# Fundamental Studies on Composition/Performance Correlations for Aviation Fuels

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Office of Naval Research Science & Technology

**Goal:** **Determine the molecular compositions for newly approved alternative aviation fuels and conventional jet fuel in order to correlate their performance with their molecular composition, including impurities**

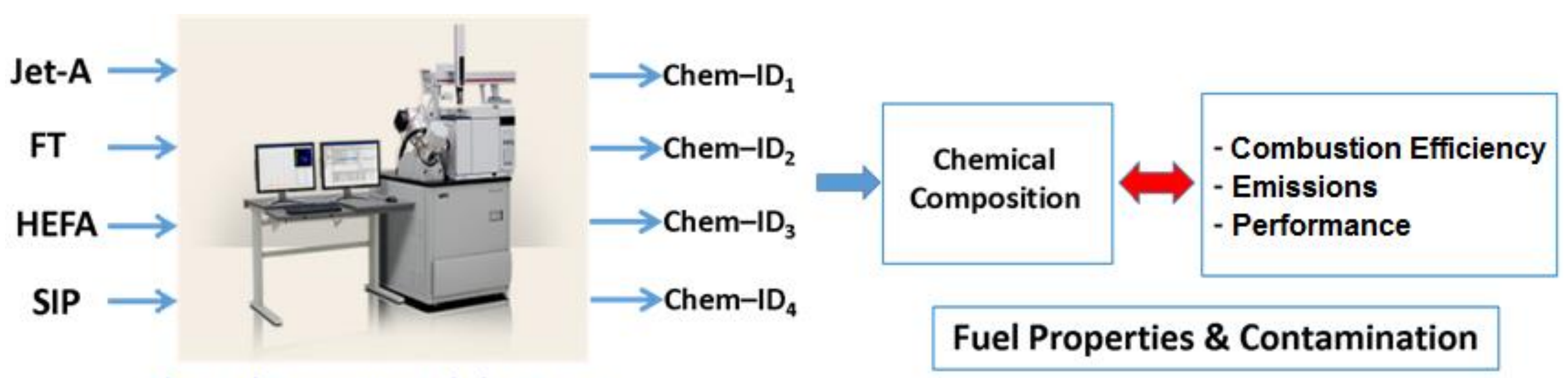

**Gozdem Kilaz**

## Introduction:

Recent advancements in bio-energy production allowed increased use of renewable liquid biofuels as aviation fuels. These "drop-in" fuels, however, also brought operational challenges as multiple novel chemicals come into contact with different airframe and power plant materials. One set of such challenges involves the performance of alternative fuels in a gas turbine engine. Correlating fuel performance with the origin of the biofuel becomes a very important aspect.

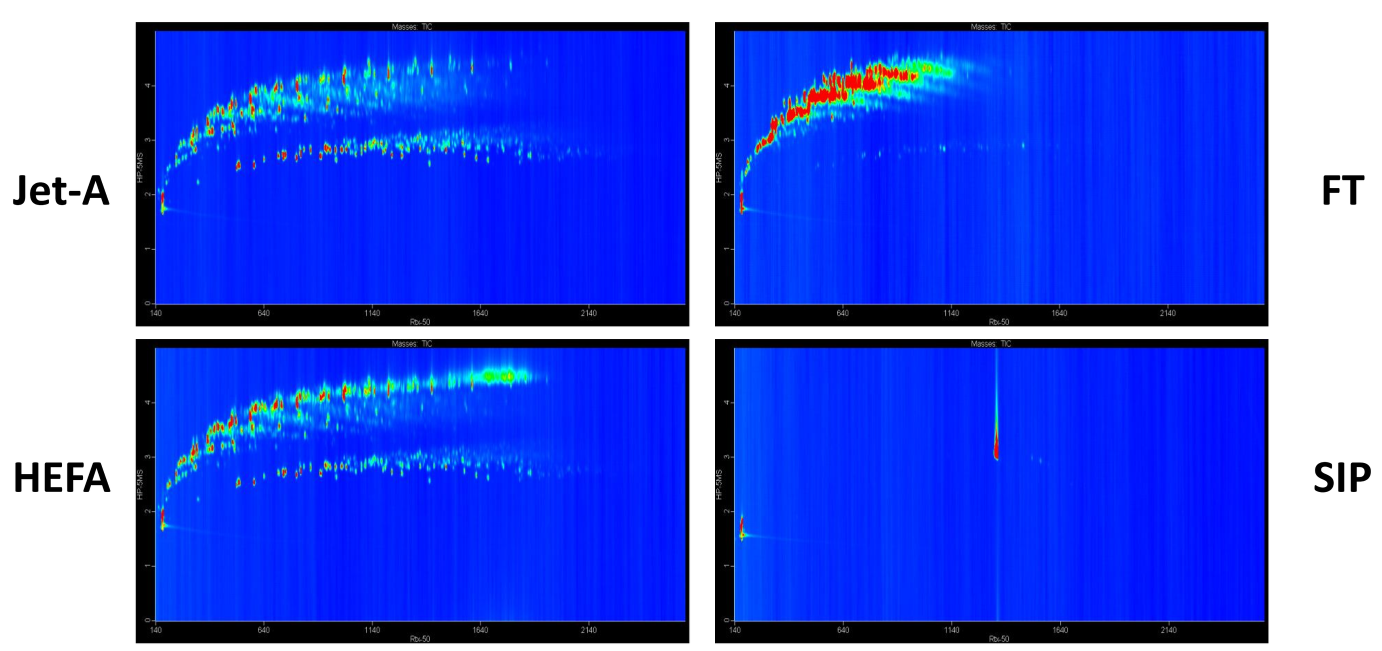
## Test Fuels (ASTM D1655 and D7566):

- Conventional Jet Fuel (Jet-A)
- Hydro-processed Esters and Fatty Acids (HEFA)
- Fischer-Tropsch (FT)
- Synthesized Iso-Paraffins (SIP)




Chemical Composition Labeling System
Pegasus® 4D GCxGC-TOFMS, www.leco.com

## Preliminary Results:




GCxGC-TOF MS spectra of Jet-A, FT, HEFA, and SIP fuels

## Next Steps:

1. Evaluate the performance differences between test fuels as they relate to combustion and emissions
2. Begin to build a database to compare the fuels performance characteristics

## References:

1. ASTM. (December 2013). D1655-13a: Standard specification for aviation turbine fuels. DOI:10.1520/D1655-13a
2. ASTM. (June 2014). D7566-14a: Standard specification for aviation turbine fuel containing synthesized hydrocarbons. DOI:10.1520/D7566-14a


**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 fuel.

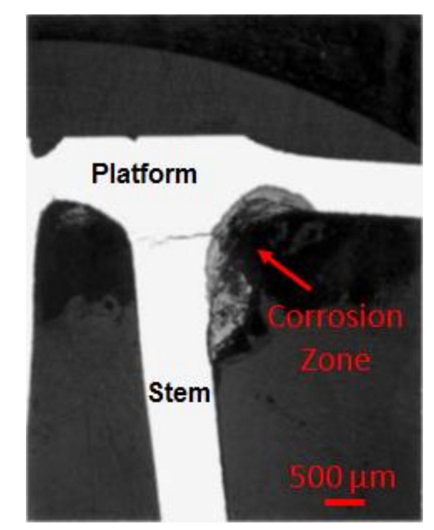
## Overview of Problem:

- Environment: Contains NaCl

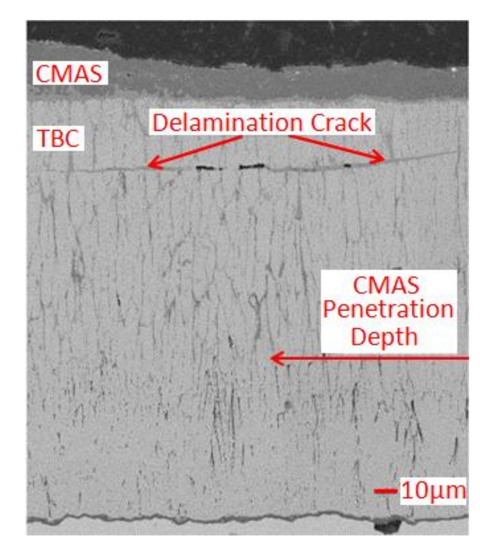
Jet Fuel JP8: Includes sulfur (0.05 wt.%)

- Na + S + O forms $Na_2SO_4$; 2 types of hot corrosion; Type I at 900°C and Type II at 700°C

- Another impurity from the environment: CMAS (CaO-MgO-$Al_2O_3$-$SiO_2$ glass) ($T_m$ ~1250°C)
- For engine temperatures greater than 1250°C, the CMAS melts and infiltrates the TBC resulting in delamination
- It doesn't take much impurity to create problems; 1 ppm contaminant = 0.45 kg entering the gas turbine every 50 hrs




Type I: Under platform corrosion




Deterioration of the TBC due to CMAS infiltration

## The Challenge of Biofuels: New Realities

Biofuels can add significant impurities into the gas turbine. These impurities include: S, Ca, Mg, Si, P and others (*e.g.,* Fe). What are the new biofuel realities? It may be possible to form CMAS without being in a middle east theater. The type of contaminant will vary based on the biomass source.

## Work to Date:

1. Working with Praxair Surface Technologies, have obtained three types of TBCs
   a. Conventional plasma spray 7 wt.% $Y_2O_3$-$ZrO_2$ (YSZ) coating on MCrAlY/Superalloy
   b. Dense vertically cracked (DVC) YSZ coating on MCrAlY/Superalloy
   c. Ultra-high purity YSZ coating on MCrAlY/Superalloy
2. Development of impurity "cocktails" for adding impurities in the liquid state
3. Modification of ablation rig for thermal cycling of impurities in YSZ coatings; added heat flux, $p_{O2}$ sensors

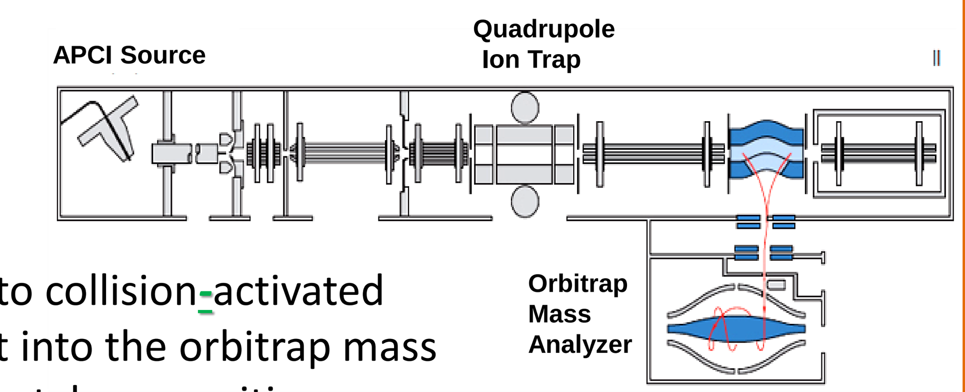
## References:

1. D.A. Shifler, ASM Handbook, 2006 (of ONR).
2. N. Eliaz, et al., Eng. Failure Analysis, [9], 2002.
3. A.D. Foster, H.E. von Doering, and M.B. Hilt, GER-3428a, 1983.


**Hilkka Kenttämaa**

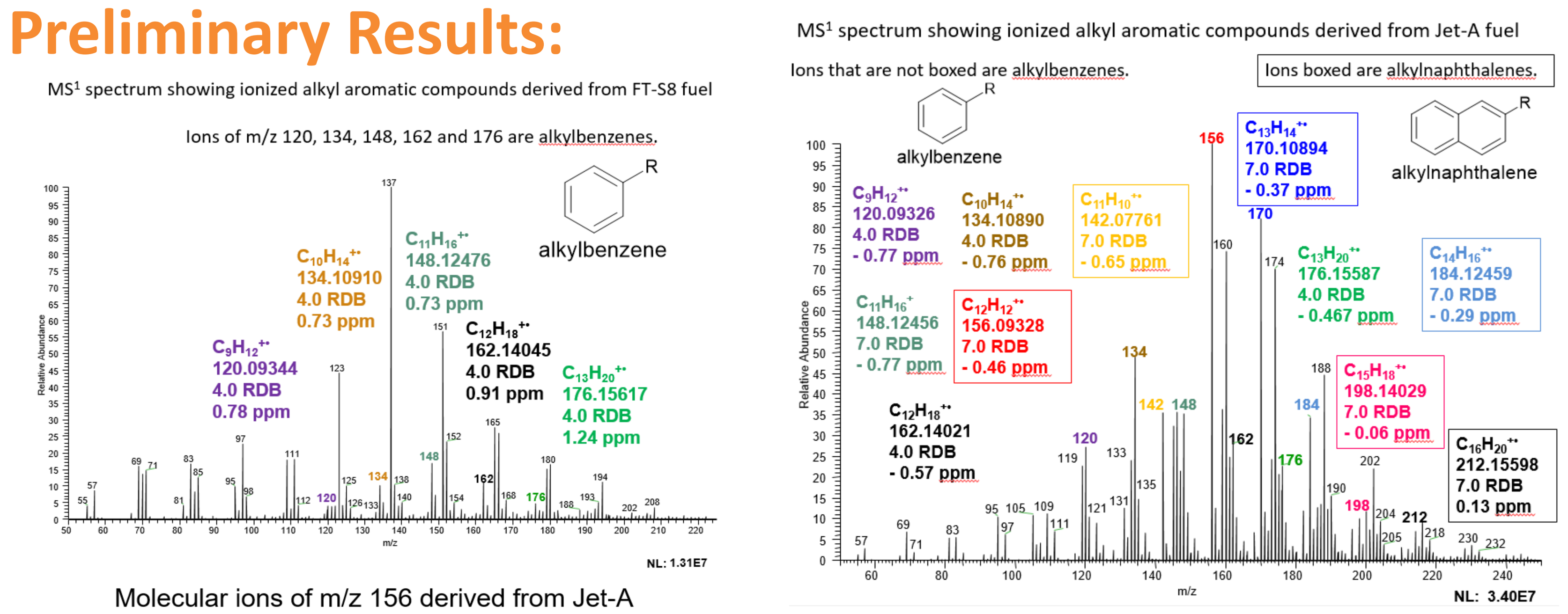
## Introduction:

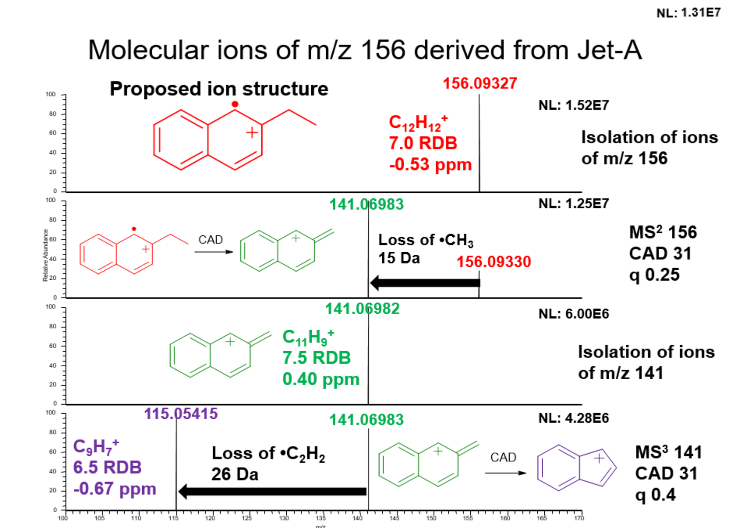
Aviation fuels are composed of hydrocarbons that provide high energy content and high combustion efficiency for peak performance. On the other hand, aromatic compounds, particularly naphthalenes, undergo incomplete combustion and produce soot and smoke. These attributes can negatively impact engine performance. Therefore, it is important to be able to structurally characterize aromatic impurities in aviation fuels.




A Thermo linear quadrupole ion trap coupled to a high resolution orbitrap is employed. Ions are first isolated in the quadrupole ion trap and then subjected to collision-activated dissociation. Fragment ions are then sent into the orbitrap mass analyzer. Each ion was assigned an elemental composition, mass error (in ppm) and ring and double bond equivalence (RDB; the degree of unsaturation: each π bond or ring corresponds to 1 RDB).

## Preliminary Results:




## Conclusions:

Jet-A and HEFA contain alkylbenzenes, alkylnaphthalenes and aromatic naphthenes. FT-S8 contains only alkylbenzenes. With fewer types of aromatic compounds, FT-S8 may produce less soot and smoke and have a higher combustion efficiency than Jet-A.

## Next steps:

Above analysis will be performed for additional fuels. In addition, polar components and saturated hydrocarbons in the fuels will be characterized (the latter by using a new high-resolution GCxGC TOF).

## References:

1 Bernabei, M., Reda, R., Galiero, R., and Bocchinfuso, Journal of Chromatography A., 985 (2003) 197-203.