

X-RAY DIFFRACTION DIFFRAC.DOUANT V2

Simplifying Advanced Quantitative Phase Analysis for Crystalline and Amorphous

Streamlined Workflow and User-Friendly Options

DQUANT, the latest BRUKER software for quantitative phase analysis from X-ray diffraction data, revolutionizes the field of X-ray powder diffraction. Utilizing one or more diffraction peaks, DQUANT establishes highly accurate calibrations based on standard reference samples.

With support for various quantitative procedures, including the ratio, addition, and Chung internal reference methods, DQUANT offers a comprehensive solution. Seamlessly integrated into the DIFFRAC. SUITE software package for measurement and data evaluation, it covers everything from calibration models to data correction and evaluation routines. Designed to cater the users of all skill levels, DQUANT provides a guided workflow from method definition to the presentation of final results. Whether interactive or fully automated analysis is preferred, DQUANT empowers the user with a single-button operation.

Ideal for both seasoned lab managers and daily operators, DQUANT combines innovative software, streamlined workflows, and method architecture to deliver maximum flexibility with unparalleled simplicity. Experience the new benchmark in quantitative crystalline-phase analysis through X-ray diffraction with DQUANT.

Introducing Version 2

DQUANT now incorporates an advanced peak profile fitting capability for precise intensity determination, especially beneficial when dealing with overlapping peaks. Amplitude and peak area, are available for subsequent calibrations. A consistent fit model is established using reference scans, ensuring accuracy, and reliability. This model is then used for the automatic evaluation of unknown samples.

Version 2 includes Partial Least Squares regression, a powerful technique for extracting sample properties, such as concentrations, from X-ray powder diffraction data. Two validation methods, test set validation or cross-validation, are offered during the training step to ensure model robustness. The software also identifies outliers and evaluates scan data that may not improve the results.

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Figure 1 Predefined calibration methods create data trees, specific to the analysis. To customize the method simply work your way through the data tree from top to bottom.

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Figure 2 Expression editor with syntax highlighting for defining concentration and intensity modules.

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Figure 3 While the expert mode allows access to the full functionality of DQUANT, the operator mode is limited to the evaluation of unknown samples.



Figure 4 DQUANT is seamlessly integradted with DIFFRAC.SUITE for automated data evaluation.

Simplified Workflow and Flexible Options: Effortless Analysis for All Users

DQUANT is designed to provide a seamless analysis experience for laboratory supervisors and operators with varying levels of expertise. Here is how DQUANT simplifies the workflow and offers flexible options:

1. Calibration and Interactive Analysis

DQUANT serves as an expert system for laboratory supervisors, guiding them in setting up calibration methods. With its intuitive graphical user interface and pre-configured data trees, the software streamlines the process for different analytical tasks. Calibration curves and intensity-drift correction can be established and verified directly in the user interface mode. Experienced users also have the option to analyze unknown samples interactively.

2. Tailor-Made Reporting and Analytical Flexibility

Concentration-modules in DQUANT allow for customized reporting of results based on calibrated concentrations. For maximum analytical flexibility, intensity-modules are available. The built-in formula editor enables easy column arithmetic of intensities, providing access to user-defined intensity corrections, peak overlap correction, and averaging techniques to reduce preferred orientation effects.

3. Drift Monitoring and Absorption Correction

DQUANT supports the establishment of drift monitors to keep calibrations up-to-date. Drift history is recorded from the initialization date, allowing additional standards to be added without re-measuring other standards. Additionally, the software supports absorption correction for samples of finite thickness, ensuring accurate determination even for micrograms of material.

4. Streamlined Data Evaluation and Results Presentation

DQUANT leverages the power of the DIFFRAC.MEASUREMENT package to simplify quantitative analysis. Measurement jobs link scan and evaluation conditions to sample IDs, including unknown samples, standards, and drift monitor samples. The data evaluation and results presentation can be triggered automatically or performed manually by the operator. The process is as simple as pushing a button.

5. Automation and Simplified Interface

For users who prefer more control, DQUANT offers a simplified user interface. Verified calibrations can be loaded, and batches of unknown samples can be analyzed without modifying the calibration. Results for multiple samples can be generated in a single run and presented according to the defined layout in the calibration project file. Various table layouts are provided, with customizable options for further export, printing, or generating documents in PDF or XPS formats.

Simplified Analysis with Partial Least Squares Regression: Harnessing the Power of X-ray Diffraction Data

Partial Least Squares Regression (PLSR) is a powerful methodology that allows you to analyze XRD data without the need for in-depth mathematical understanding. Here's how PLS Regression benefits your analysis:

1. Handling Complex Diffraction Data

Diffraction data can be complex and contain numerous variables. PLS Regression simplifies the process by extracting essential information from the data and identifying the most influential variables. It focuses on capturing patterns and relationships between variables, making it suitable for predictive modeling.

2. Multivariate Analysis Made Easy

PLS Regression excels in multivariate analysis, where you have multiple input variables (XRD data) and want to predict a specific outcome (such as concentrations, properties, or qualities). It takes into account the interdependencies and correlations among the variables, providing a comprehensive understanding of the data.

3. Predictive Modeling

One of the main advantages of PLS Regression is its ability to create robust predictive models. By identifying the relationships between XRD data and desired outcomes, it allows you to make accurate predictions and estimations. This is particularly valuable in scenarios where you want to infer properties or concentrations based on whole scan measurements.

4. Efficient Calibration and Validation

PLS Regression offers efficient calibration and validation processes. It divides the available data into subsets for model training and testing, ensuring the reliability and generalizability of the results. This approach minimizes overfitting and provides a realistic assessment of the model's performance.

By utilizing Partial Least Squares Regression, you can unlock the full potential of your diffraction data without delving into complex mathematical details. It simplifies the analysis process, enables accurate predictions, and provides valuable insights for decision-making. With PLS Regression, you can harness the power of XRD data analysis with ease and confidence.





DQUANT: Empowering Industries with Advanced Analytical Capabilities









DQUANT, the powerful software solution within the DIFFRAC.SUITE, offers a range of applications across diverse industries. Here's how DQUANT can transform your operations:

Minerals and Metals Industry:

- Accurate determination of Fe2+/Fe3+ in iron ore
- Quantification of retained austenite in steel
- Electrolytic bath control for aluminum production

Chemistry:

- Differentiation between white pigment rutile/anatase
- Precise analysis of fertilizers and other chemical compositions

Construction Materials:

- Quantification of free lime in clinker for construction materials

Workers Health Surveillance:

- Detection of breathable silica dust or asbestos deposited on filters

REACH Compliance:

- Concentration analysis of minerals like quartz in filter dust or materials such as limestone

Pharmaceutical Industry:

- Identification of amorphous and crystalline forms without crystal structure requirements
- Full compliance with cGxP/21 CFR Part 11 regulations for pharmaceutical industry needs

With its wide range of applications and compliance with industry standards, DQUANT empowers businesses across various sectors to achieve accurate and reliable analysis, ensuring optimal efficiency and regulatory compliance.

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