Instrument-Centric Workflows

Introduction

When discussing sample analysis, it is normally expected that this also includes the injection of blanks, calibration standards, check standards and so on, all combined in a series of injections, a sequence.

However, this is not always the case. For example, in the chemical or petrochemical industries, the analysis is typically driven by the need to get a fast result for an individual sample without additional injections. The main chromatography instrument used is a gas chromatograph (GC) and it is typical for one operator to use several of these instruments with each GC dedicated to a specific analysis. A calibration curve for a specific method is only required periodically, for example once every six months so running a daily blank and a check standard is sufficient to confirm the validity of the calibration.

All of this drives a more sample and instrument-centric approach to the analysis, rather than a sequence-centric view. To support these specific workflows required by (petro)chemical laboratories, Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) provides a comprehensive set of tools that streamline and simplify operation.
Instruments Overview
As mentioned before, one analyst in the laboratory can be responsible for multiple instruments. It is key that they can instantly see the status of all these instruments at a glance. Not all instruments have fully automated injection systems and may need manual interaction, for example loading a gas cylinder which was used to take the sample. Monitoring multiple instruments for their status and readiness to perform this manual action should be possible in one view.

With the Chromeleon Instruments Overview (Figure 1) the status of all the analyst’s favorite instruments are visible at once, clearly indicating which instruments are running (including run time and the operator), available for a new sample analysis or ready for a new injection. Analysts can also control the instrument queue directly from this overview.

With additional privileges, system administrators can select a range of visible instruments or have an overview of all instruments in the network (Figure 2), this can quickly identify issues, for example when an Instrument Controller is offline.
Instant sample run
From the Instrument Overview samples can be started instantly. Once a suitable and available instrument is selected for the required analysis, the run can be started in only two clicks.

1. Select the analysis method to run (Figure 3)
2. Click Finish to start the analysis (Figure 4)

Chromeleon software’s built-in eWorkflow™ procedures provide a unique framework to support this ultra-streamlined operation. They ensure that whichever instrument is selected, the correct methods and files are used for the analysis every time. This eliminates errors, simplifies operation and minimizes training requirements.
**Instrument control**
The online controls for a specific instrument can be directly accessed from the Overview pane (Figure 5A). With a single click, an ePanel opens (Figure 5B) displaying the real-time instrument status along with controls for direct operation.

**Direct data access**
In order to quickly and easily find data that was just generated, results can be directly accessed without leaving the Overview pane. One click opens the queue tab of the instrument ePanel (Figure 6A) where the recent sequence can be found. The sequence is displayed, including MiniPlots of the actual chromatograms (Figure 6B) and even custom columns, which can include results, for instant information. A double click on the sequence will open the data in the Chromatography Studio for detailed viewing or further processing if required.

**Conclusion**
By providing intelligent tools to enable operators to work with multiple instruments, start analyses quickly and review results immediately, Chromeleon CDS supports the workflows in (petro)chemical laboratories, while delivering ease of use and minimizing training requirements.
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