

AMBIENT AIR QUALITY MONITORING: PFAS DETECTION

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INTRODUCTION

Per- and polyfluoroalkyl substances (PFAS) are man-made chemicals that are widely used in consumer products and manufacturing. These compounds, often referred to as "forever chemicals", are long-lived and accumulate in the environment. Elevated levels of these species significantly degrade ambient air quality, posing risks to human health and the environment. Accurate, real-time measurement of these compounds' chemical composition, concentration is critical for effective air quality management.

Chemical ionization time-of-flight mass spectrometers (CI-TOF-MS) can perform the instantaneous analysis of VOC and VICs with exceptional sensitivity, detecting levels as low as sub-parts-per-trillion, making them suitable for real-time air quality monitoring.

In this study, we will discuss the use of CI-TOF-MS instruments for detection of PFAS.

EXPERIMENTAL

Calibration measurements of PFAS and pesticides were conducted using CI-HR-TOF with a Vocus Aim reactor. The reactor was operated at a temperature of 50°C under medium pressure of 50 mbar, facilitating field-free ionization conditions. Iodide reagent ions were generated by passing ultra-high-purity N₂ stream over a permeation tube containing a mix of photo-absorber (benzene) and methyl iodide.

For PFAS calibrations, 6:2 FTOH and 8:2 FTOH, along with 11 PFCAs, were utilized. Solutions were prepared in ethyl acetate. Experimental setup involved a 250 µL glass syringe and a syringe pump for controlled injections through a heated (130°C) Silcosteel injector (Figure 1).

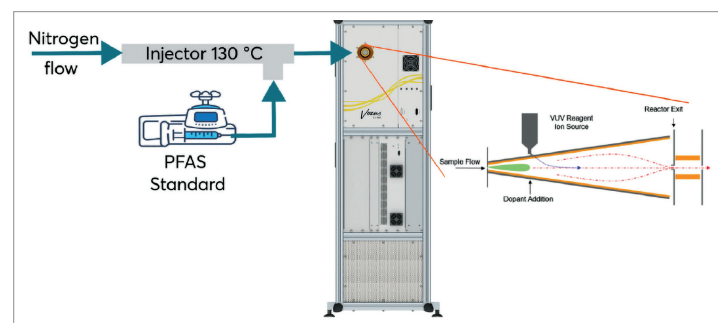


Figure 1: Experimental set-up used in the calibration of the emerging contaminants.

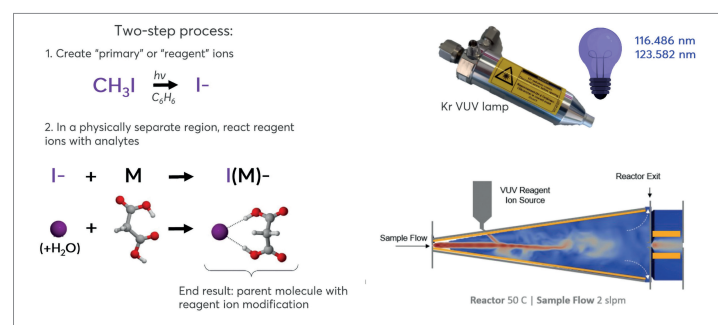


Figure 2: Principle of operation of Aim reactor.

RESULTS AND DISCUSSION

TOFWERK's versatile Vocus Aim (adduct ionization mechanism) reactor employs a soft ionization approach, which minimize fragmentation to preserve the molecular ion. All relevant PFAS compounds were detected as the parent molecular clustered with iodide reagent ions or as their deprotonated anion. Compounds were identified based on their chemical formula though precise mass-to-charge ratio measurement and isotopic pattern.

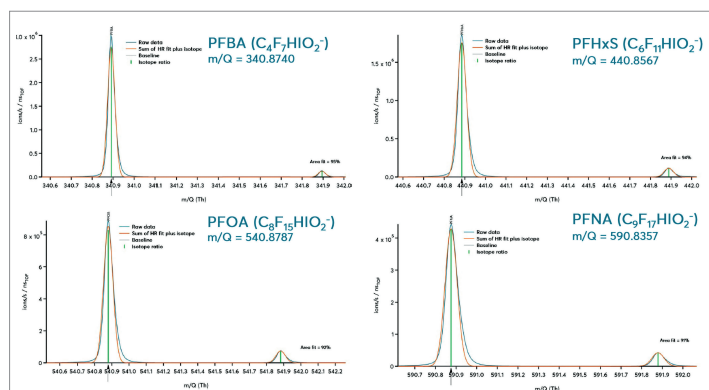
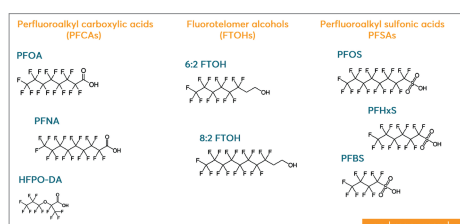


Figure 4: Identification with iodide chemical ionization mass spectrometry.

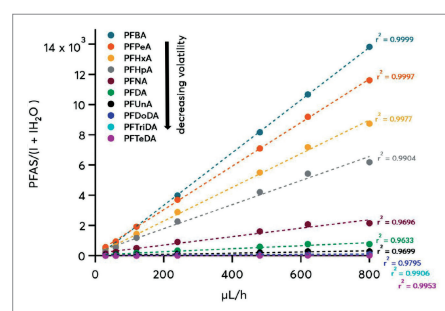


Figure 5: Calibration with iodide chemical ionization mass spectrometry.

Compound	Calibration factor (ncps ppt ⁻¹)	LOD 1s (ppt)	LOD 1min (ppt)	LOD 1min (ng/m ³)
TFA	4.30	30.0	4.0	18
6:2 FTOH	5.40	1.6	0.3	6
8:2 FTOH	5.50	1.5	0.2	4
PFBA	5.29	1.3	0.2	2
PFPeA	5.92	1.7	0.2	2
PFHxA	5.27	0.9	0.1	1
PFHpA	4.29	1.0	0.2	3
PFOA	2.77	1.3	0.3	6
PFNA	1.86	2.0	0.3	6
PFDA	0.77	3.0	0.5	11
PFUnA	0.36	3.4	0.5	13
PFDoDA	0.16	4.7	0.7	19
PFTrDA	0.06	7.6	1.2	36
PFTeDA	0.03	6.5	1.0	32
DDT	0.29	5.0	0.7	10
Pentachlorophenol	0.29	14.0	2.0	22

Table 1: Iodide CI-TOF-MS emerging contaminants calibration summary

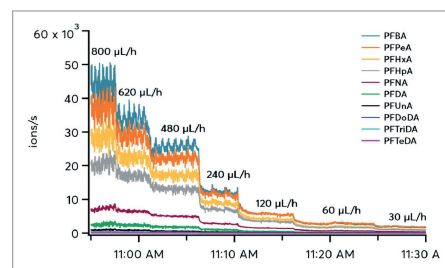


Figure 6: Real-time, continuous measurements capture rapid changes in PFAS composition.

CONCLUSIONS

Results demonstrate the use of CI-TOF-MS for the detection and quantification of selected PFAS at ultra-trace levels of parts-per-quadrillion (ppq).

Calibration data validate the reliability of our PFAS detection methodology and share illustrative examples of PFAS detection in various sample headspaces.

This real-time identification of PFAS in air introduces novel opportunities for precise tracking and management of emission sources that can be used for fast intervention and safeguarding of the environment and public health.