## A54 Fundamental Measurements for Trace Detection of Energetic Materials

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After attending this presentation, attendees will have an understanding of:

(1) the importance of thermophysical and analytical properties in the detection of explosives; and,

(2) the impact of reliable measurements and models of thermophysical properties of explosives.

This presentation will impact the forensic community by providing familiarity with thermophysical property and analytical measurements that are of importance in characterizing explosive vapors.

The continuous emergence of new and non-standard explosive compounds necessitates the need for reliable explosive detection devices. This presentaion represents the work on fundamental measurements that enable the development of such devices. Vapor detection methods for sampling and detecting energetic compounds that may be components of improvised explosive devices (IEDs) are very attractive because they are sensitive, selective, and afford non-invasive, standoff detection. To develop reliable vapor detection devices for energetic materials, it is necessary to know: (1) what; and, (2) how much is in the vapor phase above the energetic material or IED. The method presented both identifies and quantifies components (even trace components of low volatility) above energetic materials with very low uncertainty. This method, a modified purge and trap approach, makes use of cryoadsorption on short alumina-coated porous layer open tubular (PLOT) columns. To illustrate this method, headspace measurements on practical military and industrial plastic bonded explosives (PBXs) including tagged C-4, Semtex-1A, Semtex-H, detonating cord (detcord), and sheet explosive

(Detaflex) are shown. Components of the headspace were identified and quantitated as a function of temperature and are presented in the form of van't Hoff equations. The linear relationship of the recovered mass as a function of inverse collection temperature reveals the predictive capabilities of the methodology. Thus, the necessary data for standardization and calibration of current and emerging in-the-field vapor detection devices is possible. This study also presents a novel apparatus and method for detecting and quantifying the permeation of hydrogen peroxide ($H_2O_2$) through polymer barriers (i.e., plastic bottle and containers). Measurements have been performed with 35% and 50% hydrogen peroxide by weight. Polymer barriers of several thicknesses made from polyethylene terephthalate (PET), both high and low density polyethylene (HDPE and LDPE), polylactic acid (PLA), and polypropylene (PP) were tested. Analytical methods were also used to measure two fundamental thermodynamic properties, vapor pressure ($p_{sat}$) and enthalpy of adsorption ($\Delta H_{ads}$), that are critical to the detection of energetic materials. $p_{sat}$ for three mononitrotoluene compounds was measured (which are used as detection taggants in plastic explosives) with a gas saturation apparatus. In this type of apparatus a carrier gas stream is saturated with the vapor of a condensed phase. The vapor is then stripped from a measured volume of the carrier gas, the amount of vapor is determined analytically, and $p_{sat}$ is calculated by assuming ideal gas behavior. Gas-solid chromatography was used to measure the $\Delta H_{ads}$ for a variety of fuel-like compounds (acetone, benzene, n-alkanes, etc.) on concrete. This work is part of a larger project to study the surface energetics of chemicals on construction materials.

**Adsorption, Explosives, Vapor Pressure**

 ** Presenting Author*