



# Hawai'i Natural Energy Institute Research Highlights

## Alternative Fuels

### Advanced Fuel Characterization and Development

**OBJECTIVE AND SIGNIFICANCE:** The objective of this project is to systematically assess the impacts of trace quantities of heteroatomic organic species (HOS) on fuel properties and to advance the development of high-energy density (HED) fuels for future transportation applications.

New analytical methods under development can 1) evaluate the composition of fuels currently in use and those stored as strategic reserves and 2) 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 conventional petroleum and alternative fuels. The knowledge gained in this project will enhance our understanding of how HOS and fuel additives impact fuel stability and physicochemical properties, guide efforts to preserve fuel quality, reduce the cost of fuel characterization, and advance the development of alternative HED fuels.

**BACKGROUND:** Liquid fuels are, by nature, chemically complex and many fit-for-purpose and stability issues are associated with trace quantities of HOS inherent in the parent feedstock or employed as additives. Identification and quantitation of HOS and additives are challenging due to their low concentration and complex composition of the fuel matrix – necessitating the development and utilization of advanced analytical methods, such as two-dimensional gas chromatography (2D-GC).

In 2012, HNEI established a fuel laboratory with the capabilities encompassing essential analysis required by ASTM and military fuel specifications. Present capabilities include prediction of fuel properties using empirical and phenomenological modeling techniques. Research conducted in the fuel laboratory includes investigating the impacts of long-term storage, oxidative conditions, contaminants, additives, and other factors on conventional and alternative fuels and their blends. Computational methods to predict fuel properties support experimental efforts and contribute to the advancement of future transportation fuels.

In August 2018, a 2D-GC expanded the fuel laboratory's ability to identify and quantify fuel constituents present in trace amounts ( $\leq 1$  ppm). The HNEI 2D-GC employs two injectors and three detectors, i.e. mass spectrometer (MS), nitrogen chemiluminescence (NCD) and sulfur chemiluminescence (SCD), to analyze fuel components and HOS with a single injection event. Neat fuels can be injected directly without requiring solvent dilution. Data generated using this instrument is used as input to the conductor-like screening model for realistic solvation (COSMO-RS) method. These calculation techniques predict physicochemical properties of petroleum and alternative fuels based on their individual compositions and guide the design of HED fuels.

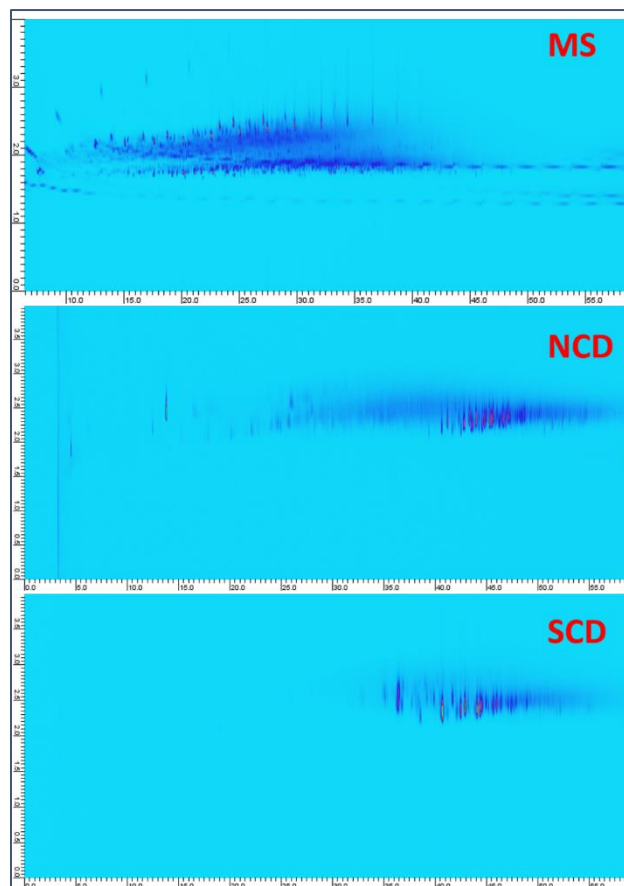


Figure 1. Comprehensive 2D-GC analysis of F-76 diesel fuel with MS, NCD, and SCD.

**PROJECT STATUS/RESULTS:** HNEI is currently collaborating with personnel from the Navy Technology Center for Safety and Survivability at the Naval Research Laboratory, Washington, DC on 2D-

GC applications for sulfur-containing compounds (SCCs) analysis.

Past activities under this project included: 1) participation in standard method development for nitrogen-containing compounds (NCCs) analysis with a 2D-GC-coupled NCD; 2) determining the impacts of antioxidant concentration on preserving fuel quality; and 3) COSMO-RS prediction of fuel boiling point, vapor pressure, density, and compatibility with fuel system polymers.

Currently, HNEI's activities include:

- Determining fuel hydrocarbon matrix;
- Exploring the influences of SCCs and NCCs on the degradation of fuel antioxidants (AOs) and the consequent impacts on fuel stabilities;
- Developing standard methods for identification and quantification of SCCs by using 2D-GC coupled to SCD and high resolution (HR) orbitrap MS;
- Calculating various fit-for-purpose properties based on the 2D-GC compositions of fuels; and
- Developing high energy density and stability fuels based on quantum chemistry and thermodynamic calculations.

To date, this project has produced the following publication:

- 2023, J. Fu, P.K. Le, S.Q. Turn, [Impacts of antioxidants on stability of biodiesel derived from waste frying oil](#), *Biofuels, Bioproducts and Biorefining*, Vol. 17, Issue 6, pp. 1496-501.

*Funding Source:* Office of Naval Research

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*Last Updated:* November 2023