Composition-Performance Correlations For Rational Development of Renewable Aviation Fuels

Mark Romanczyk1, Katherine Wehde1, Petr Vozka2, Jorge Ramirez Velasco1, Rodney Trice1, Gozdem Kilia2, Hilikka Kenttämaa1
1Department of Chemistry, 2School of Engineering Technology, and 3Department of Materials Engineering, Purdue University

Goal: Establish a databank of conventional and alternative aviation fuel constituents to be utilized to develop correlations between chemical composition, engine performance, and material performance. We also aim to seek further opportunities to collaborate with US military personnel.

Hilkka Kenttämaa
Introduction:
Thousands of molecules, most of them unknown, make up the currently used jet fuels. Using an advanced analytical separation method, two-dimensional gas chromatography, coupled with high-resolution time-of-flight mass spectrometry (GC/GC/TOF/MS), compound classes in two fuels and two drop-in components were identified and molecular structures of the compounds were determined.

Method:
Compounds in complex fuels can be separated using GC/GC with separation based on boiling point and polarity. The GC/GC separation of Jet-A is plotted on blue background on the left. The black outlines show separations obtained using only one column.

Next Steps:
1. Characterize the molecular composition of additional fuels including biofuels.
2. Develop quantification methods.

Gozdem Kilia
Introduction:
An increasing number of blending components are getting approved as an alternative pathway to enable the deployment of aviation “drop-in” fuels. This challenge has been recognized since 1980s. It is a highly agreed upon consent that fuel composition affects the performance. However, the way this relationship works is still a “black box”. We aim to de-mystify the pertinent steps. Our focus is fuel property analysis based on chemical constituent identification. Consecutive benefits in terms of cost and time saved throughout the fuel approval process are predicted to be greatly significant which will serve as the much needed incentive for future alternative fuels manufacturing.

Property-composition relationships:

Hydrocarbon groups dependence on fuel properties and its complexity

weight fractions of: n-alkanes [n], branched plus cyclic saturates [BC], and aromatics [Ar]; Vc, aromatics content; SG specific gravity; Qe, net heat of combustion; SP smoke point; % H hydrogen content; FP freezing point

Next Steps:
1. Test fuel properties via ASTM methods and build bridges per multidimensional gas chromatography findings
2. Expand the fuel specific databank to interconnect performance to chemistry

Rodney Trice
Introduction:
The gas turbine engine is of utmost importance for generating electrical power and/or thrust in Naval aircraft. The hot sections of gas turbines are typically comprised of superalloy turbine blades, many of which have additional thermal protection provided by a ceramic thermal barrier coating or TBC. Both the superalloy blades and TBC can be attacked by corrosive species found in the environment and individual constituents of CMAS that can come from Biofuels.

Simulating how impurities interact in the gas turbines:

1. Gas turbines operate at 1300°C-1400°C, always trying to increase temperature for efficiency gains; ablation process simulation capability is up to 2200°C when testing TBCs.
2. The developed process simulates how impurity atoms come into a gas turbine after burning thousands of gallons of fuel.

Microstructure comparison due to the effect of Biofuel impurities

1. For engine temperatures greater than 1250°C, Biofuels impurities melt and infiltrate the TBC resulting in delamination.
2. Biofuel impurities cause macroscopic delamination and microstructural changes.

Next Steps:
1. Quantify the contaminants that will be found in biofuels
2. Study the effect of Biofuel impurities over different TBCs (APS, HVOF, EB-PVD)