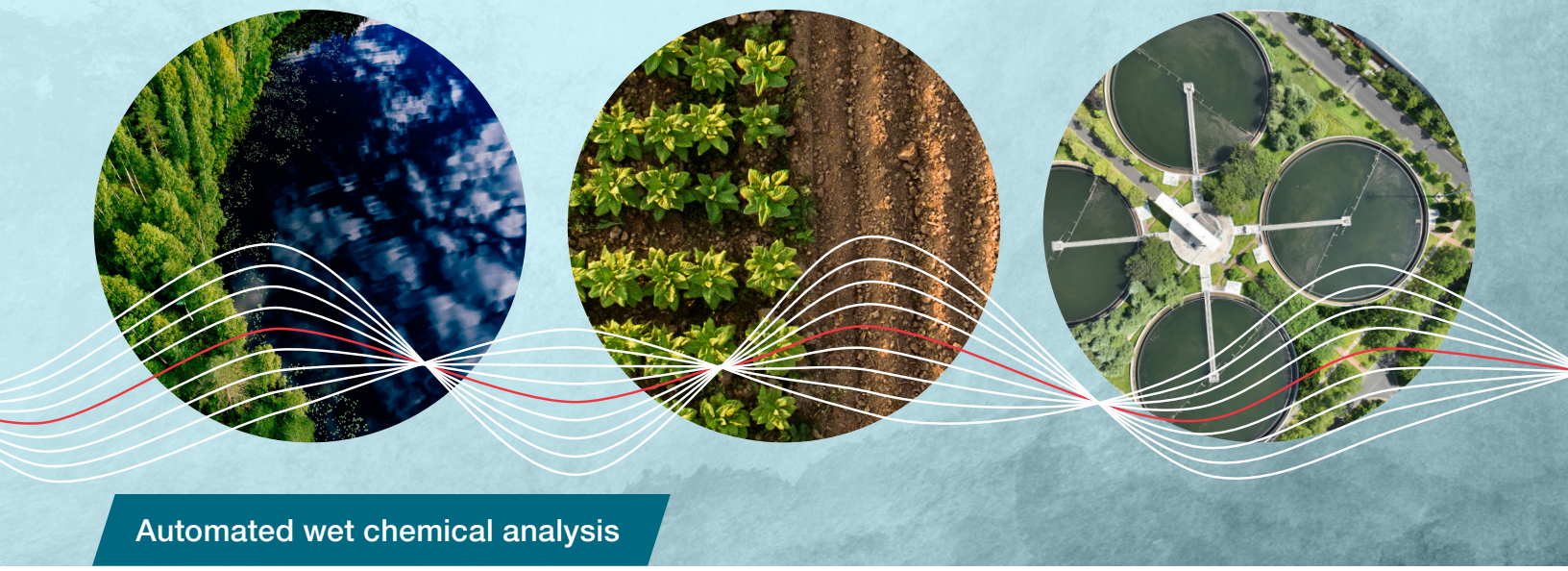


Automated wet chemical analysis

How can the Gallery Aqua Master discrete analyzers simplify water and environmental sample analysis workflows?

Questions/answers

Why is contaminant and nutrient analysis important?

Analysis of contaminant and nutrient levels in drinking, surface, and wastewater is necessary to protect aquatic habitats and maintain clean and safe drinking water supplies. Utility companies and environmental laboratories regularly measure elemental phosphorus and nitrogen in sewage water, along with a range of other pollution indicators, to ensure that discharge streams are compliant with regulatory standards. Environmental contaminants analyzed include inorganic anions, cations, heavy metals, organic pollutants, and nutrients. The United States Environmental Protection Agency (U.S. EPA) Safe Drinking Water Act (SDWA) and the Clean Water Act (CWA) are the two most important environmental laws in the US that govern water regulations. Wastewater nutrient analysis is used to assess population-level infection, including SARS-CoV-2 surveillance, to support biomarker-based population size estimates.[1]

What are the challenges associated with contaminant and nutrient analyses?

Traditional wet chemistry techniques, including titrations, flow injection analysis, and other colorimetric techniques are slow, labor-intensive, often unreliable, and involve the use of hazardous reagents that add substantial costs for waste disposal. Wet chemistry tests are time- and skilled-labor-intensive because they require many sequential and complicated manual steps. These manual steps are potentially significant sources of error, reducing overall measurement accuracy.

How do the Gallery Aqua Master discrete analyzers address these challenges?

Laboratories need accurate, efficient, and easy-to-use techniques for water and nutrient analysis. The Thermo Scientific™ Gallery™ and Gallery™ Plus Aqua Master Discrete Analyzers are integrated and highly automated platforms that provide a turnkey alternative to traditional wet-chemistry methods that is faster and safer. The platform delivers a high-throughput measurement of up to 20 parameters simultaneously, and every test is performed in a precise and predefined way. No user intervention is required once

the pre-mixed, ready-to-use reagents are loaded into the instrument. The analyzers not only improve the reliability and sensitivity of results compared to manual techniques, but they also increase laboratory productivity by freeing staff to walk away and work on other value-added tasks. In addition, automated workflows eliminate the need to handle hazardous reagents, helping to protect the health and safety of laboratory staff.

For analyses related to regulatory compliance, Gallery and Gallery Plus Aqua Master discrete analyzer workflows have been verified to meet the U.S. EPA-approved reference method requirements and international regulatory requirements for environmental wastewater and drinking water analysis. In particular, the analyzer's advanced software provides sought-after features that enable laboratories to achieve a higher degree of workflow automation and usability when following the various regulated methods and international standards.

What software capabilities are essential for streamlining workflows and complying with regulations with walkaway efficiency?

The walkaway productivity of the Gallery and Gallery Plus Aqua Master discrete analyzers is supported by custom-designed software that performs required calibration orders and relative standard error (RSE) calculations, routine quality-control (QC) schemes, automated spiking, flexible reporting, and easy rerun of samples requiring new dilution factors. These are the five most sought-after features that enable laboratories to fully automate their testing workflows while following the appropriate local regulations. Even the most complicated spiking, calibration, and QC procedures can be fully automated using the Gallery and Gallery Plus Aqua Master discrete analyzers.

Choice of automated calibration method and order with relative standard error calculation

Many regulatory bodies list the discrete analyzer methods that have been approved for drinking water and environmental analysis. These methods typically explain the approved method in detail, which can include procedures for creating the calibration curve that must be used to calculate the sample results. The most commonly specified calibration curve types are relative response factor, linear, quadratic, or weighted quadratic.[2] The approved method may also require the calibration to be performed in a specific concentration order, for example from low to high concentration to minimize carryover or vice versa. The software includes a comprehensive test-parameter configuration that allows a flexible definition of the calibration, including calibration order, to meet method-specific needs. Figure 1 shows how to select either an ascending or descending calibration order on the "Calibration" tab under the "Test definition" tab in the Gallery Aqua Master discrete analyzer software.

The industry-preferred method to determine calibration quality is the RSE. The Gallery Aqua Master discrete analyzer software automatically calculates the RSE and flags the calibration, if the defined RSE limit is exceeded, providing instant feedback about goodness-of-fit. The RSE parameters are also defined in the "Calibration" tab (Figure 1).

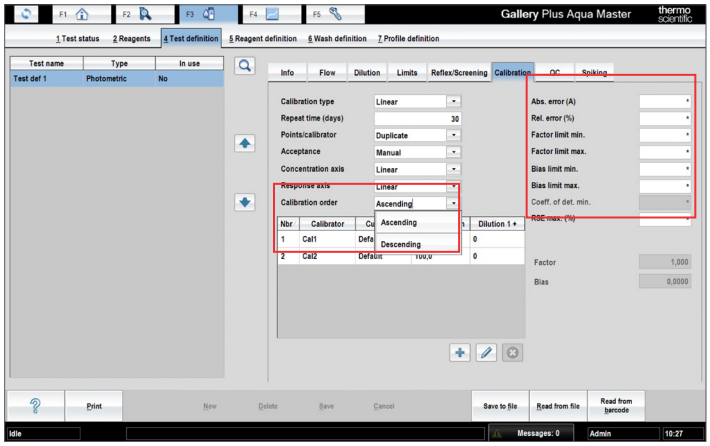


Figure 1. Choosing the calibration order to meet method requirements—either ascending or descending—is fast and easy when using the Gallery Aqua Master discrete analyzer software. The RSE limits used for automated error flagging are defined in the same software tab.

Automated quality assurance/quality control (QA/QC) procedures

QA/QC requirements, including procedures and intervals, are usually described in either the standard methods to be followed or in the instructions and guidance documentation provided by the relevant regulatory body. Common method QA/QC procedural requirements include:

- Demonstration of capability (DOC)
- Method detection limit (MDL)
- Laboratory reagent blank (LRB), also referred to as method blank (MB)
- Laboratory-fortified blank (LFB), also referred to as a spiked blank, or laboratory control sample (LCS)
- Matrix spike (MS) and matrix spike duplicate (MSD), or laboratory-fortified matrix (LFM) and LFM duplicate to assess precision, particularly if matrix interference is a concern
- Calibration (initial and continuing), also referred to as initial calibration verification (ICV) and continuing calibration verification (CCV)

The Gallery Aqua Master discrete analyzer software enables laboratories to define the QA/QC procedures that will be automatically run at what intervals, and if they should be carried out at the start or end of a run. To fulfill a variety of U.S. EPA and international regulatory and method requirements, the choice and setup of the automated QA/QC procedures are highly flexible. If multiple QC procedures must be run, their sequence is easy to define in the software.

Figure 2 shows the software's "Configuration" tab which the laboratory can select to automatically perform "Procedure specific" QC from the "QC in start and end of run" pull-down field. For backward compatibility with and to mimic previous versions of the software "Yes" or "No" can be selected from the pull-down menu. The QC procedure that triggers "Start of run" and "End of run" is configured in the "QC" tab (Figure 3). These triggers can be independently chosen and automatically applied to each QC procedure. If multiple QC procedures must be run, then the order is defined in the "Procedure" list. "Move up" and "Move down" buttons make it easy to change the order the procedure is applied.

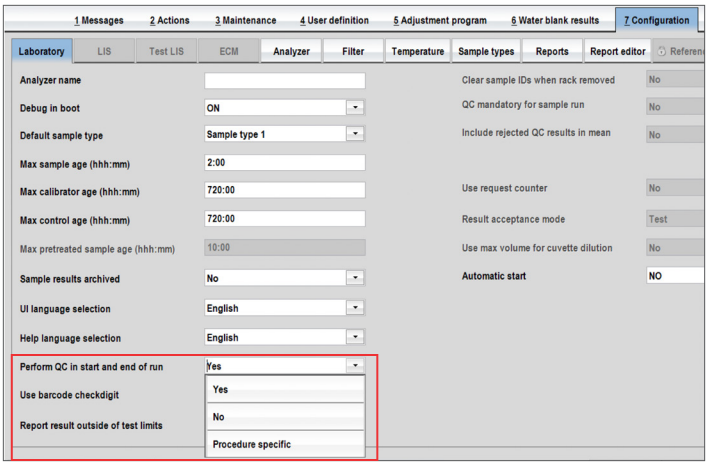


Figure 2. In the Configuration tab, it can be defined whether an additional QC at the start and end of analysis is performed.

Analytical controls provide a standard to which comparisons are made for QC purposes. Controls can be part of a specific, or of all, run groups. Each time a QC procedure is run, the software will run the controls appropriate for the current run group as defined by the user in the "QC' tab shown in Figure 3. The order for a run group is defined by the order in the table and can be readily changed using the "Move up" and "Move down" buttons. Charting QC data is essential to visualizing trends in analytical and laboratory performance. Automated collection and transfer of QC data into the Gallery Aqua Master discrete analyzer's QC Charts feature saves an enormous amount of time compared to manually transferring the data to another software (Figure 4).

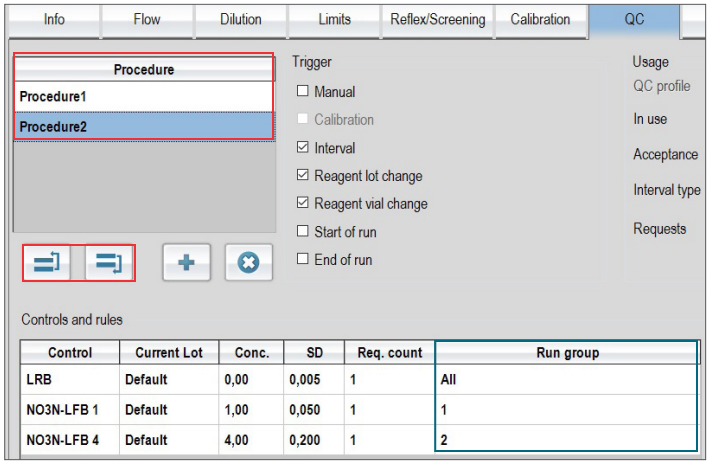


Figure 3. The "QC" tab is used to define the desired QC triggers, as well as controls and rules. If multiple QC procedures are triggered at the same time, their running order is set up in the "Procedure" list. "Move up" and "Move down" buttons make it easy to change the order of procedures or control runs.

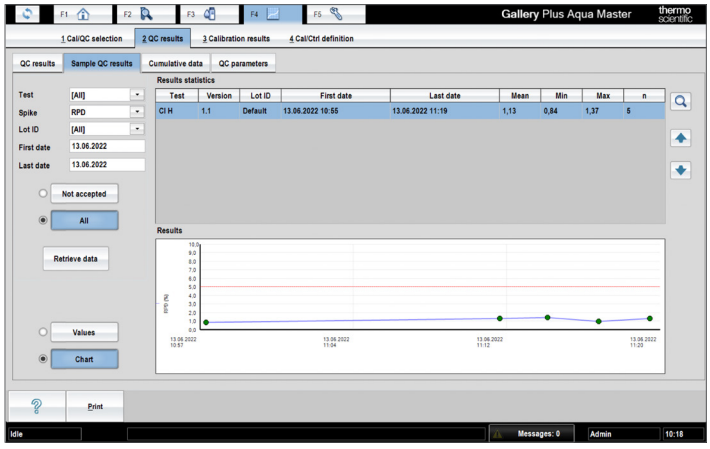


Figure 4. The Gallery Aqua Master discrete analyzer software can automatically chart QC data, making it easy to observe trends in performance.

Automated spiking procedure for easy identification of sample-matrix-related interferences

The Gallery Aqua Master discrete analyzers include an automated sample spiking procedure that can be used to streamline the identification of sample-matrix-related interferences (Figure 5). The procedure makes it easy to evaluate the performance of an analytical procedure for a specific sample matrix and the validity of the test results. To maximize flexibility, the spiking series can be automatically and repeatedly performed at user-specified intervals based on number of samples, or the laboratory can elect to spike selected samples manually.

Automated spiking saves a lot of time and reduces error compared to manual sample spiking which typically involves manually making spike samples and calculating the results in another software. The spiking series includes three samples: the native sample, spiked sample, and its duplicate. The spiked sample is prepared by adding a known quantity of analyte (spiking standard) to a sample. The spiked sample and its duplicate are then analyzed, and the quantification results calculated in the same manner as native sample. After analysis, the software calculates the analyte concentration for native and spiked samples, recovery for both spiked samples, and the relative percent difference (RPD) between the spiked samples. The software allows definition of minimum and maximum limits for percent recovery and the maximum limit for percent RPD (Figure 5). If the results obtained are not within the defined limits, the corresponding errors are displayed in the results view.

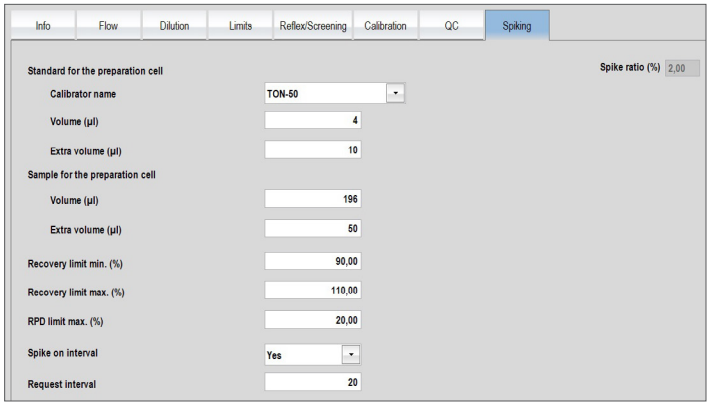
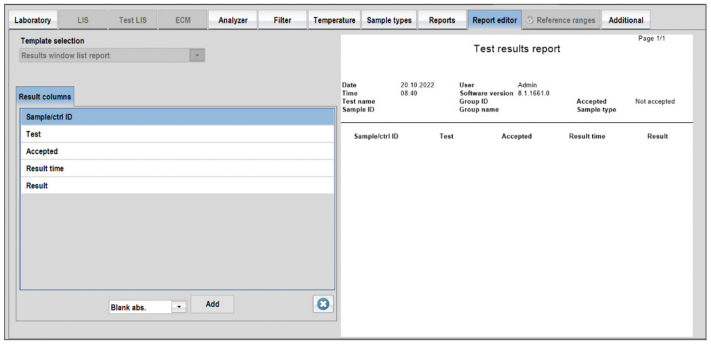


Figure 5. The Gallery Aqua Master discrete analyzer software provides for automated sample spiking that can streamline identification of sample-matrix-related interferences, including minimum and maximum limits for percent recovery and maximum limit for percent RPD.

Flexible results reporting with predefined and customizable templates

The Gallery Aqua Master discrete analyzer software offers versatile capabilities for results reporting, including predefined and easily customizable report templates that can be accessed in the “Report editor” tab (Figure 6). The easy-to-use report editor allows customization of reports in both pdf and spreadsheet formats to meet laboratory needs. Reports can be organized by sample, batch, or test. The default report templates provide fixed results-column formats, while the customizable templates enable users to select the results columns to display. The report editor also allows customization of the header texts, logos used, and more.



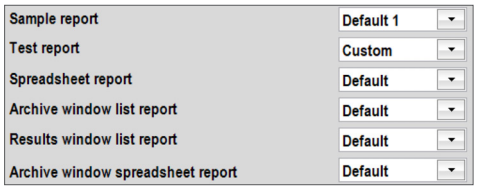


Figure 6. The report editor includes versatile capabilities to report test results, including report templates that can be easily customized to meet laboratory needs.

Easy rerun of one or many samples if a new dilution factor must be applied

If needed, the Gallery Aqua Master discrete analyzer software makes it easy to rerun samples using a new dilution factor. Simply select the samples to rerun and then enter the new dilution factor under the “Results” tab (Figure 7). Multiple samples can be rerun without having to individually define a new dilution factor for each.

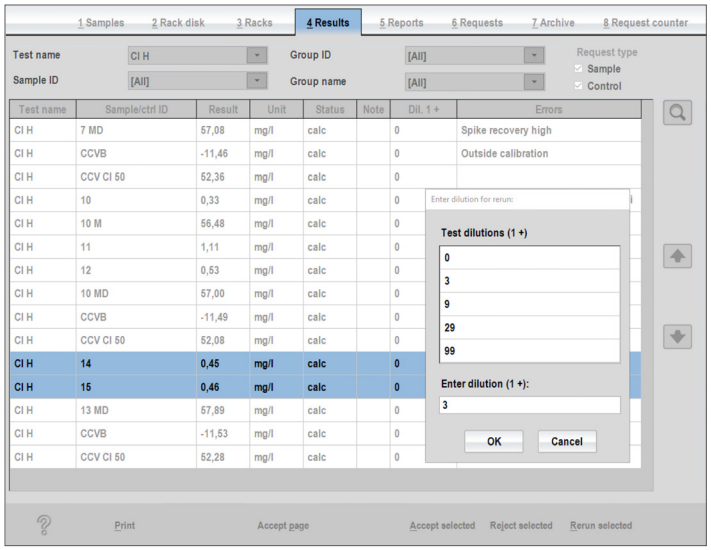


Figure 7. To rerun samples using a new dilution factor simply select the samples to rerun and then enter the new dilution factor.

Conclusion

Now it's easier than ever to streamline the flow of your laboratory's water and nutrient analyses. Master the efficiency of the Gallery Aqua Master and Gallery Plus Aqua Master discrete analyzers—easy-to-operate automated systems created specifically for simultaneous multiparameter water and nutrient analyses. The analyzers are powered by custom-designed software that helps laboratories meet local regulations, with high-throughput automation and walkaway efficiency.

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1. Thermo Scientific Smart Note. Wastewater surveillance of COVID-19. SN000035-EN 0621M. [Online] 2021. https://assets.thermofisher.com/TFS-Assets/CMD/brochures/sn-000035-da-wastewater-surveillance-covid-19-sn000035-en.pdf (accessed November 4, 2022).
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