Project ASCENT 31B

Effect of Residual Oxygenated Functional Groups on the Behavior of Alternative Jet Fuel Properties

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Motivation and Objectives

1. Research Question:
What oxygenated compounds are present in the AJFs under consideration by the FAA and industry *and what could be their impact*?
2. What are we doing?
Identifying and **quantifying oxygenated compounds** left in Alternative Jet Fuels (AJF) under ASTM certification. Evaluation of potential **impact of these compounds on jet fuel properties**.
3. Impact
Guide the stakeholders on the development of new methods to identify and quantify these compounds and on the improvement of hydro-treatment processes to avoid the presence of undesirable oxygenated compounds in alternative jet fuels.

Tasks:

1. AJF samples collection (From AFRL and UW)
2. Identification of the nature and quantity of residual oxygenated compounds in AJFs
3. Preparation of surrogate blends and evaluation of the five most important oxygenated compounds identified on fuel properties
4. Determination of lean blow out limit, NOx and sooting threshold
5. Development of fast methods for the detection of Oxygenated compounds in AJFs

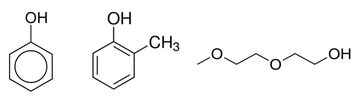
Methodology

Fuel Samples

Company	Alternative JF
Virent	SK and SAK
Kior	Hydrotreated Kerosene
Gevo	Gevo Jet Blend Stockm (2)
Amyris	Farnesane
ARA	ReadiJet (JetA)
UOP	Camelina (2) and Tallow
Sasol	FT - Coal
Syntroleum	FT - Methane
TOTAL SAMPLES	**12**

Company	Comercial JF
Shell	Jet A (Civil Jet Fuel)
Valero	JP-5 (Military Jet Fuel)
NuStar	JP-8 (Military Jet Fuel)
TOTAL SAMPLES	**3**

Molecules Chosen to Prepare Surrogate Blends:



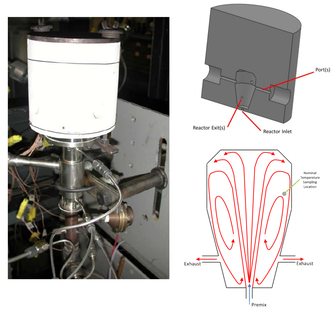
Phenol **2-methyl-Phenol** **2-methoxy-ethoxy-ethanol**

Prepare surrogate blends containing 0.01, 0.1, 1.0, 2.0 and 5.0 wt. % of the standard oxygenated compounds in a commercial jet fuel

Overall composition analysis(GC-MS, CHNO, Karl-Fisher Titration) was carried on for all Jet fuels. In addition, fuel properties were also characterized as well, including density, kinematic viscosity, water solubility, flash point, cold flow , heating value, total acid number, and carbonyl content.

Determination of lean blow out limit, NOx and sooting threshold

- Represents generic gas turbine primary zone
- Fuel/air premix introduced via sonic jet that provides intense mixing and a recirculation flow pattern
  - Recirculation provides flame stabilization mechanism, just as it does in practical gas turbine primary zones
  - Liquid fuels are prevaporized and introduces as vapors to focus only on combustion behavior
- Flame stabilization can be evaluated by exploring lean blowout points
- NO_x can be evaluated by sampling from the reactor volume.



Jet-Stirred Reactor

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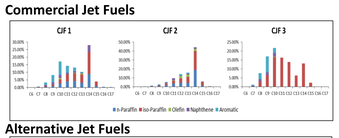
Washington State University-University of Washington
Program ManagerL Cecilia Shaw
September 27-28, 2016

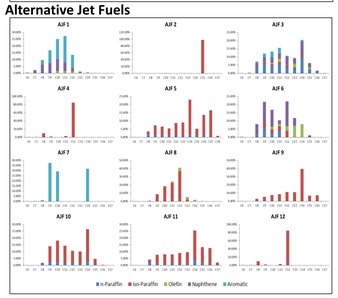
Results and Discussion

Overall composition analysis:

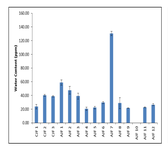
Commercial Jet Fuels



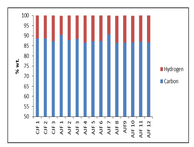
Alternative Jet Fuels



Water Content



Elemental Composition

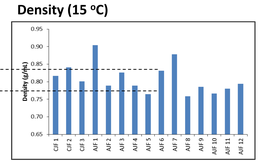


Oxygenated molecules identified in AJFs(mg/g)

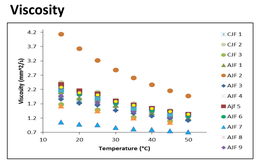
	AJF1	AJF2	AJF3	AJF4	AJF5	AJF7	AJF8	AJF10	AJF 11	AJF 12
2-Butanone, 3-methoxy-3-methyl-	-	-	-	N/S	-	0.008	N/S	-	-	N/S
2,5-dimethyl-2-hexanol	-	-	-	0.018	-	-	-	-	-	0.018
3,4-dimethyl-3-hexanol	-	-	-	0.004	-	-	-	-	-	0.004
3-Pentanol, 2,3,4-trimethyl-	-	-	-	0.004	-	-	-	-	-	0.004
3-Hexanol, 5-methyl-	-	-	-	0.012	-	-	-	-	-	0.012
2,4,4-Trimethyl-1-pentanol	-	-	-	0.004	-	-	-	-	-	0.004
Ethanol, 2-(2-methoxyethoxy)-	-	-	-	-	1.298	-	2.035	0.356	0.311	-
Ethanol, 2-(2-ethoxyethoxy)-	-	-	-	-	-	-	0.074	-	-	-
Phenol	-	-	0.024	-	-	-	-	-	-	-
Cyclohexane-ethanol	-	0.056	-	-	-	-	-	-	-	-
Phenol, 2-methyl-(o-cresol)	0.645	-	0.329	-	-	-	-	-	-	-
Phenol, 2,6-dimethyl-	-	-	0.160	-	-	-	-	-	-	-
Phenol, 2,4-dimethyl-	0.207	-	-	-	-	-	-	-	-	-
1-Pentanol, 2,2,4-trimethyl-	-	-	-	0.014	-	-	-	-	-	0.014
1-Hexanol, 4-methyl-	-	0.038	-	-	-	-	-	-	-	-
Phenol, 4-methyl-(p-cresol)	0.071	-	-	-	-	-	-	-	-	-
Phenol, 2-ethyl-	0.197	-	0.146	-	-	-	-	-	-	-
3,4-dimethyl-phenol	0.525	-	0.127	-	-	0.009	-	-	-	-
Phenol, 2,4,6-trimethyl-	0.106	-	-	-	-	-	-	-	-	-
Phenol, 2-propyl-	0.227	-	0.120	-	-	-	-	-	-	-
Phenol, 3,4,5-trimethyl-	0.199	-	-	-	-	-	-	-	-	-
4-Methyl-2-propylphenol	0.200	-	-	-	-	-	-	-	-	-
Phenol, 4-butyl-	-	-	0.234	-	-	-	-	-	-	-
Phenol, 4-pentyl-	-	-	0.374	-	-	-	-	-	-	-

Fuel Properties:

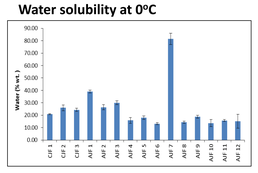
Density (15 ºC)



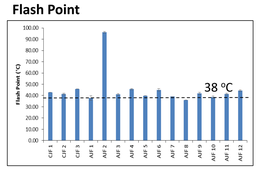
Viscosity



Water solubility at 0ºC



Flash Point

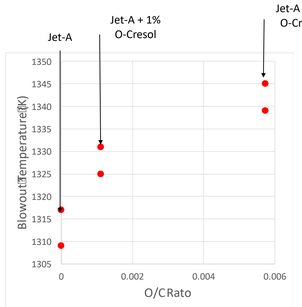


Cold Flow properties (by DSC) ,heating value , carbonyl content and total acid number (TAN).

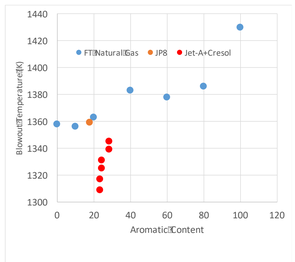
Jet Fuel	Cloud Point (°C)	Pour Point (°C)	HHV(kJ/g)	LHV (kJ/g)	CO (µg/g)	TAN (mg KOH/g fuel)
CJF 1	-53	-57	46.13	43.63	1.52	0.010
CJF 2	-58	-62	44.53	42.03	1.04	0
CJF 3	-57	-60	46.13	43.36	0.98	0
AJF 1	< -80	< -80	44.27	42.19	1.82	0.021
AJF 2	< -80	< -80	47.14	44.48	1.25	0.005
AJF 3	-48	-54	46.17	43.64	2.46	0.005
AJF 4	< -80	< -80	47.23	44.28	0.38	0.004
AJF 5	-61	-68	47.23	44.44	0.27	0.016
AJF 6	< -80	< -80	41.31	38.52	0.37	0
AJF 7	< -80	< -80	43.25	41.21	5.73	0.005
AJF 8	< -80	< -80	47.12	44.16	0.60	0.010
AJF 9	-56	-63	46.18	43.23	0.60	0.010
AJF 10	-72	-83	46.80	43.92	0.64	0.010
AJF 11	-62	-70	47.26	44.45	0.65	0.010
AJF 12	< -80	< -80	47.22	44.32	0.00	0.016

Lower Freezing point: Jet A (-40 ºC), Jet A-1 (-47 ºC):

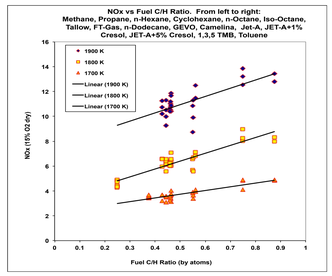
Blowout Temperature

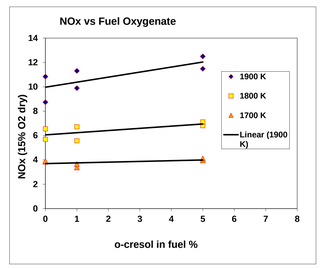


Influence of Aromatics on Blowout

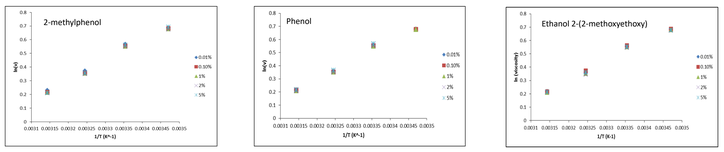


NO_X Interpretation:

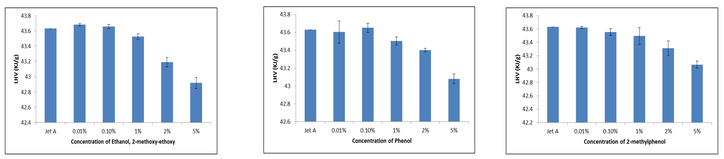




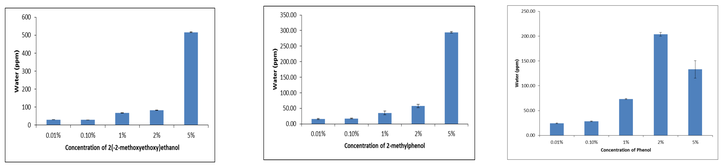
Effect of oxygenated compounds on viscosity of Jet Fuel



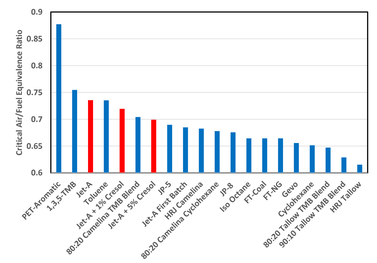
Effect of oxygenated compounds on High Heating value of Jet Fuel



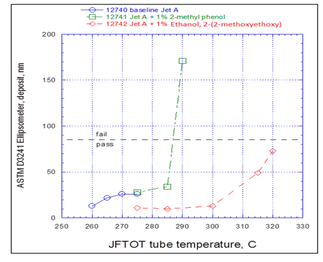
Effect of oxygenated compounds on water equilibrium(at 0ºC) on Jet Fuel



Soot Performance:



Effect of oxygenated compounds on Thermal oxidative stability of Jet Fuel



Conclusions

1. Trace amounts of oxygenated molecules were detected in the alternative jet fuels and phenols and 2-methoxy-ethoxy-ethanol were the most common ones. The content of oxygenated compounds measured is comparable in AJFs with Commercial Fuels.
2. Oxygenated molecules in the surrogated blends affected fuel properties, such as HHV, water solubility, and kinematic viscosity.
3. Addition of o-cresol results in increase in blowout temperature; Oxygenates give generally steeper NO_X dependence than predicted by C/H ratio but reduce sooting.