Composition/Property/Performance Correlations For Rational Development of Renewable Aviation Fuels

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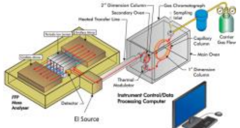
Goal: Establish a databank of conventional and alternative aviation fuel constituents to be utilized in developing correlations between chemical composition, engine performance, and material performance. Our mission is to serve towards Navy's alternative energy goals while training and educating midshipmen and US military personnel.

Introduction:

Cost and time intensive fuel certification protocol is a challenge to the deployment of alternative aviation fuels. Our research aims at mitigating this hurdle by establishing correlations between the chemical composition of fuel, its properties and its performance. Aromatic compounds, such as alkylbenzenes, are an example of compounds affecting fuel performance. We explored correlations of alkylbenzenes' structures with O-ring swelling. Parallel investigation was executed on the effects of biofuel impurities on gas turbine combustion chamber components, such as blades, vanes and other hot sections.

Methods:



- Two-dimensional gas chromatography coupled with high resolution time-of-flight mass spectrometry (GC/GC/TOF MS): identification of structures of alkylbenzenes in fuels.
- Scanning Electron Microscopy (SEM) with Energy Dispersive X-Ray Microscopy (EDS): Microstructure evaluation and surface element mapping.
- MTS Insight: O-Ring tensile test
- NiKon optometer: measurement of the thickness of o-rings

Nikon Digital Optometer

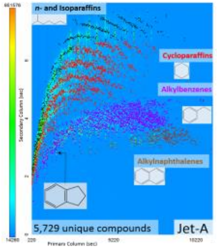
Conclusions:

GC/GC/TOF was used to identify alkylbenzenes in fuels and additives. The exact structure of alkylbenzenes doped into FT-S8 was demonstrated to influence the extent of o-ring swelling, with ethyl benzene being most effective; however when testing the tensile strength of the samples, ethyl benzene weakened the samples the most. Elemental mapping and microscopy analysis provided evidence that silica and alumina products were formed over the surface and in the cracks of the ceramic coatings, hastening delamination and premature failure of gas turbine components.

Future plans:

Measure properties of fuel samples (Jet A/alt. blending components with different classes of hydrocarbons) using ASTM approved devices and apparatuses:
- Stabinger Viscometer SVM 3001: density and viscosity
- TAG 4 Flash Point Tester: flash point
- 6200 Isoperibol Calorimeter: net heat of combustion
- K29700 Apparatus: freezing point
- Distillation apparatus: distillation profile

Hydrocarbon classes identified via GC/GC/TOF MS

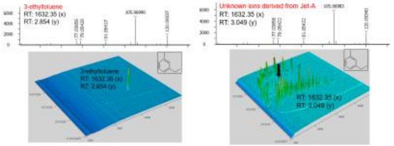


O-rings exposed to FT-S8 doped with an alkylbenzene for 48 hours

Sample tested	Chemical structure	Volume swell %
FT-S8 (neat)	Trace amounts of aromatic content	0.09 ± 0.04
t-butylbenzene		0.34 ± 0.05
sec-butylbenzene		0.43 ± 0.07
butylbenzene		0.60 ± 0.03
1,3,5-trimethylbenzene		0.65 ± 0.09
1,2,4-trimethylbenzene		0.79 ± 0.11
isopropylbenzene		0.81 ± 0.04
propylbenzene		0.96 ± 0.10
HEFA + Jet-A	Mixture of aromatic compounds	1.16 ± 0.11
ethylbenzene		1.34 ± 0.09
Jet-A	Mixture of aromatic compounds	2.60 ± 0.35

Set-up for O-ring immersion test

Identification of alkylbenzenes via GC/GC/TOF MS

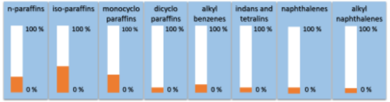


Identification of alkylbenzenes via GC/GC/TOF MS

Alkylbenzene	Jet-A	HEFA	FT-S8	CHCJ
o-xylene	X	X	X	X
m-xylene	X	X	X	X
p-xylene	X	X		
ethylbenzene	X	X	X	X
propylbenzene	X	X		X
2-ethyltoluene	X	X	X	
3-ethyltoluene	X	X	X	X
4-ethyltoluene	X	X		X
1,2,3-trimethylbenzene	X	X	X	
1,2,4-trimethylbenzene	X	X		X
1,3,5-trimethylbenzene	X	X		X
isopropylbenzene	X	X		X

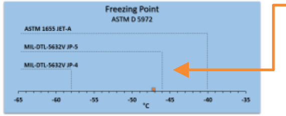
Next steps:

Identify an alkylaromatic compound/compounds ideal for renewable aviation fuels with regard to its/their ability to swell o-rings as well as other important properties.



Next steps:

We will measure the physical properties of fuel with different classes of hydrocarbons. We will expand the fuel specific databank to interconnect properties to chemical compostion.



O-Rings tensile test after biofuel exposure

Buna-N O-Ring 48 hrs of Biofuel Exposure

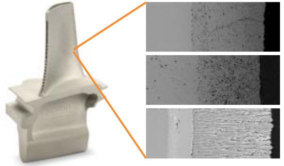
Sample tested	Ultimate Elongation (%)	Ultimate Tensile Strength (MPa)
control (non exposed)	437	38.2
SIP	438	38.3
FT-S8 + 1,2,4-trimethylbenzene	403	56.7
FT-S8 + ethylbenzene	385	18.5

- While O-rings swelling is necessary, biofuels can enhance degradation of the mechanical properties of the O-ring.

Next steps:

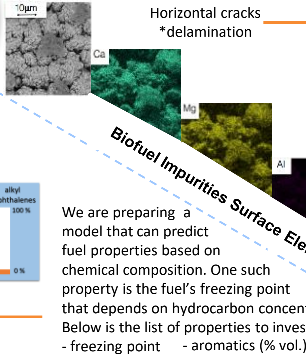
Quantitative and qualitative analysis of the corrosive glass products and damage evaluation, multifactor study of O-ring degradation.

Biofuel impurities effect in the ceramic coatings

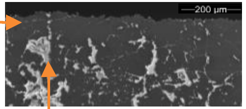


- Manufacturing process (APS, EB-PVD)
- Purity of powder used (Standard vs High)
- Structure density and surface roughness
- Dimensionally Vertically Cracked (DVC)

Thermal cycling with biofuel impurities.

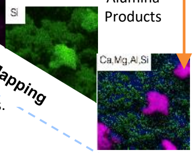


Horizontal cracks *delamination



Glass formation *corrosive Product

Silica and Alumina Products



We are preparing a model that can predict fuel properties based on chemical composition. One such property is the fuel's freezing point that depends on hydrocarbon concentrations. Below is the list of properties to investigate:

- freezing point	- aromatics (% vol.)
- density	- naphthalenes (% vol.)
- distillation	- viscosity
- flash point	- net heat of combustion