응용 자료

Improving the Longevity of PFAS Method Calibration Data with the Xevo TQ Absolute XR Mass Spectrometer

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Application Brief

This is an Application Brief and does not contain a detailed Experimental section.

Abstract

The need to rerun method calibration curves costs companies time and money, decreasing the amount of time an environmental laboratory can spend running samples that generate meaningful results or potential revenue. This creates a demand for robust method calibrations that can be used for weeks at a time, particularly in the world of per- and polyfluoroalkyl substances (PFAS) testing, where reagent standards and internal standards are costly, run times can be relatively long, and the number of concentration levels can be large. With the Xevo™ TQ Absolute XR Mass Spectrometer and waters_connect™ for Quantitation Software, environmental laboratories can be confident that their instrument will maintain accurate method calibration for up to 5 weeks while analyzing challenging matrices.

Benefits

- Up to 5 weeks of accurately calculated concentrations using the same method calibration curve with fewer interruptions for recalibration
- waters_connect for Quantitation Software faciltates the re-use of exisiting calibration curves without having to re-acquire standards
- Reduced method calibration frequency results in lower consumption of expensive PFAS reagent standards and internal standards, enabling laboratories to analyze more customer samples

Introduction

PFAS testing is now a crucial part of environmental monitoring, with companies depending on accurate results to comply with regulatory requirements and maintain quality standards. Method calibration underpins the accuracy of calculated concentrations, but it requires significant time and resources. Reducing the frequency of method calibration, while maintaining confidence in results, can offer substantial operational and cost benefits.

Many laboratories are forced to recalibrate after one week. Demonstrating that a calibration can remain valid for longer would reduce the need for repeated method calibration runs, allowing more time for sample throughput and minimizing interruptions in workflow. Moreover, when method calibration performance is validated over extended periods and across diverse matrices such as surface water, biosolids, and landfill leachate, it reinforces confidence in the robustness of the method.

As part of a robustness study using the Xevo TQ Absolute XR Mass Spectrometer, replicates of surface water, biosolids, and landfill leachate extracts were run alongside solvent QCs.[1] This data, for 42 PFAS compounds, was then reviewed against the method calibration curves acquired at the beginning of the sample set. QC standards were assessed every 10 matrix injections to see how long they would stay within a ±30% tolerance of the initial method calibration. The data presented here was acquired 10 weeks into the original robustness study to showcase how the method calibration is maintained on a system that has already run many challenging samples.

Experimental

Samples included river water, biosolid, and landfill leachate. River water was collected in Scotland, UK, from the

River Tay. Biosolid (domestic sludge, National Institute of Standards and Technology (NIST) 2781) and landfill leachate (LGC 6177) were both purchased as reference materials.

Extraction and solid-phase extraction (SPE) clean-up were carried out as outlined in previously published work [2–3] with 250 mL river water, 0.5 g biosolid, or 25 mL landfill leachate as the relevant sample sizes. Matrix injections alternated between extracts of biosolids, surface water, and landfill leachate, with QC standards injected after every 10 matrix injections. Linear, 1/x weighted calibration curves were plotted on the first day, with all data from the following days measured against these plots.

At the time of this calibration and sample set, the instrument had already completed over 7,000 matrix injections, providing a meaningful demonstration of method durability and system resilience under extended operational conditions.

Results and Discussion

Method calibrations were created for 42 PFAS analytes, with all returning Relative Standard Error (%RSE) values of <20%.[4] The calculated concentration was determined for every QC standard injection of all 42 PFAS analytes over the subsequent 35 days. This concentration was then used to plot the trueness of the calculated concentration to assess any deviation, with a ±30% tolerance. Figure 1 presents a 35-day trueness plot for 42 PFAS analytes, showing how well QC injections align with the original method calibration curves over time. The Xevo TQ Absolute XR Mass Spectrometer maintained method calibration integrity for up to 5 weeks, even after more than 7,000 injections involving complex samples like biosolids, surface water, and landfill leachate.

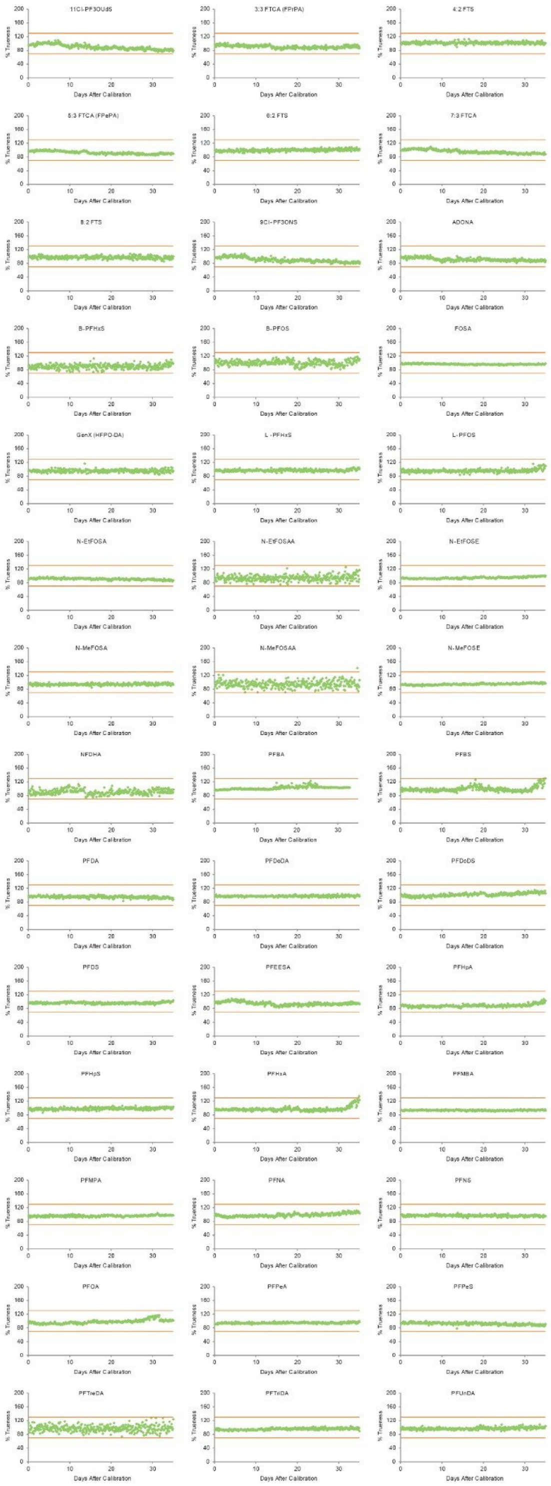

Figure 1. Trueness (%) plots for 42 PFAS with 30% tolerance lines in orange.

Table 1 shows the mean measured concentration of each PFAS for all QC injections, as well as the agreement between the measurements expressed as % RSD. The majority of analytes returned %RSD of <10% showing good precision over 35 days of QC measurements while also injecting complex matrices. The %RSE for each calibration graph is also displayed, apart from Total PFOS and Total PFHxS, which were calculated using the Totals feaure in waters_connect for Quantitation Software from their respective branched and linear isomers.

PFAS	Mean Concentration (ng/mL)	%RSD	Calibration %RSE
11Cl-PF3OUdS	0.14	11.6	8.8
3:3 FTCA (FPrPA)	0.38	5.7	6.9
4:2 FTS	0.38	3.2	3.5
5:3 FTCA (FPePA)	1.77	4.8	7.1
6:2 FTS	0.39	3.5	5.0
7:3 FTCA	1.76	6.5	7.6
8:2 FTS	0.37	4.1	6.5
9Cl-PF3ONS	0.14	11.1	7.5
ADONA	0.16	6.5	8.9
Branched-PFHxS	0.02	7.7	10.2
Branched-PFOS	0.03	7.5	7.4
FOSA	0.09	1.6	6.6
GenX (HFPO-DA)	0.19	4.0	10.4
Linear-PFHxS	0.07	3.0	5.8
Linear-PFOS	0.07	4.4	8.5
N-EtFOSA	0.09	3.4	9.8
N-EtFOSAA	0.07	8.6	6.3
N-EtFOSE	1.00	3.5	8.8
N-MeFOSA	0.09	2.7	6.6
N-MeFOSAA	0.07	11.0	7.5
N-MeFOSE	0.98	2.8	8.0
NFDHA	0.20	8.8	10.3
PFBA	0.41	4.1	7.8
PFBS	0.09	8.2	7.2
PFDA	0.09	3.5	10.3
PFDoDA	0.10	2.2	6.4
PFDoDS	0.11	5.8	9.3
PFDS	0.10	2.6	7.6
PFEESA	0.18	5.4	9.8
PFHpA	0.09	5.0	6.4
PFHpS	0.10	3.3	9.1
PFHxA	0.10	6.6	9.6
PFMBA	0.19	2.6	8.8
PFMPA	0.20	4.1	6.9
PFNA	0.11	5.4	7.8
PFNS	0.10	2.5	8.2
PFOA	0.10	5.4	9.5
PFPeA	0.19	3.0	7.7
PFPeS	0.09	4.0	8.2
PFTreDA	0.10	10.0	8.3
PFTriDA	0.10	2.8	5.5
PFUnDA	0.10	3.6	8.7
Total PFHxS	0.10	3.9	N/A
Total PFOS	0.10	4.3	N/A

Table 1. Mean concentration, %RSD and %RSE for 42 PFAS over 5 weeks from a single

method calibration.

Conclusion

The Xevo TQ Absolute XR Mass Spectrometer was challenged with 90 injections per day of complex extracts and still provided accurate QC data, within typical guidance criteria of ±30% deviation, for up to 5 weeks. This system had already been used for more than 7000 injections prior to the method calibration being established.

This gives testing laboratories long-lasting confidence in the robustness of their PFAS method calibrations on the Xevo TQ Absolute XR Mass Spectrometer and in the quality of their reported results. This study demonstrated the accuracy of the calculated concentration even when the method calibration curve was only run once. Even if a batch approach were to be followed, waters_connect for Quantitation now facilitates the re-use of existing calibration curves without having to re-acquire standards. Reduced method calibration frequency results in lower consumption of expensive PFAS reagent standards and internal standards, and enables laboratories to analyze more customer samples that generate meaningful results or potential revenue.

References

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