TD-GC×GC-LRTOFMS/FID and TD-GC×GC-HRTOFMS for the Analysis of Tobacco Heating Products

B. Savareear[a*], J.Escobar-Arnanz[a], M. Brokl[b], C.G. Wright[b], C. Liu[b] and J.-F. Focant[a]

[a]Centre for Analytical Research and Technologies (CART), University of Liege, Belgium
[b]Group Research and Development, British American Tobacco, Southampton, UK

There is an ongoing interest in the development of new forms of tobacco products for the purpose of tobacco harm reduction. Recently, new generations of tobacco heating (heat-not-burn) products (THPs) were introduced [1, 2]. Such products can vary significantly from regular combustible products and have yet to be characterized, especially in terms of total aerosol chemical composition. In addition to high chemical complexity of the aerosol emissions over a large dynamic range, the presence of certain components at extremely high concentrations (e.g. glycerin, nicotine, triacetin) often leads to saturation of the MS detector and makes the evaluation of closely eluting constituents very challenging. In this context, we have developed an analytical method based on thermal desorption and comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry and flame ionisation detection (TD-GC×GC-TOFMS/FID). The splitting of the flow between the detectors was achieved using a controlled flow splitter (CFT) with different lengths and diameters of capillary column to reach a 4:1 split ratio between FID and TOFMS, respectively. Sample introduction, GC×GC separation and MS parameters were optimized and validated to achieve reliable, semi-quantitative THP aerosol analyses. Commercial THP products were compared using supervised statistical approaches including the calculation of Fisher ratios (FRs) and application of PCA. Finally, the TD-GC×GC approach was coupled to high-resolution time-of-flight mass spectrometry (HRTOFMS) to enhance the identification of compounds of interest. The results confirm the superior capability of the developed method in analyzing aerosol mixtures generated from tobacco heating products and demonstrate the relative simplicity of THP aerosols in comparison to mainstream cigarette smoke.

[1] M.R. Smith, et.al.,Regulatory Toxicology and Pharmacology, 81 (2016) S17-S26.
[2] R.R. Baker, Prog. Energy Combust. Sci. 32 (4): 373-385.