B56 The Adsorption and Persistence of Gasoline Residues on Household Materials Investigated by Inverse Gas Chromatography

Eric Frauenhofer, Buffalo, NY 14223; Joonyeong Kim, PhD, Buffalo State College, Buffalo, NY 14222*

Learning Overview: After attending this presentation, attendees will better understand macroscopic transfer and persistence of gasoline residues on solid substrates, with reporting on estimated molar adsorption enthalpies and adsorption amounts of selected hydrocarbons in gasoline residues on household materials investigated via inverse gas chromatography. In addition, distortion effect of chromatograms due to the difference adsorption affinity of individual components in gasoline to solid substrates during sampling process will be presented.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by offering a molecular level understanding of transfer, persistence, and recovery of gasoline residues on various solid substrates in forensic fire investigations.

The transfer and persistence of ignitable liquids on human skin and various daily household materials such as clothes, shoes, carpets, and wood has attracted a lot of attention as a part of efforts to reconstruct fire investigations. Previous studies have shown that the transfer and persistence of ignitable liquids on solid substrates is affected by many factors including the compositions of ignitable liquids, temperature, air movement, and physical characteristics of solid substrates. Transfer and persistence of ignitable liquids can be viewed as the adsorption of molecules in ignitable liquids on the solid substrate. Although it is a much more complex process, adsorption is the result of molecular interactions between ignitable liquids and solid substrates under the given experimental parameters. When spiked on the solid substrate, all components in ignitable liquids will be partitioned to either a gas phase via evaporation or a solid surface via adsorption with different proportions depending on the magnitude of interactions with solid substrates.

The interactions between molecules and solid substrates mainly depend on several factors including the polarity, size, and structures of adsorbing molecules (adsorbates) and chemical compositions and structures of solid substrates (adsorbents). One of the physical quantities to measure the absolute magnitude of interactions between molecules and solid substrates is the heat of adsorption, the energy required to remove the given molecule from the surface. In addition, sorption isotherms and solubility coefficients are also useful physical quantities which represent interactions between adsorbates and solid substrates. In this respect, inverse gas chromatography is one of the techniques which can estimate molar enthalpies of sorption, sorption isotherms, and solubility coefficients between adsorbates and adsorbents.

Inverse gas chromatography is a molecular probe technique used for the characterization of surface and bulk properties of various solid materials including polymers. As the reverse of a conventional gas chromatographic experiment, inverse gas chromatography utilizes a conventional gas chromatography, with minor modifications, to measure the interactions between a pure probe (e.g. hydrocarbons) and a stationary phase (e.g., polymers) in terms of the retention time of the probe as a function of temperature. A chromatographic column (stationary phase) can be packed with the solid substrate of interest which provides potential application of inverse gas chromatography for various types of solid substrates. A small quantity of pure probe compound is injected, vaporized, and diluted in a mobile phase in a stationary phase (the column) by establishing fast equilibrium between the vapor and the stationary phase. Therefore, the retention time of the injected probe is affected by the magnitude of interactions with the stationary phase. From the measured retention times of the injected probe as a function of temperature at a constant flow-rate and column inlet pressure, various thermodynamic data as well as isotherms be estimated.

The scope of this study is the investigation of hydrocarbon adsorption on solid substrates via inverse gas chromatography for a better understanding of macroscopic transfer and persistence of gasoline residues on solid substrates. Although numerous components exist in gasoline residues, six hydrocarbons (*n*-heptane, *n*-octane, *n*-nonane, toluene, *p*-xylene, and *1,2,4*-trimethylbenzene) were selected as molecular probes in this work. Columns used in inverse gas chromatography measurements were prepared with three popularly encountered household materials, cardboard, cotton fabric and carpet. Herein, estimated molar enthalpies of sorption of six hydrocarbons on three solid substrates, isotherms of these hydrocarbons on three solid substrates measured at 40°C and the solubility coefficients of these compounds on solid substrates at 40°C as defined by Henry's law are reported in the presentation.

Inverse Gas Chromatography, Gasoline Residues, Adsorption Enthalpies