A116 Differentiation of Yellow Polyester Fibers With Different Dye Loadings Using Microspectrophotometry and Chemometrics

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After attending this presentation, attendees will gain a fundamental understanding of the application of multivariate statistics to the analysis of fibers.

This presentation will impact the forensic science community by touching upon key improvements suggested by the 2009 National Academy of Sciences Report. In particular, human observer error is a potential problem in fiber color comparisons and the use of multivariate statistics could virtually eliminate this issue.

Microspectrophotometry (MSP) is a quick, accurate, and reproducible way to compare colored fibers for forensic purposes. In turn, the use of chemometric techniques applied to MSP data can provide valuable information, especially when looking at a large dataset. As of now, routine fiber color comparisons are made by use of an MSP and the trained eye of a forensic fiber examiner, who examines the overall shape of a fiber's spectrum. Comparisons are made by overlaying the spectra from items of questioned and known origin and determining if similar spectral characteristics are observed. However, minute differences not seen by the examiner can provide valuable information in a relatively featureless spectrum. The use of chemometric techniques like agglomerative hierarchical clustering (AHC), principal component analysis (PCA), and discriminant analysis (DA) can detect these differences and make objective comparisons of complex data possible.

The purpose of this study was to use chemometric techniques to discriminate UV-visible spectra obtained from yellow polyester fibers that had different dye loadings. Research has shown that visually similar yellow polyester fibers can be discriminated based on their UV-visible spectra; however, none have determined if fibers dyed with the same dye, but with different dye loadings, can be discriminated by their UV-visible spectra alone. Background subtracted and normalized UV-visible spectra from 11 yellow polyester exemplars dyed with different concentrations of the same dye ranging from 0.1-3.5% were analyzed by AHC, PCA, and DA. Simple visualization of the overlaid spectra showed the shape of the spectral curve broadened as dye loadings increased. One fiber with an unknown dye loading was determined to have a dye loading between 0.75-1.5% based on visualization of the spectra and subsequent chemometric techniques. AHC and PCA grouped the fibers into three classes ranging from low to high dye loadings. When grouping the fibers into their three classes based on low, medium, and high dye loadings, the classification accuracy was 94%. However, when fibers were grouped individually, the classification accuracy was quite poor (52%). In addition, an external validation study resulted in higher classification accuracy when fibers were grouped into three classes instead of individual groups (95% vs. 50%). Finally, exemplars with similar dye loadings were treated like known and questioned fibers and analyzed by PCA and DA in order to determine if they could be discriminated. Three exemplar comparisons and both class comparisons were considered discriminated based on a classification accuracy of 90% or higher and a receiver operating characteristics curve score of 0.9 or higher.

Overall, chemometric analysis of UV-visible spectra provides an objective means of discriminating similar fibers with different dye loadings.

Chemometrics, Dye Loadings, Fiber Comparison

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