B130 Covariance Mapping as an Aid to Ignitable Liquids Classification and Rapid Database Searching

Michael E. Sigman, PhD, and Mary Williams, BS, National Center for Forensic Science, University of Central Florida, PO Box 162367, Orlando, FL 32816-2367*

After attending this presentation, attendees will learn a simple mathematical approach to treating GC-MS data for ignitable liquid samples that aids in the classification of the sample by ASTM guidelines and can be implemented as an automated database search routine.

This presentation will impact the forensic community and/or humanity by demonstrating presenting an improved methodology for ignitable liquids analysis and the introduction of a data analysis method that may be implemented for rapid searching of a single database or networked databases.

This presentation will focus on the use of covariance mapping as an aid in the classification of ignitable liquids by ASTM E 1618 guidelines and as a method to facilitate automated searching of ignitable liquid databases.

This presentation will impact the forensic community and/or humanity by presenting a simple mathematical approach that facilitates the examination of gas chromatography – mass spectromtery (GC-MS) data collected in fire debris analysis. The method is easily implemented for rapid database searching and can be readily incorporated into existing databases.

Under the conditions employed in electron ionization mass spectrometry, compounds of a given class (*i.e.* alkanes, aklylbenzenes, etc.) exhibit similar fragmentation patterns. Identification of the most prevalent ions in a sample and the relative amounts of the ions corresponding to different classes of compounds forms the basis for the preliminary steps in ASTM classification of an ignitable liquid. The ion-profile information can be extracted from the GC-MS data set manually with subsequent visual pattern recognition. Alternatively, the information may be conveniently obtained by calculating the covariance between the individual ion chromatograms. The computational method removes the time domain information from the dataset; however, the information is not lost and is retained in the original dataset. The resulting data matrix may be graphically presented as a solid surface which has distinguishing features that are useful in classifying the ignitable liquid. The diagonal elements of the calculated matrix are proportional to the integrated product of the corresponding extracted ion chromatogram, while the off-diagonal elements correspond to the product of two different extracted ion chromatograms integrated over the chromatographic time coordinate. When the covariance matrix is intensity-normalized, to compensate for variable sample size, and presented as a 3-D surface, different classes of ignitable liquids can be recognized by visual inspection.

Two intensity-normalized surfaces may be directly compared by defining the sum of the absolute difference, calculated element-by-element, as a “distance” between the two the surfaces. The distance will tend toward a limiting value of zero for identical surfaces and toward a limiting value of two for surfaces that are totally non-overlapping, thereby providing a measure of surface similarity. Data will be presented to show that the distance is minimized for surfaces corresponding to ignitable liquids constituting the same ASTM classification. The distance calculation provides a convenient computational method of comparing an unknown sample with database entries.

Results will be given for calculations on a series of ignitable liquids representing various classes and sub-classifications under the ASTM E 1618 standard. The method clearly discriminates between petroleum distillates, isoparaffinic products, dearomatized distillates, oxygenated solvents, naphthenic paraffinic products, and gasoline at various stages of evaporation. Discrimination between sub-classifications (*i.e.* between medium and heavy petroleum distillates) is less distinct in some cases. In addition, the advantages and limitations of the computational method for inter-laboratory data comparisons will be demonstrated and discussed, along with the utility of the method in analyzing matrix-contaminated samples.

Ignitable Liquids, Fire Debris, GC-MS Analysis