D7 Advancing Fire Debris Analysis through Chemometrics: An Overview of Research at the National Center for Forensic Science

Mary R. Williams, MS, Michael Sigman, PhD, Jennifer Lewis, BS, Erin Waddell, BS, University of Central Florida, National Center for Forensic Science, PO Box 162367, Orlando, FL 32816; and Caitlin Rinke, BS, University of Central Florida, PO Box 162367, Orlando, FL 32816-2367*

The goal of this presentation is to describe the chemometric methods currently being studied at the National Center for Forensic Science for the analysis of fire debris data and to show how the methods can assist the analyst in their casework.

This presentation will impact the forensic science community by raising the awareness of research efforts to introduce new mathematical approaches to the analysis of fire debris which facilitate the detection of ignitable liquids in the presence of interfering pyrolysis products, allow for rapid searches of ignitable liquid and pyrolysis product libraries, and support the use of probabilistic classifiers.

Current practice in fire debris analysis often relies on ASTM-E 1618-06, which defines a standard method for ignitable liquid residues analysis and classification in extracts from fire debris samples using gas chromatography-mass spectrometry. Identification of the presence of ignitable liquid residues is accomplished by the analysts' recognition of chromatographic profile patterns and target analytes. Laboratory-to- laboratory variations in chromatographic conditions can complicate the automated search of large databases and libraries that are shared between laboratories. Covariance maps of the chromatographic data and the total ion spectrum (TIS) are chromatography-invariant for a given set of analytes and therefore form the basis of robust pattern recognition and classification methods which allow spectral libraries to be searched for the identification of an unknown.

Ignitable liquid identification challenges resulting from sample contamination with pyrolysis products can be overcome by target factor analysis of a set of spectra, each containing differing contributions from ignitable liquid residues and pyrolysis products. Target factor analysis reduces the dimensionality of the dataset, producing a set of latent variables that do not necessarily resemble the spectrum of a single component in the fire debris. The abstract solutions can be tested one at a time to determine if an oblique rotation (to an angle other than 90° with respect to the latent variables) can lead to a vector that correlates strongly with a known spectrum obtained from a library. When this procedure is applied to a set of spectra of known ASTM classification comprising a library, the resulting correlations allow for the use of several probabilistic classification techniques to identify classes of ignitable liquids potentially present in the samples.

Analysis of a large set of total ion spectra from ignitable liquids (greater than 450 samples) and a set of spectra from pyrolysis products (greater than 50 common building materials) has demonstrated that the data from each set can be independently modeled and new samples correctly classified with a high degree of accuracy as either resulting from an ignitable liquid or a substrate. Further classification of ignitable liquid data to the correct ASTM class is less accurate and the correct classification rate is significantly reduced when the miscellaneous and oxygenate classes are included. The use of other chemometric methods for the implementation of hard and soft classifiers will also be discussed The chemometric methods are applied to datasets resulting from laboratory burns, large scale burns of furnished 20'x8'x8' containers designed to replicate structure fires, and from libraries of hundreds of commercially available products that are highly flammable. This presentation will provide detailed information about ongoing research conducted at the National Center for Forensic Science. Large scale burns were performed in collaboration with the Bureau of Fire Standards and Training, Ocala, FL, and the Bureau of Forensic Fire and Explosives Analysis, Tallahassee, FL.

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 U.S. Government and no official endorsement should be inferred.

Chemometrics, Fire Debris, Factor Analysis

 ** Presenting Author*