B180 The Practical Application of a Kinetic Model to Generate Predicted Reference Collection for the Identification of Ignitable Liquids in Fire Debris Samples

Briana A Capistran, BA, Michigan State University, East Lansing, MI 48824; Victoria L. McGuffin, PhD, Michigan State University, East Lansing, MI 48824-1322; Ruth Waddell Smith, PhD, Michigan State University, East Lansing, MI 48824*

Learning Overview: The goal of this presentation is to demonstrate the practical application of a kinetic model to generate a reference collection of predicted chromatograms used to identify ignitable liquids in fire debris samples.

Impact on the Forensic Science Community: After attending this presentation, attendees will understand how the kinetic model can be applied to the chromatogram of an unevaporated liquid to predict chromatograms corresponding to a range of evaporation levels. These predicted chromatograms form the basis of an extensive reference collection which, in this work, is used to identify ignitable liquids in samples collected from large-scale burns.

Fire debris samples are analyzed by Gas Chromatography/Mass Spectrometry (GC/MS) to determine the presence of ignitable liquids based on comparisons to a suitable reference collection. Identifications can be challenging due to evaporation of the ignitable liquid and the presence of interferences arising from substrates in the fire debris samples. These challenges can be overcome by including evaporated liquids in the reference collection and by using extracted ion profiles to minimize or eliminate substrate effects. However, experimental evaporations can be time consuming, with the result that not all liquids in the reference collection will be evaporated to different levels.

A first-order kinetic model was previously developed in the Michigan State University laboratory to predict evaporation rate constants for compounds in ignitable liquids as a function of retention index, which is related to boiling point. The evaporation rate constants are used to calculate the fraction remaining of each compound in a liquid, from which chromatograms corresponding to evaporated liquids can be predicted. Previous work in this laboratory demonstrated the predictive accuracy of the model for petroleum distillates, whereas recent work highlighted improvements in accuracy for gasoline. In this work, practical application of the model is demonstrated.

The kinetic model was applied to generate a reference collection of ignitable liquids from five different chemical classes defined in American Society for Testing and Materials (ASTM) 1618 (isoparaffinic, aromatic, naphthenic-paraffinic, petroleum distillate, and gasoline). Unevaporated liquids from each class were analyzed by GC/MS to generate Total Ion Chromatograms (TICs) and Extracted Ion Profiles (EIPs) of the major compound classes. The kinetic model was applied to the TICs to predict chromatograms corresponding to total fraction remaining (F_{Total}) levels of 0.9–0.1 (evaporation levels of 10%–90%) for each liquid. Predicted reference collections corresponding to the EIP for major compound classes were generated in a similar manner.

The liquids were also experimentally evaporated to different F_{Total} levels and analyzed by GC/MS. The TICs and EIPs of the experimentally evaporated liquids were then compared to the corresponding predicted reference collection, using Pearson Product-Moment Correlation (PPMC) coefficients as a measure of similarity. For example, for the TIC of paint thinner experimentally evaporated to F_{Total}=0.50, strongest correlation was observed for comparisons to predicted TICs of paint thinner, with a maximum PPMC of 0.942. Conversely, the PPMC coefficients for comparisons of the experimentally evaporated paint thinner to other liquids in the predicted reference collection were generally less than 0.500, indicating weak correlation.

To demonstrate practical application of the model, three burn cells (8ft x 16ft) furnished with carpeting and other household items were prepared. Gasoline was poured in two of the cells and paint thinner in the third cell. Each cell was ignited and allowed to burn for 8min or just past flashover. The fires were extinguished, and samples were collected and analyzed by GC/MS. The resulting TICs and EIPs were compared to the predicted reference collections.

For burn samples containing paint thinner, the maximum PPMC coefficient for comparison to the TIC reference collection was 0.862, which corresponded to the predicted TIC of paint thinner with F_{Total}=0.80. Higher correlation was observed when the EIPs were considered. For example, the maximum PPMC coefficient of 0.935 was observed for comparison to the cycloalkanes/alkenes EIP with F_{Total}=0.90. Only weak correlation was observed for comparisons to all other liquids in the TIC and EIP reference collections, with PPMC coefficients less than 0.500.

This presentation will describe the development of the predicted reference collection in more detail and application to data collected from large-scale burns. Overall, this work will demonstrate the utility of the kinetic model combined with EIPs to more accurately predict the presence of ignitable liquids in fire debris samples.

Fire Debris, GC/MS, Extracted Ion Profile

*Presenting Author