Separation and Quantification of Trace Chemical Emissions from Packaging Materials Using the Vocus PTR-TOF

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Introduction

Plastic packing materials are widely used in both industrial and everyday life activities. Possible outgassing of residual solvents, raw monomers, additives, and degraded byproducts raises concerns for occupational safety and product contamination. It is therefore desirable to screen packing materials on the production line or during shipping to ensure product quality and safety in terms of fugitive VOCs. The massive scale of production and the chemical diversity of targeted substances demands analytical instrumentation capable of high-throughput sampling and detection of a wide range of compounds.

Confident Separation in Complex Emissions

The Vocus PTR-TOF is a proton transfer reaction mass spectrometer (PTR-MS) for sensitive, real-time detection of volatile organic compounds (VOCs) from material emissions. A Vocus 2R model with mass resolving power > 12000, equipped with a headspace autosampler, is used for this application example.

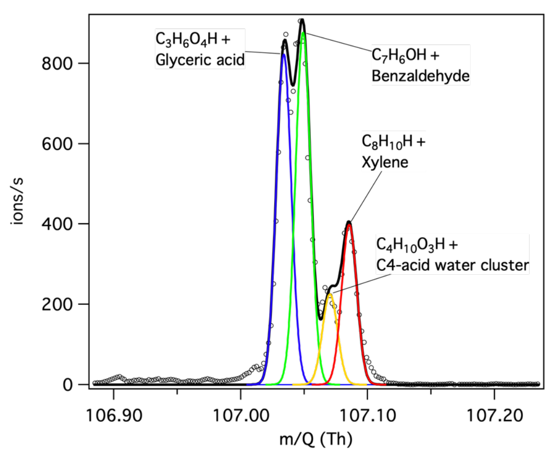

Figure 1 *An example of high-resolution mass spectrum at mass 107 with 4 isobaric compounds separated and identified from the packing material emissions.*

With market-leading sensitivity, high mass resolving power and response time, the Vocus PTR-TOF enables accurate identification and quantification of trace level VOCs emitted from materials. In Figure 1, four isobaric compounds with accurate masses ranging between 107.0 and 107.1 are clearly separated . The high mass resolving power allows confident separation of the air toxic species, such as benzaldehyde and xylenes, to ensure accurate quantification and subsequent estimation of exposure risks.

Distinct Emission Profiles

In this work, eight different packing materials were tested, including hard and soft foamed plastics, emptied air pillows, bubble wraps, wrapping sheets and sound-absorbing sponge. Some of the materials were of unknown composition. The samples were pre-baked at 50°C for several hours to minimize interferences from adsorbed VOCs. After that, each sample was placed into a sealed vial and kept at 75 °C for 30 minutes to reach headspace equilibrium. The headspace gas was then injected into a heated sampling line where constant nitrogen flow at 250 mL/min was used to deliver the headspace sample to the Vocus PTR-TOF.

Figure 2 and Figure 3 show the emission matrices of a range of chemicals emitted from

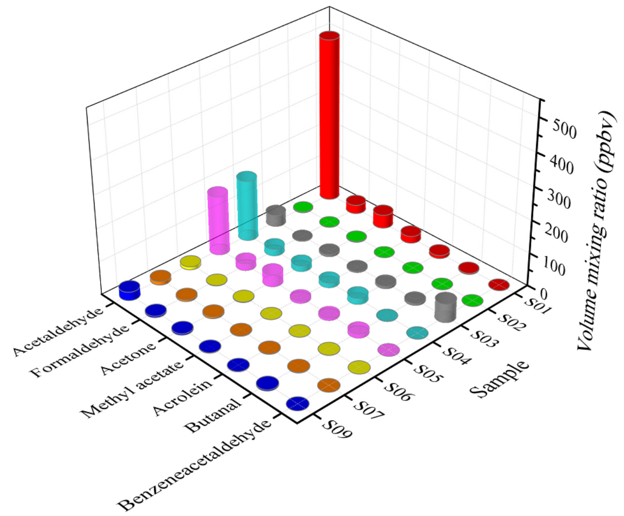

Figure 2 *Various oxygenated species detected in sample headspace. Acetaldehyde is the dominating fugitive in Sample S01, S04 and S05.*

various packaging materials. The emission profiles of different samples vary significantly. For instance, sample S03 shows high emission of aromatics and derivatives (e.g. Benzeneacetaldehyde), indicating it may be primarily made of polystyrene. The distinct emission profiles with high aldehydes and amides (e.g. formaldehyde, acetaldehyde in Figure 2 and formamide in Figure 3) in sample S01, S04 and S05 suggest their primary composition of polyurethane. Overall, sample S02 and S06, both made of polyethylene, have the lowest emissions of the suite of monitored compounds. These samples may be higher quality materials, or may emit compounds not included in the target list. For example, degradation byproducts of

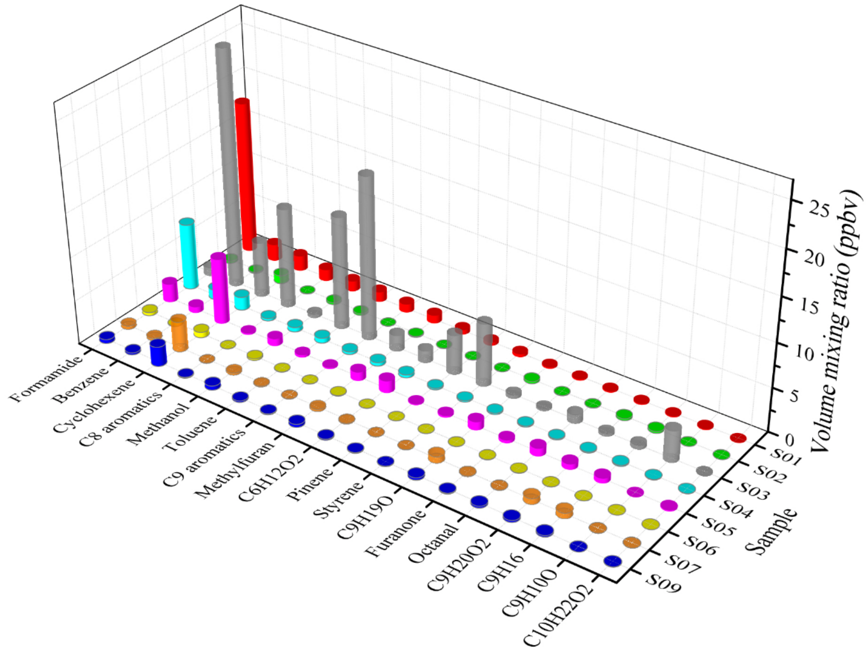

***Figure 3** Additional chemicals observed from the emissions of 8 packing material samples. Sample S03 shows high emissions in aromatics and derivatives, whereas sample S02, S06, S07 and S09 emissions are much lower. Relatively high formamide, which could be from residual process solvent, were obtained in both sample S01 and S04.*

polyethylene include small aliphatic hydrocarbons, which are poorly detected by H_3O^+ reagent ions but can be detected using other reagent ions (e.g. O_2^+ or NO^+). These are additional options for the Vocus product line.

Conclusion

The ability to separate and quantify a wide range of compounds in seconds makes the Vocus PTR-TOF an ideal tool to understand the complex emission profiles of different packaging materials. When coupled with a headspace autosampler, the Vocus PTR-TOF ensures high-throughput analysis for a large quantity of samples and offers a cost-effective method per sample for both testing labs and material manufacturers.

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