Real-time analysis of e-cigarette aerosol constituents using PTR-MS

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1. Introduction

E-cigarettes are gaining acceptance as potential alternatives to traditional tobacco products. When an e-cigarette user takes a puff, the liquid solution is heated and the aerosol, consisting of propylene glycol and/or glycerol, water, flavorings and nicotine, is inhaled. From both a regulatory and sensory point of view it is important to determine the transfer of e-liquid compounds – especially nicotine – into the aerosol, their intake during inhalation and their release following exhalation.

We use Proton Transfer Reaction Mass Spectrometry (PTR-MS; Fig. 1) for the direct sampling and analysis of volatile organic compounds (VOCs) in both the e-cigarette mainstream and exhaled breath following the use of e-cigarettes. PTR-MS is a rapid and highly sensitive tool allowing the simultaneous monitoring of VOCs without sample preparation and compound separation [1]. This is achieved by combining soft ionization techniques (proton transfer from H3O+ which mainly yields protonated parent molecules [MH+]) with a high resolution time-of-flight (TOF) mass spectrometer.

Here we show for the first time the application of PTR-MS to measure the influence of vaping behaviour (e.g. when the aerosol is inhaled into the lungs or not) on the release of e-cigarette aerosol compounds via the exhaled breath.

Instrument: PTR-TOF-MS 8000 with a detection limit of 10 parts per billion by volume (ppbv) and mass resolution of ca. 5000; sensitivity was 120 compounds/ppbv for benzene (standard calibration gas compound); the PTR-MS line of sight: p (drift): 2.2 mbar, U (drift): 600 V, T (drift): 120°C. Mass spectra were recorded in the mass-to-charge (m/z) range of 5-310 atomic mass units with a time resolution of one second.

MH+ of selected aerosol compounds: H2O2 (m/z: 21.02), nicotine (m/z: 163.12), 1,2-propylene glycol (m/z: 77.06), glycerol (m/z: 93.09), benzaldehyde (m/z: 107.05), isovaleraldehyde (m/z: 87.13), cis-3-hexenol (m/z: 101.1); m/z values were confirmed by calibration of PTR-MS with high purity standards (>99%) of said compounds (see below).

Calibration: a liquid calibration unit (LCU, [2]) was used to evaporate aqueous standards of the aerosol compounds into a gas stream, resulting in a gas flowing containing compounds at defined concentration (ppbv/ppmv level).

Volunteer measurements: Samples of “Original Flavour” Puritan e-cigarettes (nicotine 8, 16, or 20mg/g) were used (manufactured Forenem Ventures B.V.), the Netherlands; Subjects: 3 experienced e-cigarette users (closed systems/ cigalikes) age 26-41 (1 female), Puffing regimen subjects were instructed to draw for 3 s at the e-cigarette and keep the aerosol for 3 s in mouth before exhalation over “puffing” mode or II. deep lung inhalation (“inhalaion” mode) prior to exhalation into the PTR-MS inlet (Fig. 1b). For each sample, the exhaled breath of 5 individual puffs was recorded from each subject.

Data analysis: The maximum intensities (Imax) of all peaks, after subtraction of the background, in the individual mass spectra of the target compounds shown (MH+ of selected aerosol compounds) were determined; the respective intensities were normalized to the primary ion intensity (MH+). Absolute concentrations were determined from the respective regression functions (see “Calibration”). For each volunteer and compound the arithmetic mean Imax and error (standard deviation) of 5 exhaled breaths after use of an e-cigarette were determined.

3. PTR-MS calibration

Calibration of nicotine and benzaldehyde

Figure 2 shows typical calibration plots for nicotine and benzaldehyde, two representative aromatic compounds originating from the Virginia flavouring. Linear regression analysis revealed a fit with R²=0.997 (n=0.998).

Calibrations were also performed for 1,2-propylene glycol, glycerol, and additional aroma compounds selected to represent a wide range of different physico-chemical properties (data not shown). In order to accommodate the wide range of compound concentrations (ppb to ppm level), found in this study additional calibration plots covering all levels were constructed (data not shown). Again, linear regression analysis revealed a fit with R²=0.997 (n=0.995).

4. Quantification of nicotine and propylene glycol in exhaled breath

The calibration plots were used for the quantification of specific compounds in the exhaled breath of 3 subjects after the use of a Puritan e-cigarette in the “puffing” (Figures 3a, b) or “inhalaion” mode (Figures 3c, d). No exhalation after a puff or the e-cigarette is sampled via a heated transfer line for immediate ionization and analysis by PTR-MS.

5. Conclusions & future work

In this study we show for the first time the application of PTR-MS to analyse the exhaled breath of a person after the use of an e-cigarette.

Data showed that both “aeroseal compound” and “subject” have an effect on the composition of the exhaled breath and therefore on the fraction of aerosol compounds retained and/or released into the environment. As a result, the e-cigarette composition may not be a good predictor for a person’s exposure to e-cigarette aerosol compounds.

“Subject” effects can be explained by physiological differences as well as different e-cigarette user topographies. “Puffers” exhaled a large proportion of the aerosol compounds in this study whereas “inhales” retained the majority of compounds they inhaled. This may have consequences for nicotine availability and uptake. User topography may also influence the aroma composition available at the olfactory receptors and explain differences in consumer perception and preference.

As regulators and public health organization are beginning to examine potential implications that exposure to exhaled e-cigarette aerosol constituents may have on the e-cigarette user as well as bystanders and non-users, our approach may also be useful for investigating these concerns.

Please see poster session 2; poster number 82 for our work applying PTR-MS to examine the exhaled breath following use of a range of different nicotine delivery products.

References

2. R. L. Zhang et al., www.eurocarbox.com/technical CheLSA systems/liquid calibration-unit.ca

Declaration

This project was supported by Imperial Tobacco Group. The e-cigarettes used in this study was manufactured by Foronem Ventures, a fully owned subsidiary of Imperial Tobacco Group.