A169 Identification of Ignitable Liquid Classes by Target Factor Analysis of Total Ion Spectra

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The goal of this presentation is to describe a chemometric approach to identifying American Society for Testing and Materials (ASTM) E1618-06 defined classes of ignitable liquids in the presence of pyrolysis products in fire debris.

This presentation will impact the forensic science community by presenting a supplementary data analysis method that uses the total ion spectrum (TIS) method and target factor analysis (TFA) to identify classes of ignitable liquids in fire debris samples.

Current methods in ignitable liquid identification and classification from fire debris rely on pattern recognition of ignitable liquids in total ion chromatograms (TIC), extracted ion profiles, and target compounds as described in ASTM E1618-06. The total ion spectra method takes advantage of the reproducibility among sample spectra from the same ASTM class and is independent of chromatographic conditions which affect retention times of target compounds, aiding in the use of computer- based library searching techniques.[1] The total ion spectrum was obtained by summing the ion intensities across all elution times. The TIS from multiple fire debris samples were combined for target factor analysis. Principle components analysis allowed the dimensions of the data matrix to be reduced prior to TFA, and the number of principle components retained accounted for approximately 95% of the variance of the overall sample set. The latent variables were rotated to find new vectors (resultant vectors) that were the best possible match to spectra in a reference library of over 450 ignitable liquid spectra (test factors). The Pearson correlation between target factors and resultant vectors were used to rank the ignitable liquids in the library. Ignitable liquids with the highest correlation represented possible contributions to the sample. The technique of receiver operating characteristics (ROC) was used to evaluate the likelihood of identifying a specific ASTM-designated class of ignitable liquid as a contributor to the sample set.

Tests included small-scale laboratory burns of substrates with ignitable liquids as well as large scale burns in 20'x8'x8' containers complete with furnishings and flooring. Large scale burns were designed to test the identification limits of the chemometric approach to ignitable liquid identification in the presence of background pyrolysis products. Burn conditions were controlled by adjusting the volume of ignitable liquid used, the fuel load, ventilation level, and the elapsed time of the burn. Samples collected from the large scale burns were analyzed using passive headspace adsorption with activated charcoal strips and carbon disulfide desorption of volatiles for analysis using gas chromatography- mass spectrometry.

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Reference:

1. Michael E. Sigman, Mary R. Williams, Joseph A. Castelbuono, Joseph G. Colca, and C. Douglas Clark, "Ignitable Liquid Classification and Identification using the Summed-Ion Mass Spectrum," *Instrumentation Science and Technology* 36 (2008) 373-395.

Chemometric, Fire Debris, Factor Analysis

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