A102 Effect of Pulsed Pressure Injection on the Analysis of Gasoline Using Gas Chromatography-Mass Spectrometry and Chemometric Procedures

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After attending this presentation, attendees will understand the importance of a pulsed pressure injection on the precision of gas chromatography-mass spectrometry (GC-MS) data, as well as, the effect on subsequent chemometric procedures used in data analysis.

This presentation will impact the forensic science community by identifying parameters that can affect the precision of injection and by illustrating the subsequent effect on data analysis procedures. Optimizing injection parameters is essential in order to minimize non-chemical sources of variation prior to applying chemometric procedures and, hence, to ensure meaningful results. The effect of injection mode on the association of gasoline replicates with discrimination from other gasolines will be demonstrated using principal components analysis (PCA).

Chemometric procedures such as principal component analysis (PCA) are widely used in the analysis of samples of forensic interest. These chemometric tools can facilitate the rapid and reliable identification and differentiation of complex samples based on the chemical composition. However, it is necessary to minimize any sources of variance that are not inherent to the samples, to ensure that meaningful results are obtained. The purpose of this research is to investigate the effect of a pulsed pressure injection on the precision of chromatographic data and the resulting effect on data analysis using PCA.

For optimization studies, a standard mixture of five alkanes, ranging from C_8 to C_{16} was prepared. The alkane standard was analyzed by GC-MS with an automatic liquid sampler, using a standard oven temperature program. The pulsed pressure injection was firstly optimized, investigating pulse pressures up to 40 psi and up to one minute in duration. For each combination of pressure and duration, the alkane standard was analyzed in triplicate and relative standard deviations (RSDs) of peak height, peak area, and retention time were calculated for each alkane, from the total ion chromatograms. The optimal pulsed pressure method was chosen based on the combination that offered the lowest RSDs and, hence, the best precision. The alkane standard was then analyzed by the optimal pulsed pressure injection in both split and splitless modes, as well as by an unpulsed injection in both modes. Relative standard deviations of the peak height, peak area, and retention time for the alkane components were compared among all combinations of injection parameters to determine the most precise injection mode.

To demonstrate the effect of injection mode on PCA, five gasoline samples were collected from different brand service stations. Each sample was diluted 1:200 in dichloromethane and analyzed in triplicate by GC-MS, using both the optimized pulsed injection as well as a non-optimized injection. The resulting 30 chromatograms were retention time aligned using a commercially available alignment algorithm and normalized. Principal components analysis was then applied to assess the effect of injection mode on the precision of the analysis, which has consequences for the association of replicates and discrimination of different gasoline samples. Results of these studies will be presented and discussed along with the implications for forensic analyses using chromatographic data and chemometric procedures.

GC-MS, Gasoline, Principal Components Analysis

 ** Presenting Author*