B33 Fourier-Transform Infrared Spectroscopy Investigations of Smokeless Powders

Quashanna Price, National Center for Forensic Science, 12354 Research Parkway, Orlando, FL 32816-2367; Mary R. Williams, MS, PO Box 162367, Orlando, FL 32816-2367; and Michael E. Sigman, PhD, University of Central Florida, National Center for Forensic Science, PO Box 162367, Orlando, FL 32816*

The goal of this presentation is to determine whether novel smokeless powder classes can be identified beyond the single-base and double-base designations by statistical analysis of Fourier-Transform Infrared Spectroscopy (FTIR) data.

This presentation will impact the forensic science community by providing a statistically valid classification method for powders exclusive of the classic division of single-base and double-base designations.

In 2009, the National Center for Forensic Science (NCFS) developed a smokeless powders database in conjunction with the Technical/Scientific Working Group for Fire and Explosives Analysis (T/SWGFEX) regarding the analysis of smokeless reloading powders. Smokeless powders are low explosives that contain energetic materials and function as propellants in reloading ammunition and they are frequently found in Improvised Explosive Devices (IEDs) such as pipe bombs. The three main types of smokeless powders are single base, double base, and triple base, with all three types containing nitrocellulose. In addition to nitrocellulose, double-base powders contain nitroglycerin while triple-base powders contain nitroglycerin and nitroguanidine. The smokeless powders database housed by NCFS contains analytical data for a large number of commercially available single-base and double-base powders that have been analyzed through analytical methods including Gas Chromatography/Mass Spectrometry (GC/MS), stereomicroscopy, and FTIR.

For this research, FTIR data for 87 smokeless powder samples analyzed at NCFS were utilized. The percent transmittance (%T) was converted to absorbance and the intensity values for wavenumbers 400-4,000 cm^{-1} were normalized to scale 0-1. Since no prior information was known regarding potential grouping of the data, an unsupervised technique, Agglomerative Hierarchical Clustering (AHC) was used to generate dendrograms showing the clustering groups of powders based on FTIR. Hierarchical clustering utilizes a distance metric (i.e., Euclidean, maximum, etc.) to calculate the distance between samples and a linkage-metric (i.e., single, complete, etc.) to cluster data.

Further studies included defining the appropriate distance and linkage by creating dendrograms using Euclidean distance and single, complete, and ward linkage-methods to determine the best clustering. It was determined that the distance and linkage combination of Euclidean and Ward, respectively, gave partially overlapping clusters. The similarity data was then used to generate a heat map to visualize the groupings.

Preliminary results from cluster analysis identified four groups among single-base and double-base powders that do not cluster based on the presence or absence of nitroglycerin, indicating that there are additional factors influencing cluster formation. Additional research will seek to determine the chemical factors contributing to the clustering. In addition, 2D mapping studies of smokeless powder cross-sections will be performed to investigate heterogeneity throughout the kernel.

This work was supported in part by the National Institute of Justice, Office of Justice Programs, award 2013-R2-CX-K008. The content of this publication does not necessarily reflect the position or the policy of the government, and no official endorsement should be inferred. Support is also acknowledged from the University of Central Florida, National Center for Forensic Science, a State of Florida Type II Research Center.

Cluster Analysis, Smokeless Powders, Statistics