Hawaiʻi Natural Energy Institute Research Highlights

Alternative Fuels

Fuel Characterization by Multidimensional Gas Chromatography

OBJECTIVE AND SIGNIFICANCE: The objective of this project is to identify and characterize trace quantities of heteroatomic organic species (HOS) in aviation, maritime, and diesel fuels. New analytical methods under development can evaluate the composition of fuels currently in use and those stored as strategic reserves and investigate the impacts of crucial nitrogen and sulfur containing compounds and additives on fuel properties. Comprehensive fuel composition information can be further employed to replace costly experimental measurements by calculating various physicochemical properties of fuel. The knowledge gained in this project will improve the understanding of the influences of HOS and fuel additive deterioration on fuel stability and physicochemical properties, guide efforts to preserve fuel quality, and reduce the cost of fuel characterization.

BACKGROUND: Liquid fuels are, by nature, chemically complex and many fit-for-purpose and stability issues are associated with trace quantities of HOS natural existed and additives employed. Identification and quantitation of HOS and additives are challenging due to their low concentration and complex composition of fuel matrix. Multidimensional gas chromatography (MDGC) typically uses sequential separations based on differences in polarity and boiling point as the basis for fuel sample analysis. The current state-of-the-art for MDGC is comprehensive two-dimensional GC (2D-GC).

HNEI began developing a fuel laboratory in 2012 and the current capabilities include standard analysis methods required by ASTM and military fuel specifications. Research conducted in the fuel laboratory has included investigating the impacts of long-term storage, oxidative conditions, contaminants, additives, etc. of conventional and alternative fuels and their blends.

A 2D-GC was acquired in August 2018, expanding the fuel laboratory's ability to identify and quantify fuel constituents present in trace amounts (≤100 ppm). The HNEI 2D-GC employs two injectors and three detectors (i.e. mass spectrometer, nitrogen chemiluminescence and sulfur chemiluminescence) to analyze fuel components and HOS with a single injection event. Neat fuels can be injected directly without requiring solvent dilution. Quantum chemical software based on the conductor-like screening model for realistic solvation (COSMO-RS) method was employed to calculate the physicochemical properties of petroleum and sustainable aviation fuels based on their individual 2D-GC compositions.

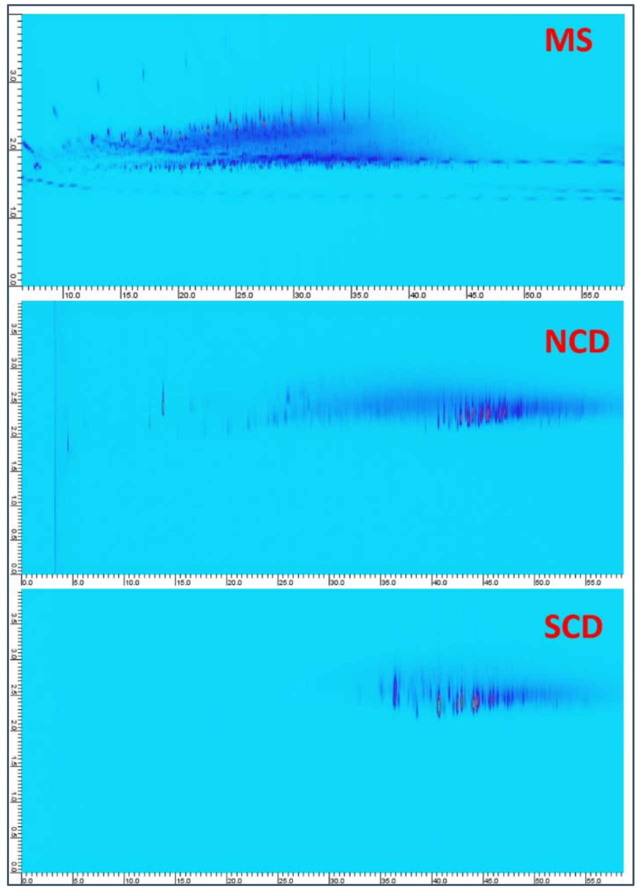

Figure 1. Comprehensive 2D-GC analysis of F-76 diesel fuel with MS, NCD, and SCD.

PROJECT STATUS/RESULTS: HNEI is currently collaborating with personnel from the U.S. Navy Fuels Cross-Functional Team at Naval Air Station Patuxent River (Pax River) and the Fuel Laboratory at Naval Supply System Command Fleet Logistic Center Pearl Harbor (NAVSUP FLC Pearl Harbor) on 2D-GC applications, including:

- Participated round robin tests on nitrogen compounds in various type of fuels;
- Predicted water solubility in fuels from -40°C to room temperature based on their individual 2D-GC compositions and COSMO-RS;
- Determining fuel hydrocarbon matrix;

- Investigating the distribution and contents of nitrogen and sulfur compounds in fuels;
- Incorporating novel separation methods to accurately qualify and quantify non-hindered and hindered phenolic species in fuel;
- Exploring the impacts of additive deterioration on fuel stabilities;
- Utilizing HOS characterization methods to investigate the potential impacts of HOS on fuel properties and fuel stability; and
- Calculating various fit-for-purpose properties based on the 2D-GC compositions of fuels.

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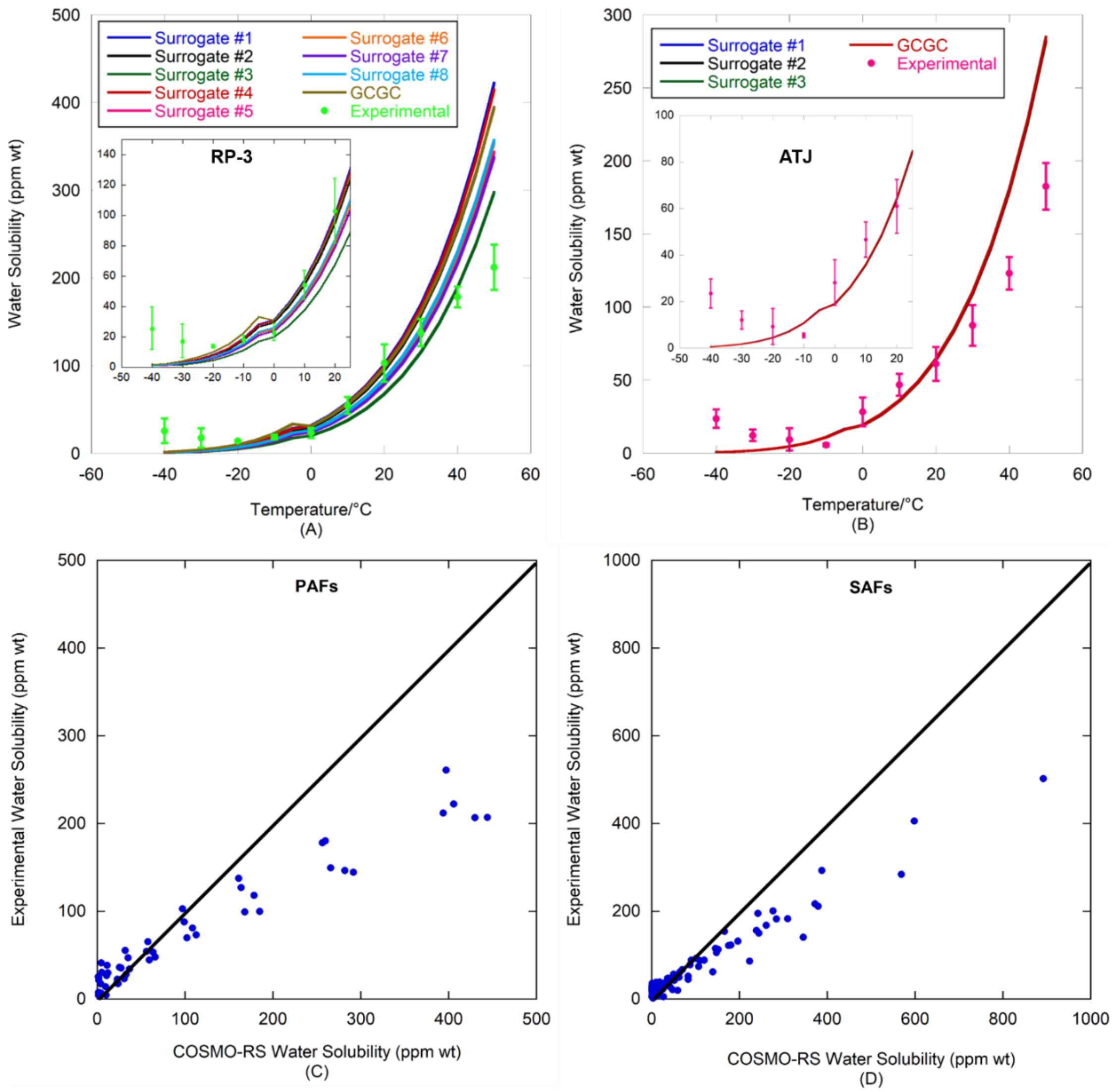

Figure 2. Correlation of COSMO-RS calculated water solubility in petroleum and sustainable aviation fuels (PAFs and SAFs) and their blends with experimental values reported by West et. al. 2018: (A)-(B) RP-3 and alcohol-to-jet with COSMO-RS calculation based on 2D-GC and surrogate data; (C)-(D) parity plots of 5 PAFs and 8 SAFs with COSMO-RS calculation based on 2D-GC data.