A179 Principal Components Analysis and Hierarchical Cluster Analysis for the Identification of Ignitable Liquids in Simulated Fire Debris

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After attending this presentation, attendees will have an understanding of how multivariate statistical procedures can be used to aid the identification of ignitable liquids in fire debris, demonstrating the use of Principal Components Analysis (PCA) and Hierarchical Cluster Analysis (HCA) for the association of simulated fire debris samples to appropriate ignitable liquid standards.

This presentation will impact the forensic science community by presenting a more objective method for the analysis of fire debris samples. The application of PCA and HCA in this manner provides a statistical basis for the comparison of forensic evidence addressing concerns regarding the subjectivity of evidence comparisons that were raised in the 2009 Report published by the National Academy of Sciences.

Following analysis by gas chromatography-mass spectrometry (GC/MS), chromatograms obtained from fire debris samples are compared to chromatograms of ignitable liquid standards to identify the presence of any ignitable liquid in the debris; however, several factors can complicate the chromatogram from the debris, making this comparison more challenging. Examples include the loss of volatile compounds, as well as the introduction of compounds that can be inherent to the debris itself or products of thermal degradation. As a result of these factors, the chromatogram from the fire debris sample may be visually dissimilar from the chromatogram of the corresponding liquid standard.

The purpose of this research was to investigate the use of multivariate statistical procedures to compare chromatograms from simulated fire debris to appropriate liquid standards, despite evaporation and the presence of matrix interference compounds and thermal degradation products. Three liquids were selected from each of three classes (naphthenic paraffinic, isoparaffinic, and alkane) as defined by ASTM International. Each liquid was evaporated to 0% and 50% by volume, then spiked onto a Kimwipe and extracted using a passive headspace procedure. A nylon carpet/carpet padding matrix was used in this research to represent a common household material. Samples of the matrix were initially burned for predefined times to determine an appropriate burn time that generated significant matrix interference compounds. To simulate fire debris, each liquid standard was spiked onto separate samples of the unburned matrix, which was subsequently burned for the appropriate time. These samples were then extracted using the passive headspace procedure, then analyzed by GC/MS.

Before analysis of the resulting chromatograms, it was necessary to perform data pretreatment procedures to minimize non-chemical sources of variance. Total ion chromatograms of the standards and debris samples were first smoothed to minimize instrument noise, thereby improving the signal-to-noise ratio. The chromatograms were then aligned to account for shifts in retention time, and finally normalized to account for slight differences in the injection volume.

The association of the simulated fire debris samples to their respective liquid standards was first evaluated using PCA. This statistical procedure is used to reduce the dimensionality of the data and identify sources of variance with the dataset. Results from PCA are shown in the form of scores plots and loadings plots. In the scores plot, chemically similar samples are positioned closely and distinctly from chemically different samples. The loadings plots are used to identify those compounds within the liquids contributing most to the variance described by the principal components. Principal components analysis was performed only on chromatograms of the liquid standards to demonstrate that the liquids could be differentiated based on liquid type and evaporation level. Then, the fire debris samples were projected onto the scores plot to investigate association to the corresponding liquid standard.

Hierarchical cluster analysis is used to assess the similarity of samples within a dataset, displaying results graphically in the form of a dendrogram. Samples that are clustered closely in the dendrogram are considered more similar. In this research, HCA was performed on the full dataset to investigate clustering, or association, of the fire debris samples with the appropriate liquid.

Using both PCA and HCA, it was possible to associate the debris to the type of liquid, despite evaporation and the presence of matrix interference compounds and thermal degradation products, from the carpet/carpet padding matrix. These procedures may provide an objective method that can be applied for the analysis of fire debris.

Fire Debris Analysis, Multivariate Stats, Chemometrics