

Lab Water: The Critical Factor You're Missing in Chemical Trace Analysis

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Chemical trace analysis is essential for detecting harmful contaminants in environmental samples like soil, air, and water. Tanja Kuschnick, Laboratory Specialist at TÜV Rheinland Energy & Environment GmbH, highlights the crucial role of ultrapure water in ensuring the accuracy and reproducibility of trace analysis and explains how her team selected their own laboratory water purification system for chromatography sample preparation and analysis.



Why Monitor Trace Contaminants?

Substances that pose a risk to human health can appear anywhere. Per- and polyfluoroalkyl substances (PFAS), for example, are widely used in industrial and consumer products and, as a result, often find their way into our environment. Their strong C-F bonds make PFAS nearly indestructible, both in the environment and in the human body, where they are linked to adverse health effects. Chemical trace analysis of environmental samples, such as soil, air, and water, is the only way to identify harmful contaminants like PFAS, pharmaceutical residues, and pesticides. It involves measuring extremely low concentrations of chemical elements or compounds in a sample, often in parts per million (ppm), parts per billion (ppb), or even parts per trillion (ppt).

This is the work of Tanja Kuschnick, [Laboratory Specialist] at TÜV Rheinland Energy & Environment GmbH in the laboratory for environmental and special analyses in Hildesheim. The laboratory under the direction of Dr. Katja Latendorf is part of a global organization offering testing, inspection, and certification services across various industries. In the lab, Tanja Kuschnick performs trace analysis on environmental substances—water, and solids such as soil samples, and air—to assess industrial and environmental conditions. Throughout this short article, she shares her perspective on the critical role ultrapure water plays in getting clean data.

Role of Ultrapure Water in Trace Analysis

The trace analysis workflow begins with sample preparation and processing, followed by analysis using highly sensitive instruments such as Headspace Gas Chromatography-Mass Spectrometry (HS-GC-MS), Gas Chromatography-Mass Spectrometry (GC-MS), High-Performance Liquid Chromatography (HPLC), and Liquid Chromatography-Mass Spectrometry (LC-MS). The results are then compiled into a report, ensuring strict adherence to documentation and quality standards.

As the largest volume component of the mobile phase in LC-based analysis, lab water plays a crucial role, affecting sample preparation, column rinsing, and elution. However, it is often overlooked compared to other reagents such as standards and organic solvents.

“Our lab relies on 50 to 100 liters of ultrapure water daily for everything from sample preparation to rinsing glassware and chromatography,” explains Kuschnick. “The water quality is critical. Tap water is unusable even for rinsing, so our lab water systems must consistently provide the highest purity. Without ultrapure water, we simply cannot perform our accredited analyses.”

A 2024 published study found that in-house utilities deionized (DI) water (commonly used due to its availability and cost-effectiveness) or even bottled LCMS-grade water can introduce contaminants that interfere with data accuracy and robustness of the system¹. Total Organic Carbon (TOC) impurities, for example, can accumulate on the column and gradually elute, leading to an upward drift in the baseline.

This highlights the importance of carefully controlled lab conditions and the use of ultrapure reagents, particularly ultrapure water, in trace analysis (see Table 1).

Criteria for Efficient Contaminant Removal

Even trace amounts of contamination can skew data, cause errors in blanks or calibration samples, and lead to artificially high sample concentrations. That is why customized water purification systems are needed to meet the strict purity standards required for trace analysis of volatile organic compounds (VOCs), PFAS, and other compounds. Kuschnick adds, “We test for contaminants like PFAS and VOCs, with thresholds varying by substance; PFAS at sub-ppt to single-digit-ppt levels, and VOCs at ppb levels. Water quality directly impacts our testing sensitivity, as even the smallest impurity can skew our data.”

Contaminant Type	Example	Reduction Target
Ionic impurities	Dissolved salts, minerals, chloride, sodium, calcium	Resistivity of 18.2 MΩ.cm
Organic compounds	Trace organics	TOC < 10 ppb
Trace elements	Bacteria, fungi, endotoxins	Undetectable levels
Particles and colloids	Particles larger than 0.22 µm	Minimized
Microbiological contaminants	Bacteria, fungi, endotoxins	Undetectable levels
Dissolved gases	Carbon dioxide, oxygen, and nitrogen	Minimized

Table 1: Water quality requirements for reliable trace analysis.



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[Laboratory Specialist LE], TÜV Rheinland Energy & Environment GmbH

When selecting an ultrapure water system, Dr. Latendorf and her team considered all contaminants that could interfere with analysis, including limits for TOCs, dissolved ions, trace metals, colloids, and microbial contaminants. Lab water purification systems incorporate various strategies to remove or reduce these impurities to undetectable levels, as described by ASTM water purity standards.

A Reliable System for Daily Testing

Dr. Latendorf and her team evaluated several water purification systems before choosing Sartorius' Arium® Pro VF Benchtop Type 1/Ultrapure Water Purification System. This system provides the highest purity water for sensitive lab applications, including chromatography. It has a UV lamp, an integrated TOC monitor, and a built-in ultrafilter. UV light prevents microbial growth and helps reduce TOC levels, which are continuously monitored by the real-time TOC analyzer. Additionally, the built-in ultrafilter uses crossflow technology to remove endotoxins, microorganisms, particulates, and nucleases (DNases and RNases), ensuring the ultrapure water meets the high sterility and low contamination requirements for critical applications.

“Aside from the reliable water quality, we love the user-friendly interface, which displays conductivity for easy monitoring and maintenance,” says Kuschnick. “It fits our needs perfectly, from the reliable dispensing to the flexible installation that adapts to our lab’s layout. We also appreciate the comprehensive support from Sartorius, including on-site assistance, which keeps our water system running.”

Arium® Pro systems are differentiated by their purification techniques (e.g., UV-light or ultrafilter), integrated features (e.g., TOC analyzer), and design (wall-mounted, integrated

under bench or benchtop). All Arium® Pro systems meet and exceed the ASTM Type 1 quality standards for ultrapure water. According to a cost analysis study, using a premium lab water system like Arium® is also more cost-effective in the long run than relying on bottled water for chromatographic studies¹.

Another system highly recommended by Kuschnick is the Arium® Smart Station for remote water dispensing. Up to three of these can connect with an Arium® Pro unit, providing a cost- and space-saving way to expand access to ultrapure water across the lab.

Conclusion

Trace analysis is vital for monitoring environmental contaminants in soil, water, and air, helping to assess pollution levels and their potential impacts on ecosystems and human health. In these labs, preventing impurities in samples and instrument blanks and standards is a milestone of acquiring accurate testing data. Sartorius plays a key role in supporting these critical applications by providing reliable flexible, and user-centric ultrapure water systems tailored to the specific needs of trace analysis.

References

1. C. Prochaska, K. Kureja, L. Morrison, I. Surowiec, Application Note: Minimizing LCMS Artifacts Using Arium® Ultrapure Water Systems, 2024.

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