A129 ASTM Classification of Ignitable Liquids and Residues by Chemometric Techniques

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The goal of this presentation is to establish a methodology with known error rates for the identification and classification of ignitable liquids in fire debris samples.

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.

Models were developed to assign ignitable liquids to the ASTM classes based on the total ion spectrum (TIS) for each sample from a library of ignitable liquid gas chromatography-mass spectrometry (GC-MS) data and a library of pyrolysis product GC-MS data. The first step of model development was to reduce the dimensionality of the data through the use of principal components analysis (PCA) to construct a set of latent variables. This was followed by linear discriminant analysis (LDA) and quadratic discriminant analysis (QDA) based on the PCA scores. Cross-validation was performed by randomly selecting 20% of the samples from each class for a test set. The remaining 80% of the samples were used to develop a model for classification by LDA and QDA. Classifications for the test set were generated from the model and evaluated by comparison to the Technical Working Group for Fire and Explosions (TWGFEX) Ignitable Liquid Reference Collection (ILRC). The cross-validation steps were repeated 100 times with a new test set being selected and classified each time. Total correct classification percentages were calculated as the sum of the cross-validation tests. All models developed on ignitable liquid and substrate library data were applied to fire debris samples.

The LDA and QDA models were developed to classify samples as: (1) ignitable liquid or substrate; and, (2) by ignitable liquid ASTM class or substrate. Models in both categories included: (a) all ASTM E1618 classes; (b) all ASTM classes other than miscellaneous and oxygenates; and, (c) all ASTM classes but combined the classes of isoparaffinics and normal alkanes as well as petroleum distillates and naphthenic paraffinics. Although the samples within the training and testing sets performed well, fire debris samples were found to have a significantly lower correct classification rate. This was attributed to the presence of pyrolysis products that led to incorrect classifications.

The influence of pyrolysis products on correct classification rates presented a major challenge in this research and has led to consideration of additional methodologies. Other methods under investigation to increase the correct classification rate of these samples include partial least squares discriminant analysis (PLS-DA), soft independent modeling of class analogy (SIMCA), and method of normalized coordinates.

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Chemometric, Fire Debris, Gas Chromatography-Mass Spectrometry

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