# Simplified real-time VOC Monitoring in air: a novel VUV PTR Ionization Reactor and Automated Instrument Performance Checks

Spiro Jorga[1], Vasyl Yatsyna[1], Felipe Lopez-Hilfiker[1], Veronika Pospisilova[1], Daniela Peroni[2]

[1] TOFWERK, Schorenstrasse 39, 3645 Thun, Switzerland

[2] SRA INSTRUMENTS SPA, Via alla Castellana 3, 20063 Cernusco sul Naviglio (MI), Italy

Volatile organic and inorganic compounds (VOCs and VICs) can be emitted into our atmosphere from natural and anthropogenic sources. Elevated levels of these gas-phase species significantly degrade ambient air quality, posing risks to human health and the environment. Accurate, real-time measurement of these compounds' chemical composition, concentration, and rapid fluctuation is critical for effective air quality management. TOFWERK's Vocus chemical ionization time-of-flight mass spectrometers (CI-TOF-MS) are developed for the instantaneous analysis of VOC and VICs with exceptional sensitivity, detecting levels as low as sub-parts-per-trillion, making them suitable for air quality monitoring. Proton Transfer Reaction Mass Spectrometry (PTR-MS) is a powerful technique for real-time monitoring of VOCs offering broad chemical coverage and high temporal resolution essential for air quality studies. However, its operation and the complexity and size of the resulting datasets pose significant challenges, often requiring extensive time and expertise for data handling.

The AirTox Monitor is a next-generation PTR-based instrument featuring a novel vacuum ultraviolet (VUV) ionization source coupled to a time-of-flight mass spectrometer with a mass resolving power of up to 3500. This innovative ion source significantly enhances measurement stability and enables rapid switching between reagent ions, expanding the range of detectable compounds. The mass resolution allows for precise peak assignment and clear distinction between isobaric species.

In this contribution we present a brief characterization of the instrument, including a comparison between postprocessed data and results directly exported via the integrated software. Furthermore, we introduce the system's automated workflows, such as background subtraction, calibration, and online mass calibration, that traditionally require manual postprocessing. These automated steps ensure high data quality while significantly reducing the time and expertise needed for analysis.

We demonstrate an instrument specifically designed for routine VOC monitoring, enabling high data quality without the need for postprocessing. Its automated operation and robust performance make it well-suited for deployment in monitoring networks, mobile platforms, and highly challenging industrial environments.

This solution allows to efficiently monitor industrial perimeter, fenceline, and stack emissions in real time with automated alarms, reporting, calibration, and system checks, enabling fully unattended operation. Continuous, sensitive monitoring of compounds of interest is possible over long periods of time.

The pre-configured list of detectable compounds includes HON-rule compounds (e.g. benzene, acrylonitrile, vinyl chloride, ethylene dichloride), small oxygenated compounds (e.g. ethanol, methylethylketone, tetrahydrofuran), chlorinated compounds (e.g. chloroethane), aromatics (e.g. toluene, styrene) and others (e.g. ethylene oxide, isoprene, hydrogen sulfide). This list is non-exhaustive and can be extended to more targets of possible interest.