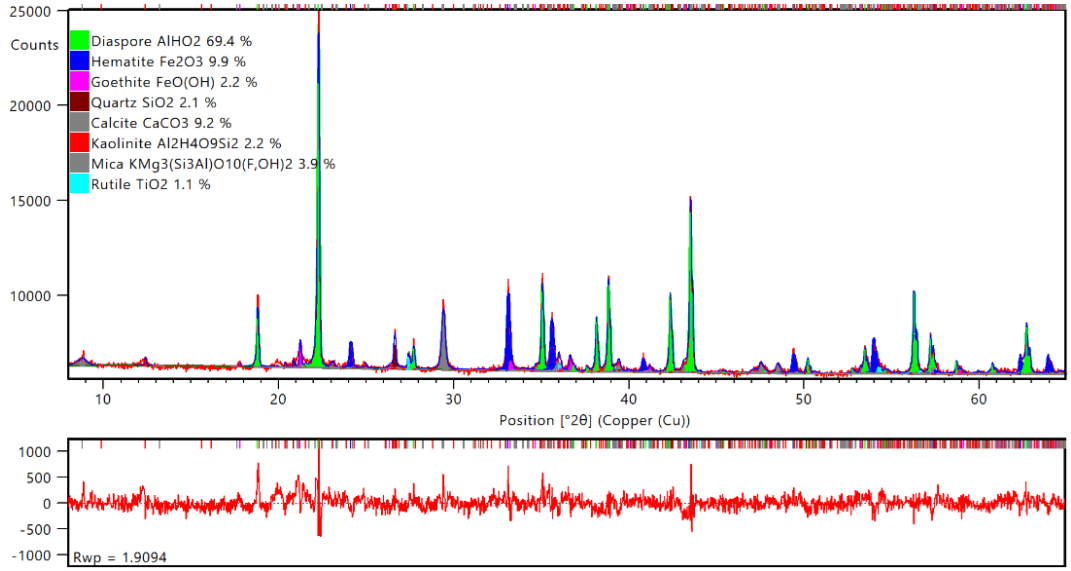


Figure 5. Quantitative XRD analysis conducted on a diasporic bauxite sample presenting the measured (pattern in red) and calculated patterns (pattern in blue) along with the difference plot (below) and the corresponding residual-weighted pattern (Rwp).

QXRD provides valuable insights into the efficiency of the Bayer process and the mineralogical complexity of the resulting residue. Figure 6 presents a representative example, showing a multi-phase assemblage dominated by quartz (28.0 wt%), Al-substituted goethite (26.2 wt%), and hematite (18.0 wt%). Alumina-bearing phases – including gibbsite (6.6 wt%), boehmite (4.1 wt%), goethite (3.6 wt%), and katoite (1.6 wt%) – collectively contribute 7.4 wt% Al_2O_3, which falls within the typical range (15.0–25.5 wt%) typically observed in red mud, depending on ore type and digestion conditions [11]. The pronounced quartz peak confirms the persistence of unreactive silica, while the abundance of Fe-oxyhydroxides indicates effective iron rejection with partial aluminium retention in iron-bearing phases.

This Si- and Fe-rich red mud is well suited for low-reactivity construction materials such as bricks, ceramic tiles, or blended cement, where its thermal stability, mechanical integrity, and pigmentation properties are advantageous despite limited pozzolanic activity [12].

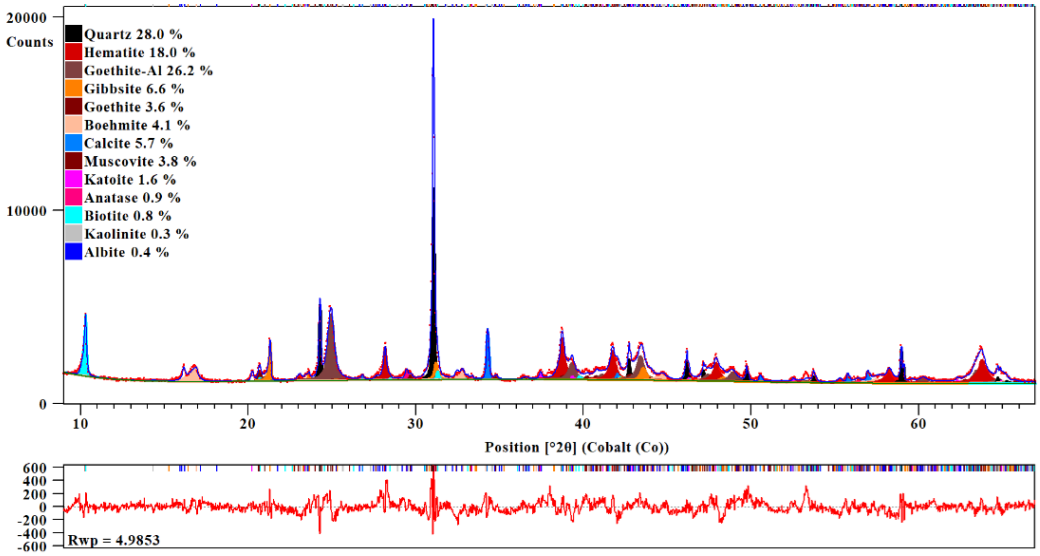


Figure 6. Quantitative XRD analysis conducted on a red mud sample presenting the measured (pattern in red) and calculated patterns (pattern in blue) along with the difference plot (below) and the corresponding residual-weighted pattern (Rwp).

3.2 Predictive Power of XRD-PLSR for Bayer-Relevant Parameters

To assess the suitability of XRD-based Partial Least Squares Regression (PLSR) for process-focused quality control, key chemical attributes of bauxite were predicted from 110 industrial XRD patterns. In the absence of replicate laboratory measurements to estimate the standard error of the reference laboratory method, 10% of the dataset withheld for external validation. While R^2 and RMSEP values were derived from the full dataset, model reliability was independently verified using this subset. Over 96% of predictions for the targeted process parameters fell within ±2 standard deviations of the reference values, and prediction errors remained within the typical repeatability range of industrial methods supporting the robustness of the model for routine use. The TEA represents the fraction of alumina readily soluble during Bayer digestion and is a key driver of process yield. The PLSR model exhibited an exceptional correlation with wet chemistry ($R^2 = 0.999$), indicating that the XRD patterns capture subtle features related to soluble Al-bearing phases such as gibbsite and boehmite. Additionally, total Al_2O_3, which encompasses both reactive and non-reactive fractions, was accurately predicted ($R^2 = 0.998$), confirming that the mineralogical features captured by XRD patterns are sufficient to approximate bulk chemical composition. Likewise, reactive silica, primarily associated with kaolinite, was well predicted ($R^2 = 0.997$) despite its typically low concentration. The LOI, representing volatiles from hydroxyl-bearing minerals and carbonates, also showed excellent agreement ($R^2 = 0.989$), further supporting the robustness of the approach. These results demonstrate that, while Rietveld-based quantification enables direct calculation of process parameters from phase abundances using stoichiometric formulas, PLSR offers a complementary approach by leveraging full-pattern statistical correlations—enhancing the utility of XRD in routine bauxite monitoring and process decision-making.

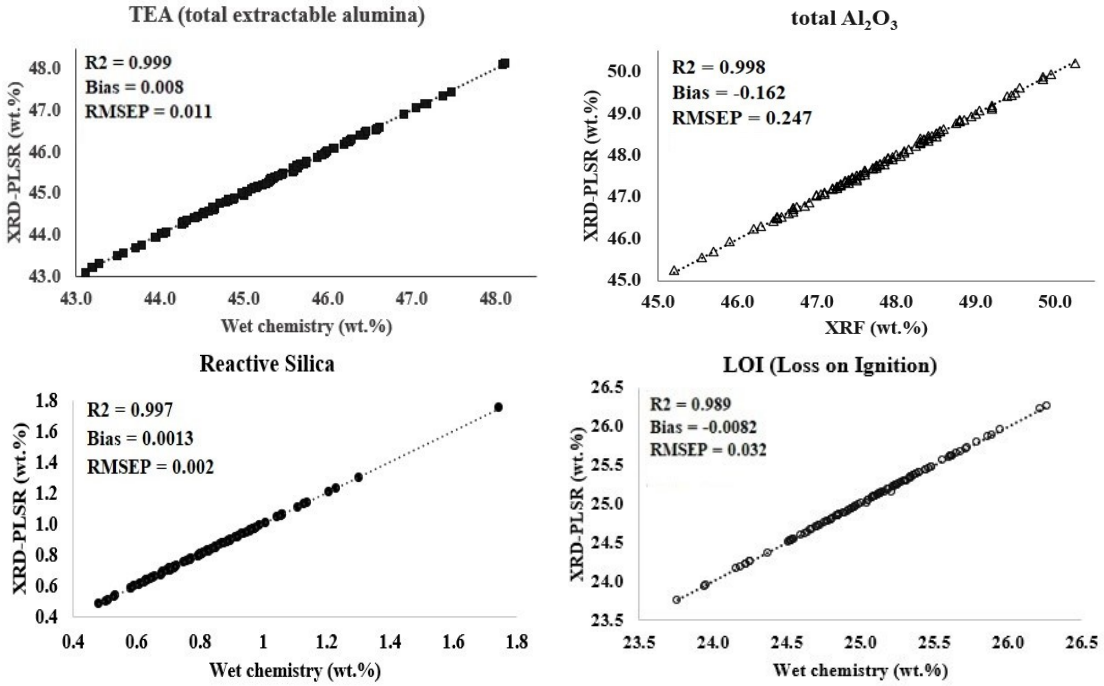


Figure 7. Correlation plots between XRD-PLSR predictions and reference values for TEA, total Al_2O_3, reactive silica, and LOI, showing excellent linearity (R^2), low root mean square error of prediction (RMSEP) and minimal bias across all Bayer-relevant parameters.

4. Conclusions

This study demonstrates the effectiveness of X-ray diffraction (XRD) for comprehensive characterization of bauxite and red mud, supporting both process optimization and sustainable resource utilization. The combined use of quantitative phase analysis (QXRD), cluster analysis, and Partial Least Squares Regression (PLSR) enabled the classification of bauxite types, evaluation of ore grade, prediction of Bayer process behaviour, and assessment of residue composition. Key methodological advances included the quantification of amorphous content using an optimized external standard approach and the estimation of kaolinite crystallinity to better predict its reactivity during digestion. PLSR models developed from industrial XRD datasets showed excellent correlation with reference values obtained via wet chemistry or XRF for process parameters TEA, Total Al_2O_3, Reactive Silica, and LOI. By integrating stoichiometric phase quantification via Rietveld refinement with pattern-based statistical modelling, the approach enables simultaneous extraction of mineralogical and compositional information. All outputs can be generated through a fully automated workflow within minutes of data acquisition, positioning XRD as a practical and efficient tool for routine quality control and process decision-making in alumina refining.

5. References

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