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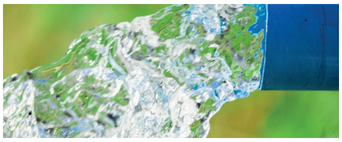

Water Analysis using ICP-MS: A New, Simplified Approach

Ed McCurdy, ICP-MS Product Marketing, Agilent UK

Routine water analysis might appear to be one of the easier applications for ICP-MS. The samples generally – though not always – have low matrix levels and the analytes do not require measurement at extremely low or high concentrations. The aqueous matrix is also ideal for ICP-MS sample introduction systems, and there is usually plenty of sample available so conventional sample preparation and handling approaches can be used. However, water analysis is now typically performed in highly competitive commercial laboratories, which brings a different set of challenges for instrument manufacturers. Throughput, productivity, and return on investment are priorities in these labs, along with ease-of-use, and fast training for new users. In this issue of the ICP-MS Journal, we discuss how Agilent is addressing these commercial priorities.

Figure 1. Agilent 7800 ICP-MS coupled to an Agilent SPS 4 autosampler – an integral part of the Agilent Water Analyzer packages.

Streamline Your Regulated Water Analysis using an Agilent ICP-MS Water Analyzer Package

Gregory Lecornet, Mark Kelinske, and Ed McCurdy, Agilent Technologies

ICP-MS in Regulated Water Analysis

ICP-MS is a firmly established technique that has been adopted/approved for regulated analysis across many industries. In the field of regulated water analysis, both US EPA 200.8 and ISO 17294-2:2016 specify ICP-MS (*1, 2*). Method 200.8 requires 21 elements to be monitored in a range of water-based sample types, while 17294-2 lists 63 elements that may be measured using the method.

Since the EPA and ISO methods were first published in 1990 and 2004, respectively, ICP-MS has seen notable improvements in matrix tolerance and control of spectral interferences. These developments enable labs to run variable, high matrix waters and other environmental samples, leading to more labs investing in the technique.

For labs that don't yet use ICP-MS, the technique is often seen as complicated and difficult to use. Even for experienced labs, development and optimization of a new method and verification of its performance for regulated analysis can take several weeks or even months. These steps may take considerably longer in labs that are new to the technique. The time and cost of training new users can be a burden for some commercial labs, where success depends on getting new equipment into production as quickly and efficiently as possible.

Streamlining the Implementation Timeline

In developing the concept for the ICP-MS Water Analyzer package, we took a new look at the traditional approach to implementing an ICP-MS method. Working closely with experts in Partner Labs in the commercial water analysis sector, Agilent ICP-MS specialists evaluated all stages of the implementation process. From this, we identified the steps that take the longest and cause the most difficulty for labs that are new to ICP-MS. We then predefined and pretested the critical method parameters, allowing us to deliver a proven analytical method, as outlined in Figure 1.

The Agilent ICP-MS Water Analyzer provides an easier way to implement ICP-MS for regulated water analysis. It includes a complete bundle of hardware, methods,

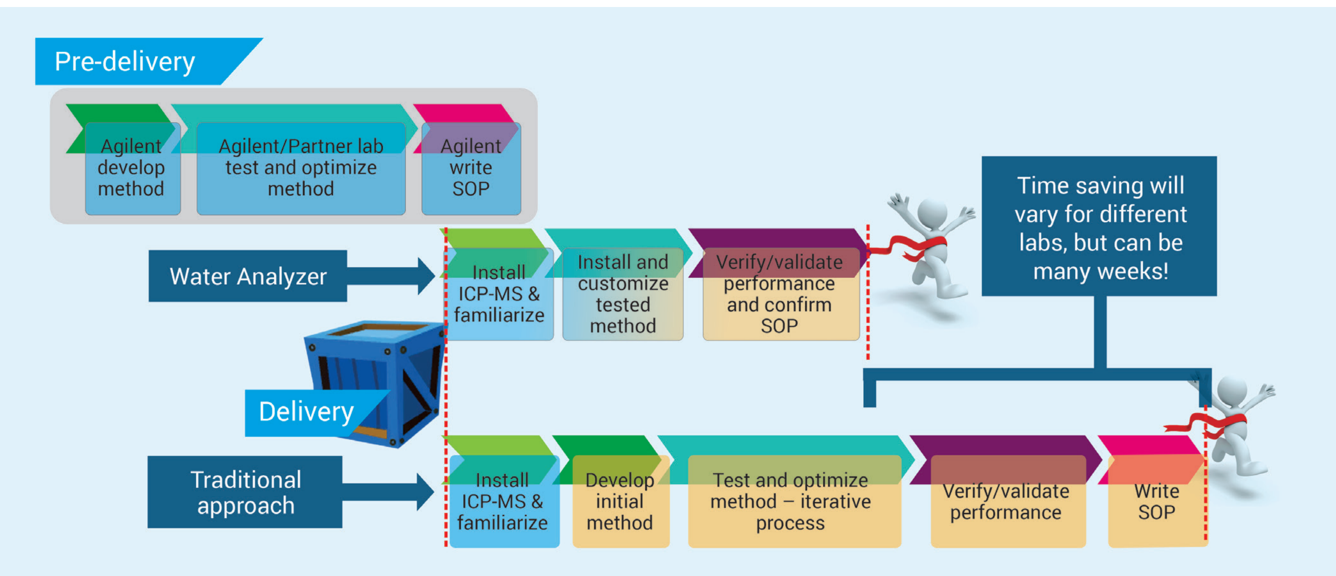

Figure 1. Installing a pretested and optimized ICP-MS method with supporting documentation and training could potentially save several weeks of work compared to developing, testing, and optimizing a new method in-house.

consumables, a simplified software interface, documentation, and a customized training package.

Figure 2. Some of the components of the Water Analyzer package.

The simplified method setup process provided by the Water Analyzer is of most benefit to labs that are new to ICP-MS. But the same concepts also benefit labs that are updating equipment or transferring methods, for example from Graphite Furnace AAS or ICP-OES to ICP-MS.

Proven ICP-MS performance

The Water Analyzer is based on the Agilent 7800 ICP-MS instrument. The 7800 ICP-MS includes Agilent's High Matrix Introduction (HMI) technology to easily handle varied, high-matrix samples. The methods use a single helium collision cell mode, providing ease-of-use as well as ensuring accuracy by controlling common polyatomic interferences. EPA 200.8 does not permit the use of collision/reaction cell modes for drinking water analysis, so the EPA 200.8 Water Analyzer includes a no gas mode method for these samples. The 7800 has a 10 orders linear dynamic range, which simplifies method setup by measuring major and trace analytes in a single run. The wide dynamic range also means fewer reruns due to over-range results.

For labs with extremely high sample numbers, throughput and productivity can be increased dramatically using the optional ISIS 3 discrete sampling device.

A Fully Operational Workflow

The Water Analyzer includes a method optimized and tested by experienced ICP-MS application engineers and Partner Lab experts. The method incorporates all the analytical, QC, and reporting requirements required by EPA 200.8 or ISO 17294-2:2016. A Standard Operating Procedure (SOP) with guide is also provided. Agilent will help you customize the SOP to your lab's specific workflow and analytical needs.

A Simplified and Easier-To-Use Interface

Agilent's ICP-MS Water Analyzers include the simplified, browser-based ICP Go software interface (as well as ICP-MS MassHunter). ICP Go's clear screen layout and simple workflow enables less experienced analysts to operate the 7800 ICP-MS with confidence. New user training can be completed in less than a day. The easy-to-use interface also makes it much easier for operators to transfer between analytical techniques, giving lab managers more staffing flexibility. More information will be given on ICP Go in the next issue of the ICP-MS Journal.

Training and Implementation Package

When your ICP-MS is ready to be installed, an Agilent Engineer will set up the instrument using agreed performance criteria, implement the method in your lab, and train your analysts on site. The engineer will follow a formal, documented process, providing the basis for the documentation that may be needed for final certification or regulatory approval.

References

1. J.T. Creed, C.A. Brockhoff, and T.D. Martin, Method 200.8, Revision 5.4 1994, accessed Nov 2018 https://www.epa.gov/sites/production/files/2015-08/documents/method_200-8_rev_5-4_1994.pdf
2. ISO 17294-2:2016 Water quality – Application of ICP-MS– Part 2: Determination of selected elements including uranium isotopes, accessed Nov 2018, https://www.iso.org/standard/62962.html

More Information

Find out more – including access to two short videos – by visiting the ICP-MS Analyzer webpage at: www.agilent.com/en/products/icp-ms/icp-ms-analyzers

The Agilent Water Analyzer and ICP Go software are currently available in North America and Western Europe only.

Optimizing ICP-MS Hardware Configuration for Reliable, Cost-Effective Routine Analysis

Ed McCurdy, Agilent Technologies Ltd, UK

Introduction

In Agilent ICP-MS Journal issue 73, we summarized some of the important factors that affect ICP-MS sample run times and cost of ownership in routine, high-throughput commercial laboratories (*1*). In this article, we show how hardware configuration and operating conditions contribute to ICP-MS usability and productivity.

These are important considerations for routine elemental analysis in industries such as food, environmental, pharmaceutical, mining, and clinical research. For many labs in these industries, ease-of-use and productivity are at least as important as ultimate detection limits.

Tolerance of High Matrix Levels

Robustness refers to the ability to successfully analyze samples containing high and variable matrix levels. Good robustness simplifies routine workflows by providing lower signal drift, fewer QC failures and recalibrations, and significantly reduced levels of routine maintenance. Robustness also contributes to lab efficiency by removing the need for specific dilutions to control the level of dissolved solids in sample digests.

Optimizing for robustness means selecting matrix-tolerant hardware and choosing operating conditions that maximize the plasma energy available for sample matrix decomposition. Key factors are:

- Nebulizer flow rate – lower solution flow reduces the sample/matrix loading on the plasma.
- Torch injector internal diameter (i.d.) – wider diameter injector means lower aerosol density and so better transfer of energy from the plasma.
- Plasma RF power – higher power increases sample decomposition.
- Flow rate of the gas that carries the aerosol through the plasma – lower flow means the sample droplets spend longer in the plasma, improving decomposition.

Sensitivity and matrix tolerance are interrelated, so must be considered together. Matrix tolerance – or plasma robustness – is monitored using the ratio of CeO^+ to Ce^+ (the oxide ratio). A low CeO/Ce ratio shows the plasma can dissociate the strongly bound Ce-O molecule, so has high enough energy to decompose the sample matrix.

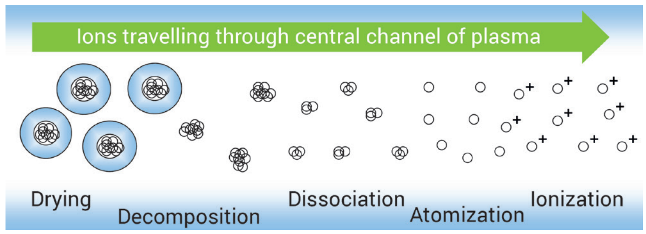

Figure 1. A robust plasma provides optimum processing of the aerosol droplets as they pass through the plasma.

Better matrix tolerance allows more variable samples to be measured in a routine analysis batch and reduces the need to matrix-match the calibration standards. A robust, high-temperature plasma also increases the degree of ionization (and therefore sensitivity) of poorly ionized analytes, such as Be, As, Se, Cd, and Hg.

Interface geometry and ion lens voltages can also be optimized for best matrix tolerance. However, increasing matrix tolerance usually reduces sensitivity.

Aerosol Dilution

Autodilution can allow higher levels of sample matrix to be presented to the instrument, but auto dilutors are expensive, complicated, and prone to leaks and blockages. Agilent's High Matrix Introduction (HMI) system uses an alternative approach called aerosol dilution to dilute the sample after the aerosol has been formed. This has several benefits compared to conventional liquid dilution. The diluent is argon gas, rather than a liquid, so the possibility of contamination is avoided. HMI also eliminates the periodic maintenance checks associated with using a liquid diluent.

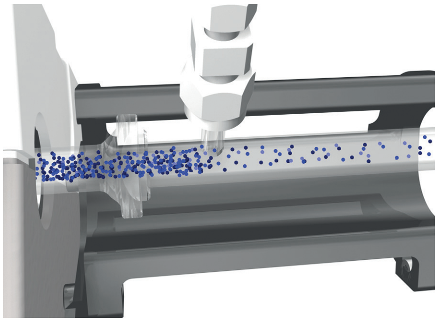

Figure 2. Schematic representation of the aerosol dilution process using Agilent's HMI. Ultra HMI (UHMI) offers extended dilution range.

HMI further contributes to productivity by improving sample decomposition and so decreasing matrix deposition on the interface cones. This improves long-term stability, reduces recalibrations, and extends the period before routine maintenance is required.

Control of Interferences

Reducing spectral interferences has obvious implications for data quality. The way interferences are controlled also has a major impact on ease-of-use and productivity.

In many routine ICP-MS applications, sample types are variable, so matrix-based polyatomic interferences vary unpredictably from sample to sample. A "universal" approach to interference control is highly beneficial as it allows consistent conditions to be applied to the analysis of different and unknown sample types.

Agilent's Octopole Reaction System (ORS) collision/reaction cell (CRC) uses an octopole ion guide in a small internal volume cell. This is the optimum design for selectively removing polyatomic ions using kinetic energy discrimination (KED) with helium (He) cell gas. He mode was pioneered by Agilent in the early days of CRCs. It is now accepted for multi-element analysis across a wide range of typical ICP-MS sample types.

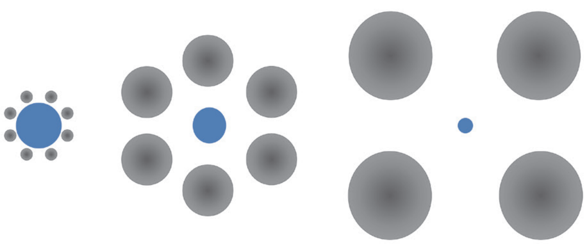

Figure 3. Illustration of how ORS octopole ion guide provides a wide ion stability region in a small internal volume cell – the ideal configuration for efficient interference removal in collision mode with helium cell gas.

Using a single He cell gas mode for multiple analytes in multiple sample types significantly improves laboratory efficiency. He mode eliminates the time-consuming, sample-specific method development required with reactive cell gases or interference correction equations. The impact is greatest in high-throughput labs where variable and unknown sample matrices are analyzed routinely, and minimal time is available for the development and optimization of specific methods.

Measurement of Major and Trace Elements

ICP-MS is usually more than capable of delivering the required method detection limits for routine applications. In many labs, measuring high concentration analytes is much more problematic. Agilent ICP-MS systems use a detector with a very wide dynamic range, covering 10 or 11 orders of magnitude. This allows major elements at concentrations of 100s or 1000s of mg/L (ppm) to be measured in the same acquisition as the trace analytes.

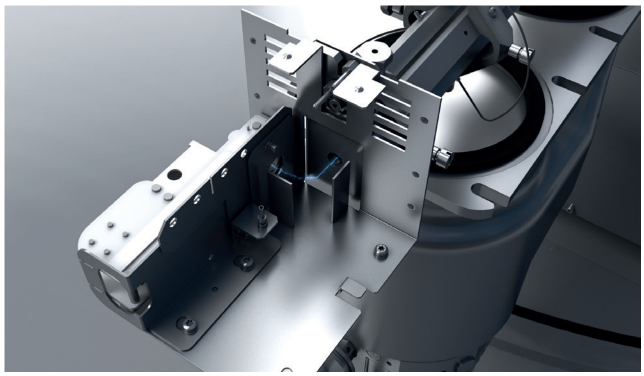

Figure 4. Agilent ICP-MS off-axis Orthogonal Detector System with wide (10 or 11 orders) dynamic range.

Agilent ICP-MS systems achieve their dynamic range without specific tuning to reduce ion transmission or detector gain, as required on other ICP-MS systems. This is crucial for ease-of-use and productivity.

Conclusions

Agilent's ICP-MS instruments have inherently high sensitivity, allowing a design focus on maximizing robustness and ease-of-use. This makes Agilent ICP-MS systems ideally suited to routine sample analysis in commercial laboratories.

Reference

Agilent ICP-MS Journal 73, 5991-9465EN

New Regulations for Trace Level Radioisotopes in Water: Resolving Peak Overlaps using ICP-QQQ with MS/MS

Glenn Woods, Agilent Technologies Ltd, UK

ISO Standard for Radionuclides in Water

Radioactive isotopes are distributed throughout the environment. Some, including Ra, Rn, Th, and U, occur naturally in radioactive minerals in rocks such as granite. Others, e.g. the transuranic elements Pu, Np, and Am, are man-made. These elements may be released intentionally or accidentally from nuclear power plants, from weapons testing, and from disposal of industrial, medical, and domestic products such as smoke alarms. Radionuclides in watercourses can enter the domestic drinking water supply, so they are strictly regulated and monitored.

The International Organization for Standardization (ISO) recently introduced a new standard, ISO 20899:2018 (*1*), for the determination of ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{237}Np in waters by ICP-MS. The method is suitable for activity concentrations in the range:

- 1 mBq/L to 5 Bq/L for ^{239}Pu, ^{240}Pu, and ^{237}Np
- 1 to 5 Bq/L for ^{241}Pu

Higher concentrations may be measured after appropriate dilution. The activity concentration is calculated from the mass concentration (in µg/L (ppb)) measured by ICP-MS, and the known specific activity (in Bq/g) for each isotope.

Importance of Abundance Sensitivity in ICP-MS

Samples that contain Np and Pu usually also contain U, even after chemical separation. Ultratrace analysis of ^{237}Np and ^{239}Pu is difficult by single quadrupole ICP-MS because of peak tailing from the adjacent ^{238}U peak.

The contribution a peak makes to its neighbors is called Abundance Sensitivity (AS). Single quadrupole ICP-MS can achieve AS of around 1×10^{-7}. This level of AS means that a peak of 1×10^{7} counts per second (cps) contributes 1 cps to the adjacent masses. High intensity peaks can therefore make a significant contribution to the peaks either side. High Resolution-Sector Field (HR-SF) ICP-MS has better resolution than single quadrupole ICP-MS, but poorer AS.

Triple quadrupole ICP-MS (ICP-QQQ) uses two mass filters (Q1 and Q2) to improve mass filtering. The AS of a QQQ is the product of the AS of the two mass filters: Q1 AS x Q2 AS – giving a theoretical overall AS of about 10^{-14}.

Neptunium by ICP-MS/MS

A standard configuration Agilent 8900 ICP-QQQ was used to determine ultratrace Np in a 10 mg/L (ppm) U matrix. A MS/MS method with O_2 reaction gas was used to mass-shift Np to NpO_2. In addition to separating the peak tail from ^{238}U, the method also resolves the various low-level UHx interferences that could compromise ultratrace level analysis of ^{237}Np .

Figure 1 shows a calibration for ^{237}Np at ng/L levels in the U matrix. The curve coefficient was 1.0000, the Detection Limit (DL) was 0.56 pg/L (ppq) and the Background Equivalent Concentration (BEC) was 0.32 pg/L. The results illustrate the suitability of the 8900 ICP-QQQ for analysis of ultratrace radionuclides in the presence of uranium.

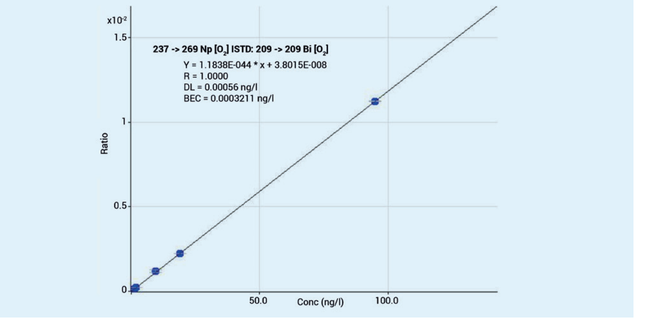

Figure 1. Calibration curve for ^{237}Np as NpO_2 in a 10 ppm uranium matrix.

Reference

1. ISO 20899:2018 water quality -- Plutonium and neptunium -- Test method using ICP-MS, accessed Nov 2018, www.iso.org/standard/69404.html

Stay Productive with ICP-MS MassHunter Software Maintenance Agreement

Alan Spilkin, Software Services Product Manager, Support and Services Division, Agilent Technologies, USA

Get Timely ICP-MS MassHunter Updates

When you buy an Agilent ICP-MS MassHunter software product, a 1-year Agilent Software Maintenance Agreement (SMA) is included. The SMA provides free software updates and upgrades, as well as unlimited telephone-based software support. After the first year, the SMA may be renewed annually, ensuring cost effective software update management over the life of the ICP-MS instrument and software.

Activate the SMA in SubscribeNet Web Portal

Agilent's SubscribeNet portal is a web-based service, which provides registered software users 24x7 access for software and SMA license management.

Registering your ICP-MS MassHunter software in SubscribeNet web portal automatically starts the 1-year SMA. Registration is quick and easy:

1. Locate the authorization code in your ICP-MS software package. Peel the label off the product packaging and place it on the Software Entitlement Certificate supplied with your instrument/software.

2. Follow the directions contained in the ICP-MS software package or visit the SubscribeNet portal: https://agilent.subscribenet.com
3. If you are already a registered SubscribeNet user, simply log into your account.
4. If you are not a registered SubscribeNet user, click the New User link at the bottom of the login page.
5. Once you have logged into your SubscribeNet account, select the "Register Software" tab on the side menu.
6. Enter your authorization code.

Your ICP-MS MassHunter software is now registered and your SMA is active.

If you bought ICP-MS MassHunter software and have not completed the software registration process, it is never too late to do so. If you cannot locate your software registration authorization code and you have not registered the software, contact your local Agilent representative to obtain a replacement code.

Stay Up-To-Date for Maximum Productivity

When you register your ICP-MS MassHunter software, the SMA begins and ICP-MS MassHunter software updates and upgrades are immediately available via download or media request. Both services are free to owners of current SMAs. Within SubscribeNet, you can opt in to receive automatic email notifications regarding new software version availability, as well as SMA contract expiration and renewal information. Maintaining your ICP-MS software on the latest version provides access to new software features, and ensures maximum software and instrument efficiency.

Talk to Agilent Software Experts

If you need software assistance, an SMA provides ICP-MS MassHunter users access to unlimited telephone-based software support. Expert help improves learning, reduces support calls, and maximizes instrument uptime.

More Information

ICP-MS MassHunter Software

Agilent Seminars, Meetings and Events: Join Us at the EWCPS 2019

Are you attending the European Winter Conference on Plasma Spectrochemistry (EWCPS) February 3-8, 2019, Pau, France? Join us at one or more events to be held during the conference. Learn how Agilent's technologies and solutions are pushing the boundaries of what is possible in research. Registration for all of Agilent's activities at the EWCPS 2019 is now open. Get your tickets for a complete Agilent experience!

- Short course: Fundamentals of MS/MS, Sunday Feb 3 at 13:30.
- ICP-MS MassHunter workshop, Monday Feb 4 at 17.30.
- Lunch seminar: Pushing boundaries of what is possible in research, Tuesday Feb 5 at 12.25.
- Company night, Wednesday Feb 6 at 19:00.
- ICP-MS MassHunter and ICP Go live demos, Monday to Friday at the Agilent booth.

Find out more and register here.

Places are limited – so book a place soon to avoid disappointment.

On-Demand Webinar

Title: How to Streamline Implementation of ICP-MS for Regulated Water Analysis
Speakers: Gregory Lecornet and Ed McCurdy
Host: Spectroscopy

Register here

Title: Tracing the Origin of Food: Establish Food Authenticity using Elemental Profiling
Speakers: Susan Ebeler, Courtney Tanabe, and Jenny Nelson
Host: Separation Science

Register here

Agilent ICP-MS Publications

- **Application note:** Analysis of Ultratrace Impurities in High Purity Copper using the Agilent 8900 ICP-QQQ: Low-ppt determination of alkali metals in high matrix samples using the optional m-lens, 5994-0383EN
- **Application note:** Accurate Analysis of Trace Mercury in Cosmetics using the Agilent 8900 ICP-QQQ: Effective removal of tungsten-based interferences on five Hg isotopes using MS/MS, 5994-0461EN
- **Flyer:** Agilent EPA 200.8 Water Analyzer, 5994-0193EN
- **Flyer:** Agilent ISO 17294 Water Analyzer, 5994-0194EN
- **Flyer:** Agilent ICP Go Software-Elemental Analysis Made Easy, 5994-0213EN
- **Brochure:** Solution-ready Agilent 7800 ICP-MS, 5991-5874EN

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