A170 Clustering of Medium Petroleum Distillate Products: A Self Organizing Feature Map (SOFM) Approach

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The goal of this presentation is to discuss an artificial neural network technique to differentiate medium petroleum distillate samples. Attendees will understand the basic idea of self organizing feature map (SOFM), an unsupervised pattern recognition neural network most commonly used for revealing natural clustering within multi-variables dataset.

This presentation will impact the forensic science community by introducing a new approach to classify and discriminate ignitable liquid samples within the same class. This presentation proposes an alternative to "conventional" multivariate analysis for example principal component analysis and hierarchical cluster analysis.

SOFM can aid the investigator in the assignment of weathered (evaporated) medium petroleum distillates to their source.

This work involves the GC/MS analysis of medium petroleum distilates and the chemometric analysis of the derived data.

The identification of liquid accelerant is a complex problem in fire debris analysis. Many techniques can be utilised in order to obtain the ignitable liquid residue from the submitted debris. It is also of increasing importance that the analysing laboratory compiles a reference collection of relevant ignitable liquids. The reference collection should also contain weathered or evaporated samples of ignitable liquids scene these are more commonly encountered in debris. The comparison of ignitable liquid residues extracted from fire debris samples is generally based on class characterisation, hence a systematic grouping of ignitable liquids has been established by the American Standard Testing and Material (ASTM) International which in principle, groups ignitable liquids on the basis of hydrocarbon compositions, boiling point, and raw material source. [1] Medium petroleum distillate (C_8-C_{13} hydrocarbon range) includes

products such as paint thinners, white spirits and paint brush cleaners are

quite common in arson cases, although they may not be as frequently encountered as petrol and kerosene.

Chromatographic profiles and mass spectral data of medium petroleum distillates, in fact most ignitable liquids from the same

classification class, often have high degree of similarity in terms of their chromatographic pattern. Therefore, examination by visual comparison of chromatographic profiles for classification and identification purposes can be very challenging, and sample individualization, arguably, unachievable.

A number of multivariate analysis techniques have been applied to differentiate ignitable liquids. These types of analysis enable more than one variable to be measured and the conclusions about these data can be presented as 2D or 3D graphical trends. This work details the mechanism by which SOFM can be utilized for chromatographic data analysis. SOFM is an artificial neural network computation which performs unsupervised multivariate analysis. Among its many applications, it is used for dimension reductionality but at the same time preserves the original data and is applicable with linear or nonlinear datasets. [2] It is perhaps the most popular unsupervised pattern recognition ANN.

A reference collection from various brands of MPD products was compiled. MPD samples were analyzed using GC-MS and their chromatographic data was examined. Automated comparison between data derived from different brands of MPD was carried out using a som software. The outcome from SOFM provided a topological map for easy visualization; hence the interpretation of the outcome is straight forward. Furthermore, the dataset variables could be studied closely from within the SOFM structure (known as component planes) to gather information about the clusters proposed. Results revealed that SOFM was capable of objectively discriminating between product brands using chromatographic patterns from unevaporated and evaporated MPD samples.

References:

1. Stauffer, E.; Lentini, J. J., *Forensic Science International 2003*, *132*, 63-67.
2. Zupan, J.; Gasteiger, J., *Neural networks in Chemistry and Drug Design*. Second Edition ed.; Wiley-VCH: Weinheim, 1999.

SOFM, Medium Petroleum Distillates, Pattern Recognition

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