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Field measurements of human VOC bioeffluents using PTRMS

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SUMMARY

Human-emitted volatile organic compounds and other trace gases often dominate concentrations of occupied indoor atmospheres. With the application of real-time mass spectrometry, it has become possible to measure time-resolved behaviour of breath metabolites, skin emanations including oil oxidation products and microbial VOCs, and other bioeffluents. The temporal and mass spectral resolution enables deeper understanding of their impact on air quality, VOC exposure, and sensory perceptions. Per-person CO_2 and VOC emissions derived from similar groups of students indicate consistencies in major breath metabolites. Skin-emitted VOCs can be differentiated from volatilization of consumer care products by their distinctive diurnal patterns. Here we synthesize recent approaches to time-resolved measurements of human bioeffluents by PTRMS to inspire new research directions in indoor air science.

KEYWORDS

VOCs, human volatilome, breath metabolites, indoor air, skin

1 INTRODUCTION

Human bioeffluents consist of a complex mixture of, among others, volatile organic compounds spanning orders of magnitude in concentrations and reactivities, and they impact air quality in densely populated and/or low-ventilated spaces (Weschler, 2016). Due to the high diversity of human emissions and incomplete understanding of factors influencing them, comprehensive quantification of human source contributions to indoor air spaces is challenging. However, studying time resolved human bioffluents is now increasingly possible owing to the advent of real-time chemical ionization mass spectrometers. New research shows that exposure to human-emitted CO_2 and VOCs can affect cognition (Allen et al., 2016), while there is also evidence that human emotions or stress can influence human emissions (Williams, Pleil, 2016). Human exhaled air and dermal emissions can be measured directly and separately from individuals (Mochalski et al., 2014) or as ensemble emissions from larger groups of people as in a classroom (Tang et al., 2016). A recent study evaluating breath and dermal emissions separately demonstrated that dermal emissions are more responsible than exhaled breath for adverse sensory perceptions (Tsushima et al., 2018). We focus here on understanding behaviour of human bioeffluents based on time-resolved measurements in classrooms and residences. Not only volatile but semivolatile organic gases and particles are emitted by humans. We synthesise the new knowledge from recent campaigns and collaborations.

2 METHODS

Emissions from engineering students in a university classroom were monitored in real time by Proton transfer reaction time of flight mass spectrometer (PTR-ToF-MS), switching every 5 min between classroom and supply air. Further details can be found in Tang et al. (2016). The PTR-ToF-MS is a valuable tool to measure time-resolved concentrations from crowds of people, and the emissions can be calculated using material balance. An interesting aspect is discrimination between endogenous and exogenous human emissions, where real-time capability is particularly useful. The shortcoming of PTR-ToF-MS (also common to other chemical ion-

ization mass spectrometers) is lack of specificity of the detected signal for providing explicit structural information of measured chemical formulas. Although in many cases the structural isomer seems evident from the measured molecular formula, PTR-MS methods might also benefit from being combined with time-integrated gas chromatography for the enhancement of speciated information. On the other hand, PTR-ToF-MS allows for quantified real-time measurements of a range of VOCs, including oxidized VOCs, which are typically difficult for measurement using gas chromatography without customized approaches (e.g. derivatization). The low detection limits and typically excellent linearity of a wide range of concentrations (from ppt to ppm) makes this method promising for the future human emission research for indoor air.

3 RESULTS AND DISCUSSION

Time resolved concentrations and emission factors for hundreds of compounds are reported from classroom students. Acetone was most strongly correlated with CO_2 indicating the predominance of exhaled breath, with relatively minor contributions from squalene ozonolysis (skin oil oxidation). Dermally emitted compounds can be separated into directly emitted, microbial VOCs, and emissions from consumer care products. The time-resolved sampling approach allowed differentiation between discrete subsources of the human volatilome based on time-resolved correlation with breath CO_2 variability, skin oil oxidation tracers and synthetic compounds (personal care products) applied to human skin and/or hair. Discrete measurements of skin bacterial cultures allowed for tracking human VOC emissions from the skin microbiome. Dermal source factor correlated with microbial VOCs identified in direct measurements from cultures of skin microbes. In less occupied residences, human VOC signature is still prominent but cannot rival with enormous VOC emissions from human activities (see abstract by Nazaroff et al.). Measurements of individual person emissions sampled from the thermal plume above the head of seated individuals showed relatively smaller source strength than breath but indicated compounds from shampoos and possibly from the human microbial cloud (Meadow et al., 2015).

4 CONCLUSIONS

Recent research advances with PTR-ToF-MS are allowing for revolutionary progress in understanding human bioeffluents, microbial emissions, and other VOC sources affecting indoor chemistry and exposure. Synthesis of recent results suggests that it is important to elucidate factors (e.g., temperature, presence of ozone) associated with bioeffluent emissions so as to model human emissions accurately in residential and work settings. The next decade will see a breakthrough in understanding interactions of the human volatilome with indoor environments.

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