



### A168 Chemometric Assisted Detection and Classification of Ignitable Liquids in Fire Debris

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The goal of this presentation is to describe the use of chemometric techniques to aid in the detection of ignitable liquid residue in fire debris, and to assist in the correct classification of ignitable liquids residues that may be present.

This presentation will impact the forensic science community by introducing an objective method to be applied to ignitable liquid and pyrolysis product classification in fire debris analysis. The methods investigated are intended to provide statistical support for current laboratory practices.

This research will examine the use of principal components analysis (PCA), discriminant analysis, and soft independent modeling of class analogy (SIMCA) for the classification of fire debris samples containing ignitable liquids and/or pyrolysis products. Ignitable liquid classes followed the American Society for Testing and Materials (ASTM) E 1618 standards.

This presentation will focus on the development of two models from a library of ignitable liquid GC-MS data and a library of pyrolysis product GC-MS data. The models were developed for: (1) the classification of the total ion spectrum, TIS, from a single sample as an ignitable liquid, IL, or a substrate pyrolysis, SP, product; and, (2) classification of a single sample TIS as an SP product or an IL from a specific ASTM classification. One data set was developed for ignitable liquids falling into all ASTM classes and substrates based on 452 ignitable liquids and 60 substrates, DS 1. Another data set incorporated ignitable liquids in ASTM classes other than the broadly defined miscellaneous and oxygenate classes based on 288 ignitable liquids and 60 substrates, DS 2. The influence of including the miscellaneous and oxygenate classes was evaluated. The models were tested on samples of ignitable liquids and burn samples created in a laboratory and field trials.

The first step of model development was to reduce the complexity of the dataset by selecting a group of ions from the total ion mass spectra that had the largest ratio of between group variance to within group variance (the largest F values). Modeling then proceeded by further reducing the dimensionality of the data through the use of principal components analysis (PCA) to construct a set of latent variables that explained known amounts of the variance in the data. The pretreatment of the F-selected data (prior to PCA) was varied by mean centering and autoscaling (mean centering with standardization of the variance of each variable).

**Model 1:** Initial results for DS 1 show that 98% of the autoscaled samples can be correctly classified as IL or SP, using 65 high-F ions and reducing the data dimensionality to 27 latent variables required to account for 95% of the variance. DS 2 results show that 98% of the autoscaled samples can be correctly classified as IL or SP, using 67 high-F ions and reducing the data dimensionality to 24 latent variables required to account for 95% of the variance. Reducing the number of latent variables to three for DS 1, which only accounts for 47% of the variance in the data, results in 86% and 70% correct classification into only the IL and SP classes, respectively. Reducing the number of latent variables to three for DS 2, which only accounts for 49% of the variance in the data, results in 92%

and 72% correct classification into only the IL and SP classes, respectively.

**Model 2:** DS 1 ASTM classes include aromatic; gasoline; heavy, medium and light petroleum distillates; isoparaffinics; naphthenic paraffinic; normal alkanes; miscellaneous; and oxygenates. DS 2 uses the same classes but excludes miscellaneous and oxygenates. Subclassification of the DS 1 IL samples into their ASTM classes, using 65 high-F ions and three latent variables, gave 55% correct classification for SP and 82% correct classification for all of the IL ASTM classes with the exception of the miscellaneous and oxygenate classes which were correctly classified for 17% and 56% of the samples, respectively. The lower correct classification rate for the miscellaneous and oxygenate IL classes is seen to result from the broad definitions of these classes and the resulting population of the classes by ignitable liquids having diverse properties. Subclassification of the DS 2 IL samples into their ASTM classes, using 67 high-F ions and three latent variables, gave 66% correct classification for SP and 89% correct classification for all of the IL ASTM classifications with the absence of the miscellaneous and oxygenate classes. Increasing the number of latent variables will increase the overall percent correct classification.

These results will be compared to other hard and soft chemometric techniques.

This work was supported by the National Institute of Justice, Office of Justice Programs. The content of this publication does not necessarily reflect the position or the policy of the Government and no official endorsement should be inferred.

**Fire Debris, Principal Component Analysis, Chemometric**