

Automated, Rapid Profiling of Trace Compounds in Complex Chemical Headspace Using the Vocus CI-TOF

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Materials can emit toxic and odorous chemicals. To ensure occupational safety and product quality during manufacturing, trace levels of these chemicals need to be identified and quantified. Standard analytical protocols use chambers and sorbent tubes followed by GC-MS analysis. This procedure is very time consuming and often difficult to interpret or use for comparison to other studies.

The Vocus CI-TOF offers ultra-low (sub-ppt levels) detection of a large range of volatile organic compounds (VOCs) within only a few seconds. This allows for real-time, instantaneous information about emission profiles from various materials. Coupling with a PAL headspace autosampler system greatly accelerates and simplifies the analytical process resulting in

an automated high-throughput method for quantifying material emissions.

The Vocus CI-TOF PAL headspace autosampler system has the capability to continuously analyze tens to hundreds of samples per hour. The autosampler is integrated into the Vocus acquisition and control software creating an end-user-friendly system for operation.

As a proof of concept measurement, 12 different polyurethane (PU) based artificial leather and 2 foam samples (all made in China) were placed in the vials of the PAL autosampler for analysis. In addition to volatile amines, ketones, aldehydes and aromatics, PU materials are known to emit residual solvents such as Dimethylformamide (DMF) and Dimethylacetamide.

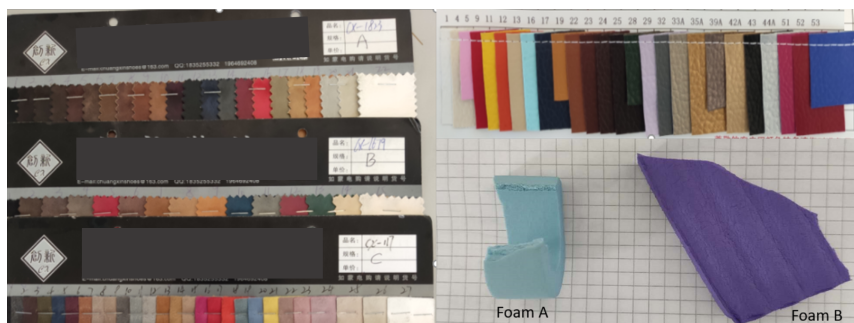


Figure 1. Overview of artificial leather samples and 2 foam materials which was chosen as test subjects.

Chronic exposure to these compounds leads to toxic metabolites and potential liver damage.

Where conventional analytical methods typically take 10 - 60 minutes per sample, the Vocus CI-TOF is capable of quantifying a wide range of potentially dangerous chemicals within sub-second temporal resolution. The 14 samples were measured within 40 minutes, including movement of the autosampler arm between samples, equilibration time, and blank measurements. In Figure 2, the 3-dimensional matrix of selected

chemicals sampled from static headspace of different leather and foam samples is shown. The chemical levels from each sample vary over a wide range.

Common volatile organics such as acrolein, acetaldehyde or acetone are identified based on their accurate masses. Further, material F1 shows a high level of formamide and $C_5H_{10}N_2$ (tentatively assigned as dihydropyrazoles or imidazolines). The emission level of toluene is significantly higher in both D28 and D39A samples compared to the rest.

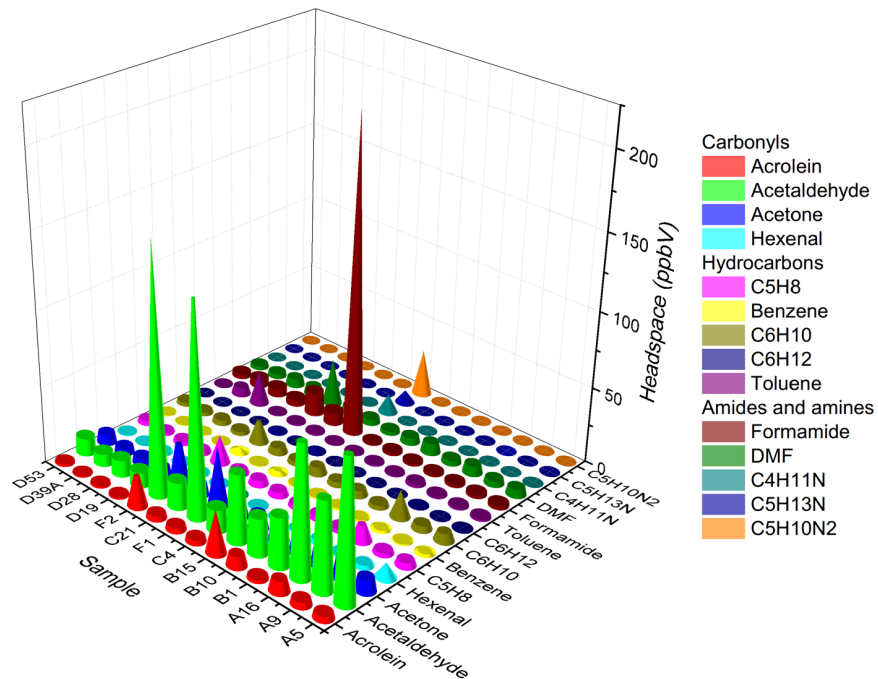


Figure 2. Selected substances emitted from synthetic leather samples (A5, A9, A16, B1, B10, B15, C4, C21, D19, D28, D39A and D53) and foam materials (F1 and F2).

The automated Vocus CI-TOF system can easily be used for monitoring compound emission profiles over a longer period. Figure 3 shows the cyclohexene emission of 14 distinct samples from continuously repeated measurements over 34 hours. The experiment was entirely automated and unattended. A decrease in the measured cyclohexene concentration was uniquely observed for sample F2, indicating that the surface of sample F2 was contaminated by cyclohexene.

A similar setup can be valuable in other applications for characterizing temporal variation, such as online analysis of product emission on product lines or real-time VOC monitoring from reaction chambers in the lab. The ability to identify and quantify a wide range of compounds in seconds makes Vocus CI-TOF an ideal tool for fast screening of large batches of samples in quality control processes, rapid feedback for improving material emission levels during research and development, and characterization of compound emission profiles over time.

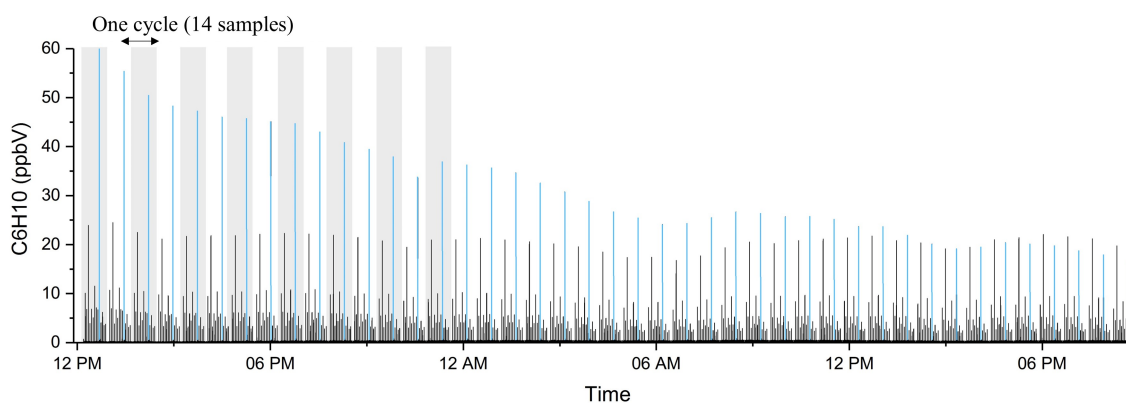


Figure 3. Long term measurements (43 measurement repeats in 34 hours) of leather and foam headspace. Each cycle consisted of 14 sample vials and two vial blanks to avoid potential carryover when highly concentrated sample being measured. The concentration of Cyclohexene ($C_{10}H_{16}$) from sample F2 (colored in blue) decayed during the course of the measurement while others stayed relatively constant.

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