B156 A Combined Approach of Gas Chromatography/Mass Spectrometry (GC/MS) and Chemometric Strategies for Fire Debris Investigation Purposes

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After attending this presentation, attendees will better understand how to combine GC/MS data with multivariate data analysis strategies for fire debris investigations.

This presentation will impact the forensic science community by illustrating that, even though in a preliminary stage, this study seems to emphasize the employment of multivariate strategies targeted at potentially helping the interpretative process of fire debris investigations.

In fire debris investigations, a largely debated issue deals with the possibility of recognizing whether or not the collected evidence is related to the occurrence of an arson.[1] In practice, data from GC/MS analyses performed on collected fire debris may be compared to those from ignitable liquids (e.g., that found in possession of a suspected arsonist). With the goal of evaluating the use of gasoline as a fire accelerant, several gasolines sampled from different gas stations located within the area of Turin, Italy, were analyzed by Solid-Phase Microextraction (SPME) -GC/MS.[2] Fresh and weathered samples were analyzed and compared to standard mixtures and protocols, namely American Society for Testing and Materials (ASTM) 1618.

The collected mass chromatograms were subsequently interpreted using a variety of targeted and untargeted approaches of multivariate data analysis, using both raw and semi-quantitative data. A data set including 150 GC/MS analyses relative to 30 gas stations was used for multivariate analysis. Gasoline samples were analyzed both as pure liquids and as mixtures of fresh and weathered mixtures at different percentages (i.e., 25%, 50%, 75%, and 95%). Several multivariate data analysis procedures were tested and their results were compared. The use of chemometric strategies allowed the building of explorative, classification, and likelihood ratio models, indicating the probabilities that fire accelerants have actually been employed. Once the chromatograms had been collected, different chemometric approaches were tested on both raw and semi-quantitative data. Principal component analysis located the fresh gasoline samples within a scores plot according to their origin (i.e., the different gas stations). *N*-way strategies were tested to determine how multivariate strategies were able to assess the occurrence of fire accelerant in an arson scene. To this purpose, whole tridimensional GC/MS data collected in scan mode were compared with those obtained from different gas station gasoline samples. Similar investigative approaches have been used with the integration of Bayesian's logic. Further development of multivariate feature-based and score-based likelihood ratio models built on the collected GC/MS spectra are in progress. In particular, principal component analysis, Self-Organizing Maps (SOM), and partial least squares – discriminant analysis, as well as *N*-way models, proved successful with the goal of identifying the usage of fire accelerant.[3,4]

Even if in a preliminary stage, this study seems to emphasize the employment of multivariate strategies aimed at potentially helping the interpretative process of fire debris investigations.

Reference(s):

1. Borusiewicz R., Zieba-Palus J., Zadora G. The Influence of the Type of Accelerant, Type of Burned Material, Time of Burning and Availability of Air on the Possibility of Detection of Accelerants Traces. *Forensic Sci Int.* 2006:160(2-3):115-26.
2. Doble P., Sandercock M., Du Pasquier E., Petocz P., Roux C., Dawson M. Classification of Premium and Regular Gasoline by Gas Chromatography/Mass Spectrometry, Principal Component Analysis and Artificial Neural Networks. *Forensic Sci Int.* 2003:132(1):26-39.
3. Bro R. PARAFAC. Tutorial and Applications. *Chemometr Intell Lab Syst.* 1997:38(2):149-71.
4. Ballabio D., Consonni V. Classification Tools in Chemistry. Part 1: Linear Models. PLS-DA. *Analytical Methods.* 2013:5(16):3790-98.

Fire Debris Investigation, GC/MS, Multivariate Data Analysis

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