ENHANCED MULTIVARIATE ANALYSIS OF HEAD-SPACE VOLATILES FROM PARTICULATE PHASE MAINSTREAM TOBACCO SMOKE BY HS-SPME GC×GC-TOFMS

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Tobacco smoke is an aerosol containing an extremely complex mixture of chemicals.[1] It consists of liquid/solid droplets, often referred to as the particulate phase (PP), suspended in a mixture of gases and semivolatiles – the vapour phase. Tobacco smoke is formed during overlapping processes of oxidation, pyrolysis, pyrosynthesis, distillation, sublimation, condensation, filtration and elution.[2] Mainstream smoke contains over 6000 currently identified compounds[3] and some reports claim that the total number of compounds might reach 100,000.[4]

In this study, head-space volatiles from mainstream particulate phase smoke were collected on a glass fiber filter and analyzed by means of comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (GC×GC-TOFMS). A comparison was made of six commercially available Solid Phase Micro-Extraction (SPME) fibers to collect and retain volatile substances from the smoke particulate phase. Multivariate response surface methodology was used to optimize experimental evaluation of SPME conditions.

To develop a strategy for the analysis of large numbers of samples from different cigarette types, a pixel-based software package was used to analyze and align 24 chromatograms. For multivariate analysis, the Fisher ratio (FR) and principal component analysis (PCA) were used to identify significant variations within specific classes of compounds from 2 types of cigarette differing in filter design. PCA allowed a clear differentiation of the studied cigarette types while FR analysis allowed identification of compounds that were most highly correlated with the chemical differences between the cigarette samples.

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

[4] Wakeham, H. In *162nd National Meeting, American Chemical Society*; Schmeltz, I., Ed.; Plenum Press: Washington, DC, 1971, p 1.