Highly Reproducible and Reliable Results with the Vocus B Mass Spectrometer

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In chemical ionization mass spectrometry, calibration can be a significant challenge. Databases of sensitivities and ion distributions are only useful when the absolute and relative responses of individual instruments are similar. Thus, different instruments with very similar sensitivities and responses provide a range of advantages to the user. Not only do comparable results across instruments indicate a high reproducibility of results and excellent ionization control, but they also dramatically simplify processes such as calibration, saving time and maximizing sampling opportunities.

Given these advantages, we wanted to know how comparable the Vocus CI-TOF B with Aim Reactors really are. We measured the individual responses of many different compounds on four different instruments using three different ion chemistries to evaluate the absolute and relative variability of the Vocus Aim Reactor on the Vocus B chemical ionization mass spectrometer.

Vocus B Instrument Setup

To test the level of agreement between TOFWERK Vocus B instruments with the Aim ion source, the instruments were connected to the same sample inlet as shown in Figure 1. They were configured with the same interface settings, and signals were normalized only to regent ions. Experiments were conducted under closely controlled conditions in a laboratory environment as well as four days of atmospheric monitoring over a long weekend.

Each instrument switched through four reagent ions every two seconds and was operated with the same interface voltages, reactor pressure and temperature and therefore with the same reaction conditions. The interface conditions were identical to minimize changes in the tuning of the instrument in the regions of the ion optics where ion-

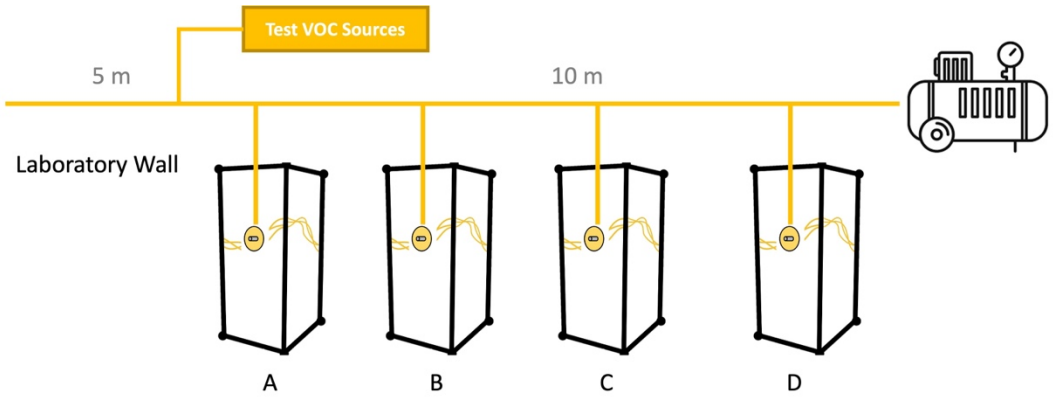

Figure 1. *Four TOFWERK Vocus B instruments were all connected to the same sample inlet as shown in the diagram. Each instrument sampled from either calibration gas or ambient air drawn through a 3/8" PFA inlet with a sample pump.*

neutral collisions still occur. We expect that by controlling each of these key instrument parameters, the resulting performance should be very similar across compound type, functional group, and ionization method. By measuring in parallel with four different instruments, the degree to which ionization conditions are controlled can be directly assessed.

Laboratory Comparison

To measure the relative response of the individual instruments, they were all exposed to a series of concentrations of hydrocarbons, solvents and simple organic acids. A multi-component gas standard was used as a source of TMB and a-pinene, while formic acid was introduced by passing clean air over a permeation tube. In each case, all instruments measured the mixtures simultaneously as shown in Figure 1.

Figure 2 shows the intercomparison results measured by the four different Vocus B instruments. The normalized instrument responses are plotted against the average response for TMB, a-pinene and formic acid. The figure demonstrates that, even without time-consuming and error-prone instrument optimizations, consistent instrument response can be achieved by using reagent ion normalization which results in errors less than +/-10%.

Ambient Sampling

To assess the instrument performance in a more challenging scenario, the second experiment consisted of four-day atmospheric ambient air measurement over a long weekend. Air was sampled out the window of TOFWERK headquarters in Thun, Switzerland via a high-flow, 15-meter sampling line. Figure 3 demonstrates that the instruments showed excellent absolute and temporal correlations,

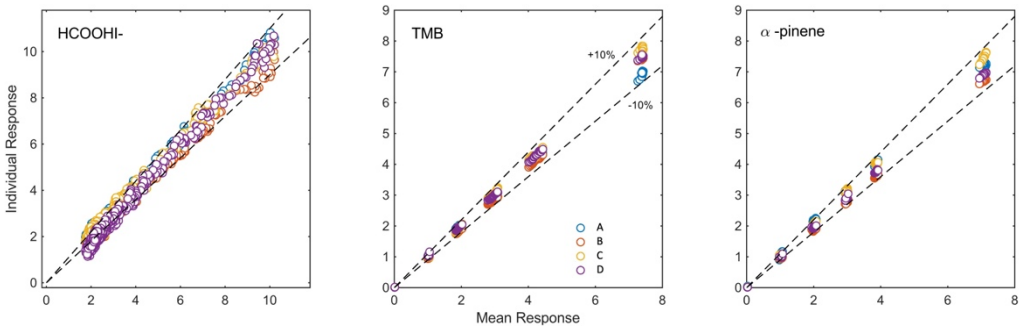

Figure 2. *Normalized instrument signal for TMB, alpha pinene and formic acid for each of the four Vocus B instruments on the y-axis plotted against the mean response of all instruments on the x-axis. Data points are color coded based on the instrument. Each compound shows strong correlation among all four instruments. Dashed lines show the +/-10% variability band in response*

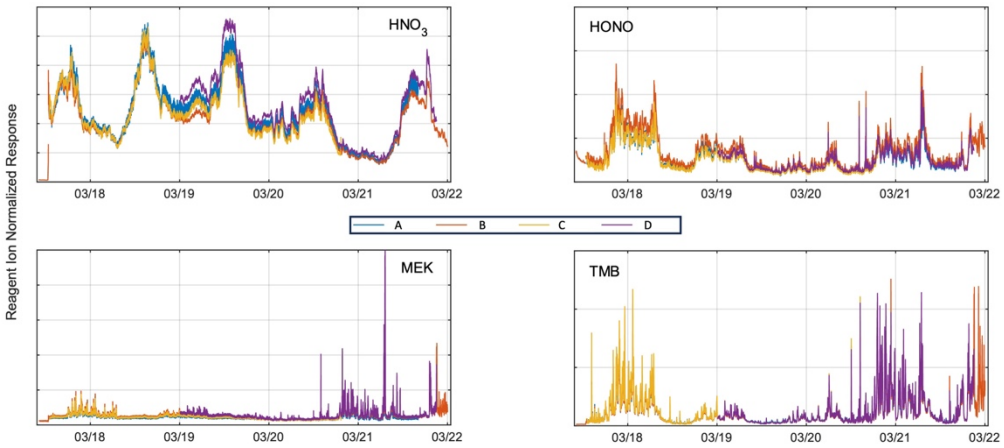

Figure 3. *Ambient sampling demonstrating the measurement of nitric acid, trimethylbenzene, methylethylketone (MEK) and HONO measured by four different Vocus B instruments. The signal on the y-axis corresponds to the normalized response of each compound to the reagent ions. Iodide anion chemistry was used for the detection of nitric acid and HONO. TMB was detected using benzene cations and MEK was detected as an adduct using protonated acetone dimers.*

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even in a complex matrix and for notoriously difficult (sticky, reactive) compounds. The top two panels show the evolution of nitric acid and HONO detected using iodide anions, while the bottom two show TMB and MEK detected by benzene cations and protonated acetone, respectively. The results of all four instruments are highly correlated and show an almost indistinguishable normalized response.

Conclusion

This experiment shows that four TOFWERK Aim ion sources coupled

with Vocus B instruments produced remarkably similar results in both laboratory and atmospheric environment sampling environments. Extremely reproducible instruments such as these can minimize setup time for the end user by simplifying the calibration process and allowing for extrapolation from one instrument to the next. This also demonstrates excellent control of reaction time, temperature, pressure, and flow rates in the Aim for an overall highly reproducible and robust measurement system.

The control and reproducibility of Aim is particularly powerful coupled with the Vocus B fast polarity-switching mass spectrometer. Millisecond reagent ion switching allows the user to overcome the Aim's selectivity and take advantage of comprehensive measurements, simplified mass spectra and highly reproducible results.

This combination is therefore an excellent choice for field and industrial deployments where space, cost and power can otherwise be limiting factors. A single Vocus B instrument with an Aim ion source offers the reliability and compound coverage of multiple traditional mass spectrometers, all in one compact package.

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