

Characterization of Ignitable Liquids in Simulated Fire Debris Using Dynamic Vapor Microextraction, NMR Spectroscopy, and Sensitivity Analysis

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After a structural fire, debris is often analyzed for the presence of ignitable liquid (ILs) using passive headspace concentration methods. The most common concentration method requires debris to be placed inside of a sealed container along with an activated carbon strip (ACS), which is then eluted using carbon disulfide, a hazardous neurotoxin. In addition, the ACS method is known to result in vapor distortion, where the ignitable liquid eluted from the carbon strip is not representative of the vapor headspace sampled. An alternative to the ACS method is dynamic vapor microextraction (DVME), where a carrier gas is used to drive vapors from the headspace of the sampling container through a chilled adsorbent capillary where they are trapped. The major advantages of this approach are the ability to elute the capillary column with less harmful solvents such as acetone and the ability to monitor vapor distortion. In this work, we describe our approach to understanding, optimizing, and validating IL collection and analysis for simulated fire debris using DVME. Using a fractional factorial design approach, we examine the impact of both instrument and sample conditions on the procedure and compare the simulated fire debris collection and elution to reference gasoline samples. Furthermore, we separate the data into several chemical classes present in gasoline: alkanes, cycloalkanes, aromatics, indanes, and polynuclear aromatics and evaluate how the factors influence IL collection and detection. Finally, we discuss a set of novel nuclear magnetic resonance (NMR) experiments aimed at understanding the kinetics and adsorption behavior during dynamic headspace sampling. These experiments rely on model mixtures which are passed across adsorptive capillaries using a flow of nitrogen gas. The flowthrough is monitored in real-time using a benchtop NMR spectrometer allowing us to determine which components pass through the column unabated. Solvent rinses of the capillary column after halting the flow of nitrogen provides confirmation of the components that were trapped on the capillary during the measurement.