X-RAY DIFFRACTION
DIFFRAC.EVA V7

## Introducing Workflow Automation for Powder X-ray Data Analysis

The power of workflows allows for the repetition of recorded commands. A standardized sequence of EVA commands can be recorded and played back whenever needed. Workflows can be initiated using the drop-down list in the toolbar. Command parameters within a generated workflow can be modified using the edit button. The use of workflows enhances efficiency, accuracy, reproducibility, and collaboration capabilities, resulting in a more streamlined and productive data analysis experience.

Creating Workflows

Creating a workflow in EVA is easy and intuitive. It starts with a trained person initiating a recording that captures all the steps of the analysis as if it were a one-time analysis. During recording, over 120 EVA commands and actions are available. The necessary parameters are easily adjusted through visual data inspection or numerical algorithms.

Once the recording is complete, the workflow can be saved, and user guidance text can be added. Use the RUNNER to adjust parameters and set breakpoints, allowing for dynamic interactions and user data entry.

Workflows cover all steps of analysis. From data input to data evaluation to creating graphs and tables, to saving or printing final reports. With EVA's user-friendly workflows, anyone can efficiently perform comprehensive analyses without extensive technical expertise.
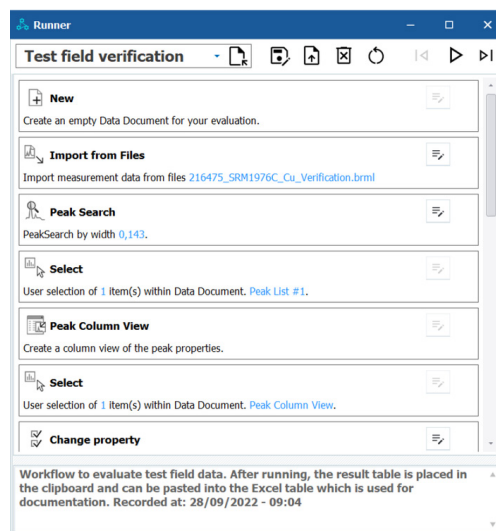
The Seven Benefits of Workflows in DIFFRAC.EVA

■ **Increased Efficiency:** Workflows allow users to record and replay a sequence of commands, saving time and effort in executing repetitive tasks. By automating complex or frequently performed operations, workflows streamline the analysis process and enhance overall efficiency.

■ **Consistency and Reproducibility:** Workflows ensure consistency and reproducibility in data analysis by capturing the exact sequence of commands used during a specific analysis. This feature is particularly valuable when working on collaborative projects or when revisiting previous analyses.

■ **Reduced Operator Training:** Workflows reduce operator training requirements and enhance accessibility, particularly for non-expert users. The pre-configured data evaluation paths eliminate the need for extensive technical knowledge, allowing to follow a simplified, intuitive approach. As a result, new users can swiftly adapt to the software and efficiently execute XRD tasks with confidence, significantly shortening the learning curve.

■ **Error Reduction:** With workflows, there is a reduced risk of human error during data analysis. Since recorded workflows execute predefined commands accurately, the likelihood of mistakes or omissions is minimized, leading to more reliable and trustworthy results.

■ **Simplified Operation:** Workflows simplify the execution of complex analysis procedures by breaking them down into a series of manageable steps. Users can execute the entire workflow with a single click, eliminating the need to remember and execute multiple commands manually.

■ **Flexibility and Customization:** Workflows offer flexibility and customization options to suit individual analysis requirements. Users can modify and fine-tune recorded workflows by adjusting parameters, allowing for adaptability and tailoring to specific analysis needs.

■ **Streamlined Collaboration:** Workflows facilitate collaboration among researchers by providing a standardized approach to data analysis. Recorded workflows can be easily shared with team members, ensuring consistency across multiple users and enabling seamless collaboration on projects.

Executing Workflows

EVA workflows are easily executed to evaluate measurement data stored in the computer file system or instrument database. The database capability also makes workflows compliant with 21 CFR Part 11 controlled environment requirements, including user rights, digital signatures and audit trail capability. There are two convenient ways to run EVA workflows:

1) The INSTANT RUNNER

Within the DIFFRAC.EVA graphical user interface, all available workflows are contained in drop-down menu lists. Selecting a workflow from this list triggers the "Instant Runner", which executes the workflow until user interaction is required, either to load new data or to execute interactive commands.

2) Integration with Results Manager

For users who use the DIFFRAC.SUITE Results Manager as their central data and reporting hub, EVA workflows can be started directly on the data selected using the query functionality. Evaluation results are automatically stored in the database for easy access and later reporting. The seamless execution of EVA workflows increases efficiency and ensures accurate data evaluation in different operational scenarios.

Workflow Examples

Typical EVA applications that are well suited to be run by workflows include

- Degree of Crystallinity
- Crystallite Size determination
- Peak/Background or Signal/Noise evaluations
- Peak or Phase Monitoring via area tool or profile fit
- Lattice Parameter refinement.

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