Investigation of emissions from heated tobacco with comprehensive two-dimensional gas chromatography with mass spectrometry detection

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Cigarette smoke is a highly complex dynamic aerosol system generated by distillation, pyrolysis and combustion reactions when the tobacco is burnt. As the burning tip of a cigarette reaches temperatures of up to 1000ºC, more than 6800 compounds have been identified in mainstream smoke[1]. Heating tobacco to temperatures lower than 300ºC and limiting the range of chemical reaction to distillation processes simplifies the composition of emissions[2].

The aim of the present study is to investigate THP complexity, focusing on particulate phase (PP), by means of comprehensive two-dimensional gas chromatography (GC×GC) coupled to time-of-flight mass spectrometry (TOFMS). A headspace solid-phase micro extraction (HS-SPME) method has been optimized by means of design of experiment (DoE) in terms of most efficient extraction of PP constituents of THP.

Emissions from heated tobacco were generated using an A14 smoking engine (Borgwaldt, Germany) according to the Health Canada Intense regime (method T-115, Health Canada) applying 12 bell shaped puffs of 55ml volume, 2s puff duration and 30s interval between the puffs. The particulate phase of smoke was collected on a standard Cambridge filter pads for head space solid-phase micro extraction (HS-SPME) analysis.

Different SPME fibres including 85 µm polyacrylate, 50/30 µm divinylbenzene/carboxen/polydimethylsiloxane, 85 µm carboxen/polydimethylsiloxane, 65µm polydimethylsiloxane/divinylbenzene and 100 µm polydimethylsiloxane were evaluated. The GC×GC-TOFMS system consisted of an Agilent 7890GC with Gerstel MPS2 (equipped in SPME and CIS4) and a Pegasus 4D with quad jet thermal modulator and secondary oven. The column set comprised RTX-5MS (30m x 0.25 mm ID x 0.25µm df) and Rxi17Sil MS (1.0m x 0.15 mm ID x 0.15µm df) from Restek. LECO ChromaTOF® software (4.50) was used for data acquisition. GC Image™ software package (2.5b6) was used for GCxGC data processing. For design of experiments The Unscrambler X 10.3 was used.

For the most abundant compounds, MS data and LRIs of each blob were compared to MS and LRI libraries (NIST14, AromaOffice 2D) for tentative identification. Amongst the 200 compounds tentatively identified, 68% were previously reported as constituents of tobacco leaves and 73% were either flavour and fragrance agents or natural substances and extractives[1].

References

1) Perfetti T.A, Rodgman A. The chemical components of tobacco and tobacco smoke, Second edition, CRC Press (2013)

2) Forster et al., Chemistry Central Journal 2015, 9:20