15th Scientific/Research Symposium with International Participation
„METALLIC AND NONMETALLIC MATERIALS“, Zenica, B&H, 24th-25th April 2025

EVALUATION OF PROFEX SOFTWARE FOR PHASE ANALYSIS OF CEMENT, CLINKER, AND LIMESTONE: A COMPARATIVE STUDY WITH TOPAS

Marina Jovanović, Adnan Mujkanović
University of Zenica, Faculty of engineering and natural sciences
Travnička cesta 1, Zenica
B&H

Nevzet Merdić, Nedžad Haračić
Heidelberg Materials Cement BiH
Selima efendije Merdanovića 146, Kakanj
B&H

Vinko Baranašić
University of Zagreb, Faculty of mining, geology and petroleum engineering
Pierottijeva 6, Zagreb
Croatia

Keywords: X-ray diffraction, quantitative phase analysis, Rietveld refinement, Profex, Topas, cement, clinker, limestone

ABSTRACT
X-ray diffraction is a crucial method for characterizing crystalline materials, widely employed in the analysis of both products and raw materials in the cement industry, including clinker, cement, and limestone. Quantitative phase analysis via X-ray diffraction necessitates sophisticated computational tools to accurately interpret diffraction patterns. While commercial software like Topas is renowned for its precision, its high cost can be unaffordable for many academic and small-scale laboratories. This study assesses the reliability of Profex, an open-source graphical user interface for the BGMN Rietveld refinement engine, by comparing its performance against Topas in analyzing clinker, cement, and limestone samples. Our comparative analysis focuses on the quantification of major and minor phases, as well as the weighted profile R-factor as a measure of fit quality. Results indicate that Profex provides comparable accuracy to Topas in quantifying major phases such as alite, belite, and calcite. However, discrepancies arise in the quantification of minor phases and in Rwp values, suggesting potential limitations in Profex's refinement algorithms and peak fitting procedures. Despite these differences, Profex demonstrates potential as a cost-effective alternative for quantitative phase analysis, though caution is advised when interpreting results.

1. INTRODUCTION

X-ray diffraction (XRD) is a valuable analytical technique frequently used for mineral identification and analysis, playing a crucial role in numerous fields of science, engineering, and technology. The fundamental principle of XRD involves the diffraction of X-ray waves elastically scattered by a series of atoms arranged in a specific pattern within a crystalline structure. This technique provides essential information about the atomic arrangement of crystalline solids, making it one of the key standard laboratory methods for material analysis [1-5]. Among several X-ray methods Powder diffraction is the most effective method for analysing multi-phase mixtures and determining the relative concentrations of various phases. This rapid, non-destructive analytical technique characterizes multi-component mixtures without extensive sample preparation. The method identifies crystalline solids by comparing diffraction patterns to established databases, such as the Powder Diffraction File (PDF) or the Cambridge Structural Database (CSD). Each crystalline material produces a distinctive diffraction pattern, serving as its fingerprint. Recent advancements in optics and fast detectors have significantly improved the speed and analytical capabilities of powder diffraction. Effective XRD analysis requires fine-grained powders (10 - 50 μm) to ensure a good signal-to-noise ratio, avoid intensity fluctuations, minimize spottiness, and reduce preferred orientation effects [6-11]. Qualitative XRD analysis identifies phases in a specimen by comparing them with standard patterns and estimating phase proportions based on peak intensities. In contrast, accurate quantitative analysis involves modeling diffraction patterns to match experimental data, which requires precise determination of peak positions and intensities. Successful quantitative methods depend on high-quality sample preparation, good data, and a deep understanding of potential experimental errors. Calibration with known standards is essential for accurate peak intensity ratios. Advanced computational software, often expensive, supports pattern modelling for quantitative analysis. Fortunately, cost-effective or free alternatives, though less user-friendly, offer effective analytical capabilities [12]. XRD is essential in the cement industry for analysing raw materials, optimizing clinker production, and studying cement hydration. It provides fast, automated phase identification, ensuring quality control and efficient kiln operation. Combined with XRF, it offers a comprehensive understanding of material composition, enhancing cement performance and manufacturing efficiency [13-17].

Commercial software packages are renowned for their advanced optimization routines and extensive profile modelling capabilities, and offer state-of-the-art solutions. Among the available software solutions, Topas has established itself as a powerfull and proven tool in various industrial and research applications. Its advanced algorithms, flexible profile fitting routines, and comprehensive treatment of microstructural effects make it the benchmark for high-precision quantitative phase analysis in complex multiphase systems [18]. Topas integrates various profile-fitting techniques, enabling single-line and whole-powder pattern fitting, indexing, structure determination, and refinement. The software is built around a non-linear least-squares system that supports Bragg diffraction and pair-distribution function (PDF) data from multiple sources, including X-ray and neutron data. Topas integrates three key techniques for structure analysis: global Rietveld refinement, charge flipping, and pair-distribution function analysis [19]. However, due to their high costs, many academic institutions and small-scale laboratories are often unable to afford these commercial software packages. Recently, several open-source software tools have emerged, providing researchers worldwide with the opportunity to perform QPA without the burden of costly licenses. One of the most promising is Profex. Profex is a graphical user interface (GUI) designed for the Rietveld refinement program BGMN, enhancing usability while preserving powerful scripting features. Developed by Jörg Bergmann, it applies Monte Carlo modelling to accurately simulate peak profiles by considering wavelength, geometry, and sample-related influences. BGMN is known for its stable convergence, automatically optimizing refinement parameters and deactivating unnecessary models when data is insufficient. Profex, combined with BGMN, is a powerful tool for academic and research applications in powder XRD analysis. The open-source licensing of both programs ensures their continued availability and development in the scientific community [20]. Nevertheless, while Profex is generally appreciated in academic settings for its ease of use, its ability to handle complex samples with overlapping phases requires further evaluation.

The objective of this study is to assess the reliability of Profex for testing clinker, cement, and limestone by directly comparing its output with that of Topas. By applying both software packages to the same set of samples, we aim to determine whether Profex can deliver accurate and reproducible quantitative results under conditions typically encountered in industrial quality control. This comparison is critical for determining if the cost-effective and accessible nature of Profex can meet the rigorous demands of structural characterization in the construction materials industry without compromising on precision.

2. MATERIALS AND METHODS

The materials utilized in this study include clinker and CEM II 42.5N cement, both produced by Heidelberg Materials Cement BiH d.d. Kakanj, Bosnia and Herzegovina, as well as limestone obtained from the Ribnica Kakanj quarry. The chemical composition of the samples was determined using the X-ray fluorescence (XRF) method. Mineralogical analyses of samples were performed using X-ray diffraction analysis of powder on XRD diffractometer Brucker D8 ENDEAVOR. For both XRF and XRD analyses, the samples were first ground into fine powders to minimize particle size effects and ensure homogeneity. Subsequently, these powders were pressed into tablets, a standard preparation method that ensures analytical accuracy by providing uniform sample presentation. The software used for data processing at Heidelberg Materials Cement BiH d.d. Kakanj is TOPAS BBQ version 6. The software that is freely available on the Internet and used for processing the same data is PROFEX version 5.2.

In this study, clinker and limestone were treated as fully crystalline materials, while cement CEM II 42.5N—containing approximately 30% fly ash—exhibits a significant amorphous fraction due to the glassy constituents of the fly ash. Amorphous phases cannot be directly detected by X-ray diffraction (XRD) because they do not produce distinct peaks but rather increase the background intensity. Conducted by the software specifically designed for cement characterization, our Topas analysis accounted for both crystalline and amorphous phases, thereby enabling accurate quantification of the amorphous content. In contrast, in our study Profex was limited only to crystalline phase analysis. To facilitate a comparative analysis between Profex and Topas, we focused solely on crystalline phases in both analyses. This approach involved excluding the amorphous phase data in cement obtained by Topas and recalculating the crystalline phase percentages to ensure their sum equals 100%.

3. RESULTS AND DISCUSION

3.1. Chemical analysis

The table 1 provides the chemical composition of four different clinker samples, obtained by XRF analysis. The chemical compositions of examined clinkers are within typical ranges for Portland cement clinker.

Table 1. Chemical composition of clinker

Composition (%)	Material			
	Clincer 1	Clinker 2	Clinker 3	Clinker 4
SiO_2	20.96	20.61	20.88	20.56
Al_2O_3	6.12	6.13	6.12	6.16
Fe_2O_3	3.36	3.38	3.43	3.38
CaO	66.57	66.12	66.40	66.27
MgO	1.19	1.18	1.18	1.17
SO_3	0.89	1.29	1.00	1.29
Na_2O	0.05	0.07	0.06	0.06
K_2O	0.58	0.74	0.63	0.74
MnO	0.158	0.165	0.162	0.162
TiO_2	0.243	0.24	0.242	0.24
P_2O_5	0.094	0.10	0.099	0.097
Cl	0.009	0.015	0.012	0.018
Sum	100.224	100.04	100.215	100.147

The table 2 presents the chemical composition of four samples of cement CEM II 42.5 N, showing minimal variations in components content.

Table 2. Chemical composition of cement CEM II 42.5 N

Composition (%)	Material			
	Cement 1	Cement 2	Cement 3	Cement 4
SiO_2	27.51	27.54	27.25	27.49
Al_2O_3	10.04	10.04	9.94	9.93
Fe_2O_3	4.73	4.72	4.70	4.72
CaO	52.06	52.04	52.20	52.25
MgO	1.68	1.69	1.67	1.69
SO_3	2.77	2.70	2.75	2.67
Na_2O	0.127	0.128	0.124	0.124
K_2O	0.95	0.95	0.95	0.93
MnO	0.114	0.116	0.126	0.126
TiO_2	0.371	0.37	0.365	0.368
P_2O_5	0.131	0.132	0.131	0.132
Sum	100.483	100.426	100.206	100.43

The table 3 presents the chemical composition of four different limestone samples. Limestone 4 demonstrated the highest purity, characterized by elevated calcium oxide (CaO) content and minimal levels of impurities such as silicon dioxide (SiO_2), aluminum oxide (Al_2O_3), and iron oxide (Fe_2O_3). Limestone 2 and 3 had moderate impurity levels, while Limestone 1 had the lowest CaO content and the highest levels of SiO_2, Al_2O_3, and Fe_2O_3.

Table 3. Chemical composition of limestone

Composition (%)	Material			
	Limestone 1	Limestone 2	Limestone 3	Limestone 4
SiO_2	13.17	12.99	10.57	4.00
Al_2O_3	3.85	1.10	1.18	0.60
Fe_2O_3	1.14	0.79	0.73	0.15
CaO	43.80	47.03	48.14	52.53
MgO	0.37	0.33	0.32	0.41
SO_3	0.08	0.02	0.08	0.07
Na_2O	0.14	0.00	0.00	0.00
K_2O	0.39	0.12	0.10	0.02
$CaCO_3$	78.18	83.95	85.93	93.77
LOI	34.38	36.87	35.25	41.61
Sum	97.32	99.25	96.37	99.39

3.2. Mineralogical analysis

Figure 1 displays the X-ray diffraction pattern of a cement sample, while the detailed mineralogical compositions of four clinker samples, as determined by two analytical approaches Topas ands Profex, are presented in Table 4.

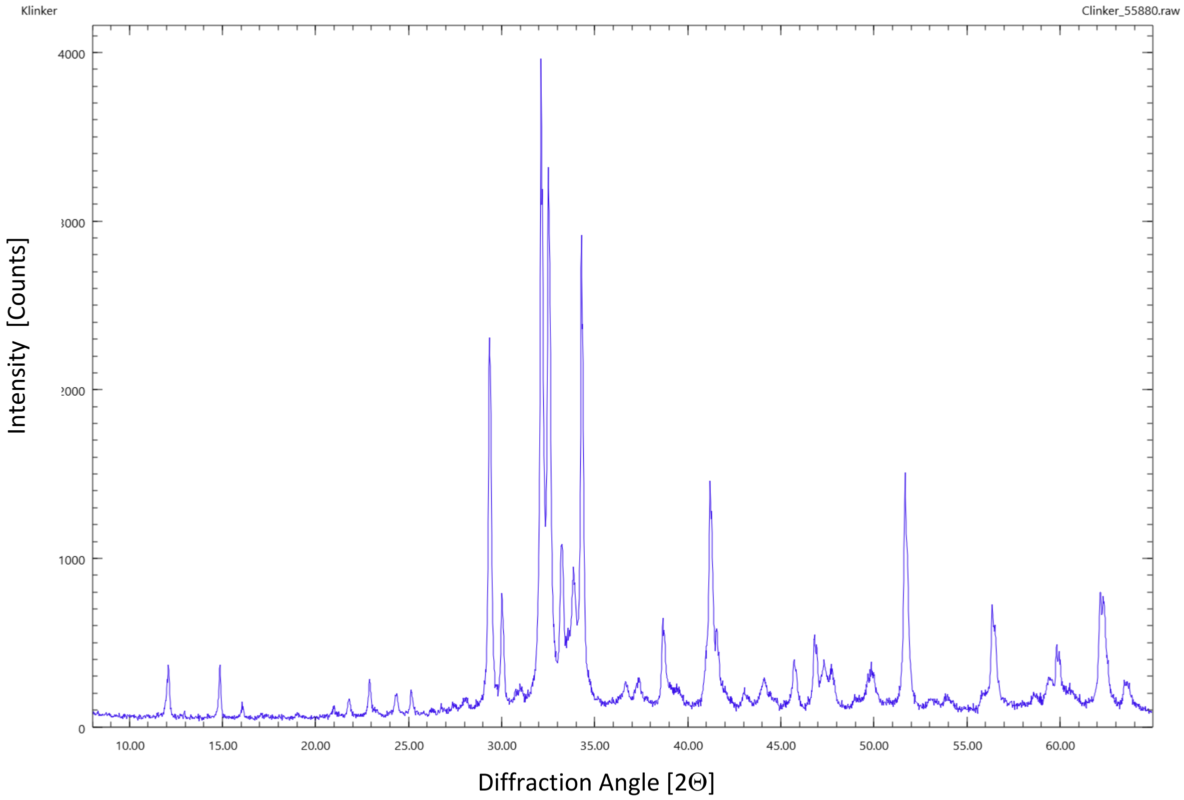

Figure 1. XRD pattern of Clinker Sample No.1 in Profex

Table 4. Mineralogical composition of clinker

Composition (%)	Material							
	Clinker 1		Clinker 2		Clinker 3		Clinker 4	
	Topas	Profex	Topas	Profex	Topas	Profex	Topas	Profex
Alite	64.64	69.27	61.54	65.08	67.34	72.00	57.36	61.67
Belite	12.60	8.70	16.87	11.91	11.04	6.20	18.25	14.23
Aluminate	6.97	8.04	5.74	7.89	5.93	8.17	6.61	7.98
Ferrite	11.71	11.18	11.45	10.91	12.40	11.70	11.20	11.04
Lime	0.91	0.48	2.03	1.59	0.78	0.00	2.65	2.51
Portlandite	0.02	0.36	0.0	0.46	0.1	0.31	0.07	0.41
Periclase	0.19	0.05	0.13	0.08	0.16	0.05	0.16	0.04
Quartz	0.10	0.03	0.03	0.03	0.08	0.09	0.09	0.09
Arcanite	1.05	0.58	1.00	0.54	1.07	0.52	1.24	0.51
Apthtiatalite	0.40	0.59	0.37	0.65	0.39	0.58	0.47	0.65
Langbeinite	0.42	0.39	0.57	0.37	0.41	0.44	0.79	0.29
Thenardite	0.64	0.34	0.00	0.49	0.00	0.21	0.73	0.58
Sum	99.86	100.01	99.73	100.0	99.70	100.27	99.62	100.0

The comparative analysis of the clinker samples revealed a consistent trend between the two software tools. Topas, serving as our benchmark, generally reported lower alite percentages and higher belite and arcanite values compared to Profex. For instance, in clinker 1, Topas indicated 64.6 % alite versus 69.3 % by Profex, while belite was quantified at 12.6 % in Topas compared to 8.7 % in Profex. Similar trends were observed across all samples: Profex consistently yielded higher alite and aluminate contents and lower belite and arcanite percentages.

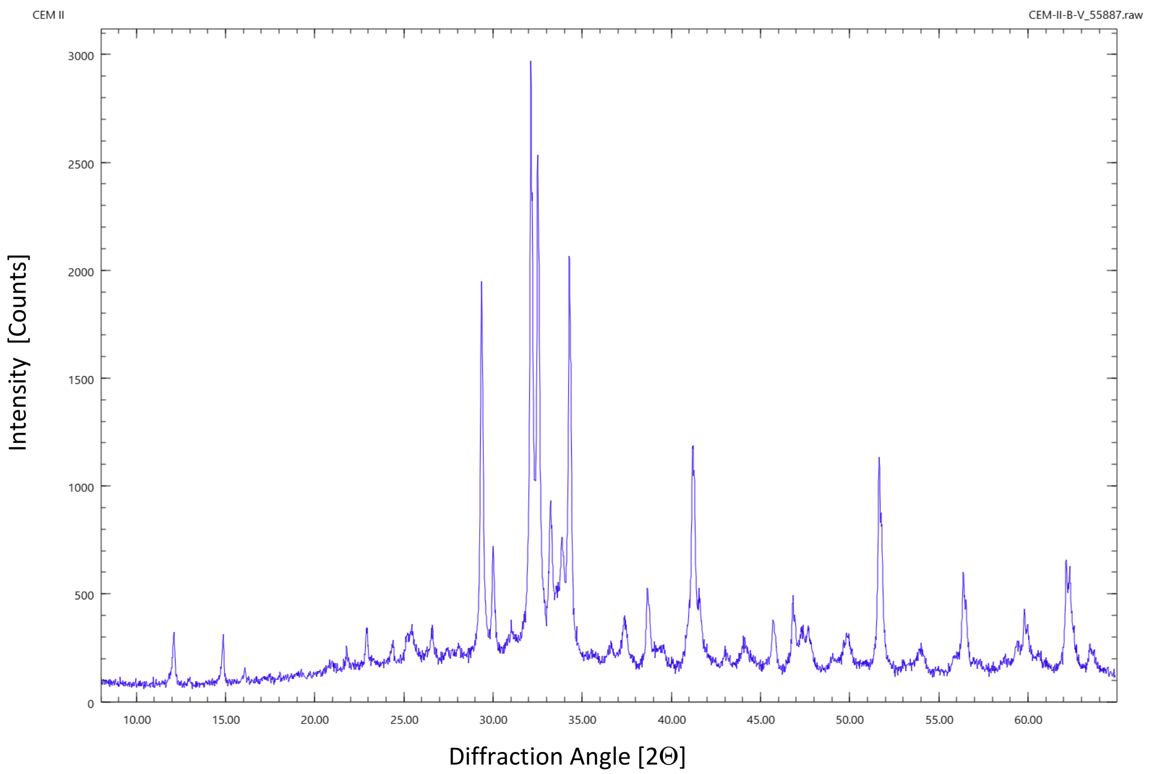

Figure 2. XRD pattern of cement 1 in Profex

Figure 2 depicts the X-ray diffraction pattern of a cement sample, while Table 5 details the mineralogical compositions of four cement samples as determined using Topas and Profex. Topas calculated the amorphous phase content to be 26.54%, which was excluded to facilitate comparison with the results generated by Profex, as outlined in the Methods and Materials section.

Table 5. Mineralogical composition of cement CEM II 42.5 N

Composition (%)	Material							
	Cement 1		Cement 2		Cement 3		Cement 4	
	Topas	Profex	Topas	Profex	Topas	Profex	Topas	Profex
Alite	54.87	61.10	54.31	60.64	54.62	60.70	56.66	62.61
Belite	13.33	10.65	14.75	9.75	14.09	9.83	14.24	9.50
Aluminate	5.95	7.20	5.27	7.55	4.94	7.56	5.81	7.39
Ferrite	11.69	10.73	12.43	12.08	11.61	10.87	10.71	11.19
Lime	1.52	1.82	1.55	1.56	1.52	1.44	1.59	1.46
Periclase	0.26	0.25	0.30	0.23	0.35	0.33	0.49	0.31
Quartz	0.97	1.21	1.16	1.24	1.06	1.19	1.11	1.11
Arcanite	1.24	0.22	1.13	0.40	1.05	0.35	1.45	0.60
Apthtiatalite	0.65	0.52	0.52	0.40	0.70	0.64	0.60	0.12
Langbeinite	1.92	0.67	1.49	0.71	1.64	0.81	1.53	0.67
Thenardite	1.13	0.18	0.82	0.24	1.09	0.43	1.00	0.00
Gypsum	0.00	0.04	0.00	0.00	0.02	0.11	0.02	0.00
Hemihydrate	0.00	0.83	0.00	0.49	0.03	1.14	0.03	0.77
Anhydrite	2.14	1.85	1.84	1.71	2.00	1.83	1.95	1.85
Calcite	1.88	0.00	1.74	0.00	2.72	0.00	0.79	0.00
Dolomite	0.88	1.49	0.82	1.34	0.79	1.04	0.71	1.26
Mullite	0.57	0.74	0.90	1.06	0.62	0.85	0.32	0.71
Magnetite	0.33	0.32	0.55	0.35	0.60	0.71	0.58	0.38
Hematite	0.64	0.15	0.36	0.28	0.51	0.19	0.35	0.13
Sum	99.97	99.97	99.94	100.03	99.96	100.02	99.94	100.06

The QPA of four cement samples reveals systematic differences between Topas and Profex. For instance, Topas quantifies alite in the range of approximately 54 – 57 %, whereas Profex reports notably higher values (60 – 63 %). Conversely, belite percentages are lower in the Profex results (around 9.5 – 10.7 %) compared to Topas (approximately 13 – 14.7 %). Similar discrepancies are observed for aluminate, with Topas yielding values of roughly 5 – 6 % and Profex in the 7 – 7.6 % range. These differences extend to minor phases as well. For example, arcanite and thenardite are consistently quantified at higher levels by Topas than by Profex. In contrast, phases like ferrite, lime, periclase, and quartz show only minor variations between the two methods, indicating that both software packages capture these well.

Figure 3 presents the X-ray diffraction profile of one of the limestone samples, and Table 5 summarizes the mineralogical composition of four limestone samples as determined by the two analytical methods.

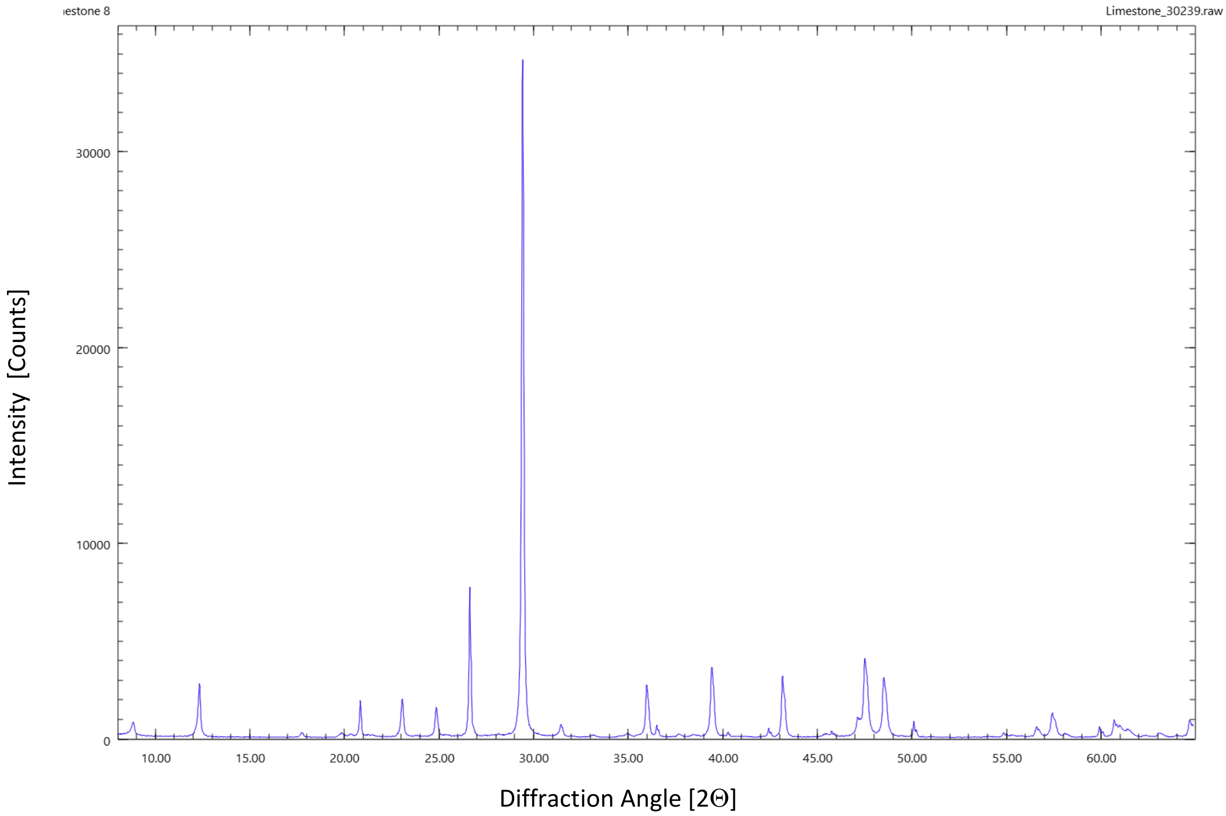

Figure 3. XRD pattern of limestone 1 in Profex

Table 6. Mineralogical composition of limestone

Composition (%)	Material							
	Limestone 1		Limestone 2		Limestone 3		Limestone 4	
	Topas	Profex	Topas	Profex	Topas	Profex	Topas	Profex
Quartz	12.09	10.96	5.56	5.38	10.92	9.39	3.45	3.09
Calcite	75.38	69.90	90.63	84.73	87.44	76.40	96.55	83.80
Dolomite	0.00	0.00	0.15	0.00	0.24	0.00	0.00	0.00
Pyrite	0.22	0.31	0.00	0.10	0.00	0.07	0.00	0.10
Illite	6.79	1.15	1.93	0.18	0.00	0.22	0.00	0.15
Kaolinite	5.53	12.28	1.72	7.48	1.40	12.30	0.00	11.80
Albite	0.00	0.11	0.00	0.29	0.00	0.00	0.00	0.00
Ankerite	0.00	0.10	0.00	0.94	0.00	0.47	0.00	0.83
Anorthite	0.00	0.26	0.00	0.25	0.00	0.61	0.00	0.00
Magnesite	0.00	0.40	0.00	0.03	0.00	0.13	0.00	0.08
Orthoclase	0.00	0.58	0.00	0.57	0.00	0.44	0.00	0.14
Siderite	0.00	0.06	0.00	0.05	0.00	0.05	0.00	0.02
Muscovite	0.00	3.89	0.00	0.00	0.00	0.00	0.00	0.00
Sum	100.01	100,00	99.99	100,00	100,00	100,08	100,00	100,01

The analysis of limestone samples using the two analytical methods reveals systematic differences in phase quantification between the two software packages. Topas consistently reports higher calcite contents—for example, limestone 4 shows 96.55 % calcite by Topas compared to 83.80 % by Profex—while Profex tends to assign lower percentages to calcite and quartz. Conversely, clay minerals such as kaolinite and muscovite are often quantified at higher levels in the Profex results. In limestone 1, for instance, Profex detects 12.28 %

kaolinite and 3.89 % muscovite, whereas Topas reports only 5.53 % kaolinite and no muscovite. Similar trends are observed in limestone 2 and 3, where Profex also indicates the presence of minor feldspar phases (anorthite and orthoclase) that are either absent or reported at lower levels by Topas.

Table 7 presents Rwp of our samples for both methods. Rwp (%) refers to the weighted profile R-factor, a key goodness-of-fit parameter in Rietveld refinement. It quantifies how well the calculated diffraction pattern matches the observed data in a least-squares refinement process. A lower Rwp (%) indicates a better fit.

Table 7. Paramter Rwp (%) calculated by Topas and Profex

	Cl. 1	Cl. 2	Cl. 3	Cl. 4	Cem. 1	Cem. 2	Cem. 3	Cem. 4	Lim. 1	Lim. 2	Lim. 3	Lim. 4
Topas	11.14	11.62	11.99	11.03	10.67	10.47	10.24	10.53	9.37	9.37	9.49	12.18
Profex	10.28	10.09	10.13	9.89	8.12	8.31	8.22	8.14	10.09	10.76	11.62	10.11

For the limestone samples, the Rwp values show a mixed trend. Limestone 1, 2, and 3 yielded lower Rwp values with Topas (9.37 – 9.49 %) compared to Profex (10.09 – 11.62 %), suggesting that Topas's sophisticated background and peak shape modeling may provide a slightly better fit for these samples. However, limestone 4 is an exception, where Profex achieved a lower Rwp (10.11 %) relative to Topas (12.18 %), indicating that under certain conditions or sample characteristics, Profex's approach can outperform Topas. In contrast, for clinker and cement samples, Profex consistently delivered lower Rwp values than Topas. Clinker samples refined with Profex ranged from 9.89 % to 10.28 % compared to Topas values of 11.03 % to 11.99 %. Similarly, cement samples showed Rwp values of approximately 8.12 – 8.31 % with Profex, while Topas recorded values in the range of 10.24 – 10.67 %.

Table 8 consolidates the observed differences between Topas and Profex for the three material types—clinker, cement, and limestone—based on our quantitative XRD analysis.

Table 8. Comparison Topas vs. Profex

Material	Mineral group	Topas observation	Profex observation
Clinker	Alite	Generally lower	Generally higher
	Belite	Generally higher	Generally lower
	Aluminate (and similar phases)	Slightly lower	Slightly higher
	Ferrite	Similar values	Similar values
	Lime and Periclase	Generally higher	Generally lower
	Quartz	Similar values	Similar values
	Sulfate & minor phases	Slightly higher	Slightly lower
Cement	Alite	Generally lower	Generally higher
	Belite	Generally higher	Generally lower
	Aluminate and Portlandite	Lower	Higher
	Ferrite	Similar values	Similar values
	Lime	Generally higher	Generally lower
	Accessory phases (e.g. arcanite, thenardite)	Slightly higher	Slightly lower
Limestone	Calcite	Generally higher	Generally lower
	Quartz	Generally higher	Generally lower
	Dolomite	Consistently low	Consistently low
	Clay minerals (illite, kaolinite, muscovite)	Lower	Higher
	Accessory phases (e.g. pyrite, ankerite, etc.)	Similar values	Similar values

Our evaluation of QPA indicates that Profex, while exhibiting systematic differences in absolute phase percentages compared to Topas, demonstrates a consistent and reliable performance overall. Profex generally reports higher alite and lower belite values in clinker and cement, as well as lower calcite and quartz and higher clay mineral contents in limestone relative to Topas. These discrepancies are systematic across multiple samples and are attributable primarily to differences in the underlying refinement algorithms. The differing strategies for background subtraction and peak-shape modeling between the two software packages appear to be the main cause of the observed variations. Despite these differences, both methods consistently capture the relative trends across samples, suggesting that Profex reliably differentiates between material variations.

4. CONCLUSION

This study evaluated the efficacy of Profex, an open-source software interfacing with the BGMN engine, in performing QPA on cementitious materials, specifically clinker, cement, and limestone. By benchmarking its performance against the established commercial software Topas, several insights were obtained:

- Major Phase Quantification: Profex demonstrated competency in accurately quantifying major phases such as alite, belite, and calcite across the tested samples. The results were largely consistent with those obtained from Topas, indicating that Profex can serve as a reliable tool for analyzing predominant components in cementitious materials.
- Minor Phase Discrepancies: Notable differences emerged in the quantification of minor phases between the two software packages. Profex tended to overestimate or underestimate certain minor constituents, which could be attributed to its refinement algorithms and peak fitting procedures. These discrepancies highlight the need for cautious interpretation when analyzing trace phases using Profex.
- Weighted Profile R-factor (Rwp): The Rwp values obtained from Profex were generally higher compared to those from Topas, suggesting a less optimal fit between the observed and calculated diffraction patterns. This observation points to potential limitations in Profex's ability to model complex diffraction data with the same precision as Topas.
- Accessibility and Cost-effectiveness: Despite certain limitations, Profex offers a significant advantage in terms of accessibility and cost. Its open-source nature makes it an attractive option for academic institutions and laboratories with limited funding, enabling broader participation in materials characterization research.

In conclusion, while Profex presents itself as a viable, cost-effective alternative for QPA, users should exercise caution when interpreting results related to minor phases and consider corroborating findings with additional analytical methods or more advanced software to ensure accuracy.

ACKNOWLEDGEMENT

We gratefully acknowledge the financial support of the Ministry of Education and Science of the Federation of Bosnia and Herzegovina for Project "Calcined Clay Use in Cement and Concrete Production Aimed at Reducing Greenhouse Gas Emissions" (Grant No. 05-35-2116-1/22), which was essential to the successful completion of this research.

REFERENCES

[1] Ali A., Chiang Y.W., Santos R.M. X-ray Diffraction Techniques for Mineral Characterization: A Review for Engineers of the Fundamentals, Applications, and Research Directions. Minerals 2022, 12, 205. https://doi.org/10.3390/ min12020205

[2] Zhao P., Lu L., Liu X., De la Torre G. A., Cheng X. Error Analysis and Correction for Quantitative Phase Analysis Based on Rietveld-Internal Standard Method: Whether the Minor Phases Can Be Ignored? Crystals 2018, 8, 110; doi:10.3390/cryst8030110

[3] Jovanović M., Mujkanović A. Karakterizacija opekarskih glina. Univerzitet u Zenici, Metalurško-tehnološki fakultet. Zenica 2021.

[4] Petrovski P. Uvod u rentgensku difraktometriju i mineralna rentgenska analiza cementa. Hijatus, Zenica 2006.

[5] Simonnet T., Grangeon S., Claret F., Maubec N., Fall M. D., Harbac R., Galernea B. Phase quantification using deep neural network processing of XRD patterns. IUCrJ (2024). 11, 859–870. https://doi.org/10.1107/S2052252524006766

[6] Ameh E.S. A review of basic crystallography and X-ray diffraction applications. Int. J. Adv. Manuf. Technol. 2019, 105, 3289–3302.

[7] Bish D.L., Reynolds R.C. Sample Preparation for X-ray Diffraction. Mod. Powder Diffr. 2018, 20, 73–100.

[8] Černý R. Crystal Structures from Powder Diffraction: Principles, Difficulties and Progress. Crystals 2017, 7, 142.

[9] Bergmann J., Le Bail A., Shirley R., Zlokazov V. Renewed interest in powder diffraction data indexing. Zeitschrift für Kristallographie. 2004, 219, 783–790

[10] Lee M. X-ray Diffraction for Materials Research from Fundamentals to Applications; CRC Press: Boca Raton, FL, USA, 2021.

[11] Bish D. L., Reynolds R. C. Sample Preparation for X-ray Diffraction. Mod. Powder Diffr. 2018, 20, 73–100.

[12] Xiao J., Song Y., Li Y. Comparison of Quantitative X-ray Diffraction Mineral Analysis Methods. Minerals 2023, 13, 566. https://doi.org/10.3390/ min13040566

[13] Ramírez-Casas J., Gómez-Val R., Buill F., González-Sánchez B., Navarro Ezquerra A. Forgotten Industrial Heritage: The Cement Factory from La Granja d'Escarp. Buildings 2025, 15, 372. https://doi.org/10.3390/ buildings15030372

[14] Stutzman P. E., Feng P., Bullard J. W. Phase Analysis of Portland Cement by Combined Quantitative X-Ray Powder Diffraction and Scanning Electron Microscopy. Journal of Research of the National Institute of Standards and Technology Volume 121 (2016) http://dx.doi.org/10.6028/jres.121.004

[15] Chauhan A., Chauhan P. (2015) Usage of Powder XRD Technique for Material Characterization and Analysis of Portland Cement. J Anal Bioanal Tech 6:e123 doi:10.4172/2155-9872.1000e123

[16] Mukhopadhyay A., Ganesh R. M., Liu K., Deng Y. Direct determination of cement composition by x-ray diffraction. Technical Report 0-6941-R1. (2019) Texas A&M Transportation Institute. http://tti.tamu.edu/documents/0-6941-R1.pdf

[17] Walenta G., Füllmann T. Advances in Quantitative XRD Analysis for Clinker, Cements, and Cementitious additions. Powder Diffraction Vol. 19 Number 1 – March 2004.

[18] Coelho A. A. TOPAS and TOPAS-Academic : an optimization program integrating computer algebra and crystallographic objects written in C++. J. Appl. Crystallogr. Vol. 51 No. 1, 210–218, . 2018, doi: 10.1107/S1600576718000183.

[19] https://www.bruker.com/en/products-and-solutions/diffractometers-and-x-ray-microscopes/x-ray-diffractometers/diffrac-suite-software/diffrac-topas.html (25/2/2025)

[20] Döbelin N., Kleeberg R. Profex: a graphical user interface for the Rietveld refinement program BGMN. Journal of Applied Crystallography 48 (2015), 1573-1580. doi:10.1107/S1600576715014685