E103 Self-Organizing Maps to Analyze the Relationship of Ignitable Liquids and Substrates

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Learning Overview: After attending this presentation, attendees will understand how the components of substrate backgrounds relate to components of the American Society of Testing Materials Standard Test Method for Ignitable Liquid Residues in Extracts from Fire Debris Samples by Gas Chromatography/Mass Spectrometry (ASTM E1618-14) ignitable liquid classes.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by providing an easy-to-visualize graphical representation of the relationship between two reference databases to better inform the analyst of where problematic class overlap can occur and types of substrate background that may interfere with the interpretation of casework samples.

Fire debris samples are currently analyzed according to ASTM E1618-14, which makes use of the total ion chromatogram, extracted ion chromatogram, and target compounds. Ignitable Liquid (IL) residues are classified as one of the following seven classes given by ASTM E1618-14: gasoline, petroleum distillate, isoparaffinic, aromatic, naphthenic-paraffinic, normal alkane, and oxygenate. The chromatographic profiles and the relative presence of the major compound types are used to determine which classes the IL residue falls into. Any ignitable liquids that do not fall into these classes are designated as miscellaneous and have characteristics of multiple classes. Even with the guidelines provided by ASTM E1618-14, determining the presence of IL residues is still a time-consuming manual pattern recognition process for the analyst and is highly subjective in nature. To counteract this, automated chemometric methods that use the Total Ion Spectrum (TIS) are being developed. The TIS is the time-averaged mass spectrum across the total chromatographic profile and allows for comparison within or between labs due to the absence of the retention time variation. This work makes use of the Extracted Ion Spectrum (EIS), a subset of the TIS, which is generated using the ions in Table 2 of ASTM E1618-14. These ions are representative of the major compound types present in each of the ASTM classes and include: normal alkanes, branched alkanes, cycloalkanes, aromatics, polynuclear aromatics, ketones, and oxygenates.

Self-Organizing Maps (SOM) are a type of artificial neural network used for the visualization of large datasets and can be easier to visually interpret than principal component analysis for complex data. In a previous study, it has been shown that IL group according to their ASTM class designations using the EIS of ASTM ions and the SOM. This work expands on previous work and uses SOM to examine the relationship of substrates and IL from the National Center for Forensic Science (NCFS) Substrate and Ignitable Liquid Reference Collection (ILRC) databases. Substrates grouped in the center of the map with the ASTM classes surrounding them. However, significant overlap was observed between substrates and the oxygenate class. Substrates were labeled according to their major polymer type and whether they are derived from wood or non-wood materials. Ground truth samples were also projected onto the map to examine the potential of the trained map to classify fire debris samples. There was a reasonable trend observed for the position of the ground truth samples on the map with respect to the ratios of the individual components used to create them. This study demonstrates the power of unsupervised machine learning methods to be used as a quick screening tool in forensic science and allows the analyst to qualitatively assess the class or components of a casework sample.

Fire Debris, Chemometrics, Machine Learning