Low Volume Evaluation of Alternative Jet Fuels and Data Library

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CAAIFI Biennial General Meeting (CBGM) & Integrated ASCENT Symposium Agenda

Marriott Metro Center, Washington D.C.

5 December 2018
Alternative Jet Fuels Evaluation: Problems, NJFCP Objectives and Achievements

Focus on streamlining, reduce cost, time and fuel volume requirement and combustor performance

<table>
<thead>
<tr>
<th>Problem</th>
<th>NJFCP Objectives</th>
<th>NJFCP Achievements</th>
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<tbody>
<tr>
<td>2-4 year approval cycle with large costs ($$M)</td>
<td>Streamline current ASTM approval process</td>
<td>- Early Prescreening Process</td>
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<tr>
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<td>for alternative Jet fuels</td>
<td>- Proposed streamline to ASTM fuel evaluation process</td>
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<td>- Demonstration in progress</td>
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<td>Initial fuel costs are high (&gt;5 gallon); large quantities required (3,000-10,000 gal). Who pays?</td>
<td>Reduce fuel quantities required for approval</td>
<td>-&quot;100 gallons and $100K&quot; with NJFCP referee rig</td>
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<td>- May reduce Tier 3/4 tests (3000 gallons), in progress</td>
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<td>OEMs design for hardware not fuel variability. They must protect their own hardware.</td>
<td>Reduce engine OEM risk/uncertainty in decision making process</td>
<td>- NJFCP Referee Rig (at AFRL) captures all OEM observed engine behavior</td>
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<td>- Experiments demonstrate and analysis explains transition amongst chemical and physical control of key 'Figures of Merit'</td>
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<td>Limited knowledge for assessing fuel impacts on combustor performance</td>
<td>Improve industry modeling and design tools</td>
<td>- Enhanced referee rig with procedures that characterizes fuel-dependent lean blowout and ignition limits</td>
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<td>- LBO predictions captured well, based on physical interpretations</td>
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<td>- CFD simulation tool for predicting LBO in progress</td>
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A strong community including international (European JetScreen) participants from 40+ entities
NJFCP: Relating Fuel Properties to Jet Combustion Operability

Key properties impacting combustor safety performance identified

Critical Engine Performance impacted by Fuel

Fuel property effects are evaluated at relevant conditions to estimate alternative fuel behavior on Figure of Merit (FOM) performance.

- Lean Blowout (LBO)
- Cold Start Ignition
- Altitude Relight

Six Critical Fuel Properties that impact FOMs

- Atomization: viscosity, density, surface tension*
- Evaporation: distillation curve
- Chemistry: DCN (Derived Cetane Number)*

Relative importance changes, depending on operating conditions and combustor design

* Novel NJFCP Contributions

Gas Turbine Engine Schematic

The $T_3$-$P_3$ curve determines the thermodynamic conditions of interest for fuel testing.

Normal design constraint
### Major Accomplishments Perceived by OEMs
(in understanding fuel impacts on combustor operability)

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<th>now</th>
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<tbody>
<tr>
<td><strong>Geometry Variation</strong></td>
<td><strong>All rigs show condition consistent trends</strong> <em>(HON APU, GE TAPS, Referee Rig, and research reactors)</em></td>
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<tr>
<td>Can a generic rig capture OEM product trends?</td>
<td></td>
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<tr>
<td><strong>Fuel Property Sensitivity</strong></td>
<td></td>
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<tr>
<td>• Chemistry... important at all?</td>
<td>Chemistry is important</td>
</tr>
<tr>
<td>• Surface tension... important at all?</td>
<td>More important than previously thought</td>
</tr>
<tr>
<td>• Viscosity... how important?</td>
<td>Dominant property leading to ignition</td>
</tr>
<tr>
<td>• Distillation curve... how important?</td>
<td>Dominant property in some circumstances</td>
</tr>
<tr>
<td><strong>Model Applicability</strong></td>
<td>Models can predict some FOM behavior, additional work is still needed</td>
</tr>
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</table>
NJFCP: Contributions to Prescreening and Proposed Revisions to ASTM Approval Process for Alternative Fuels

Prescreening for Blend Limits and Far-Term FastTrack Implementation

- **Tier α**
  - mls
  - Property Predictions & Blend Estimations
    - GCxGC
    - IR absorption, and/or
    - NMR

- **Tier ‘ZERO’**
  - ~1 liter
  - Critical Properties & Blend Limits
    - DCN
    - Density
    - Distillation Curve
    - Viscosity
    - Surface Tension

- **Tier 1, 2**
  - α
  - ~10^-2

- **Tier 2.5**
  - ‘ZERO’
  - ~10^-1

- **Tier 3 & 4**
  - α
  - ~10^2

- **Tier 2.5**
  - 200 gals
  - (100 Tier 1&2, 100 Tier 2.5)

- **0 gals?**
  - Potential ASTM FastTrack Applicability
  - Could this be a future possibility?

- **Fuel Requirements**

<table>
<thead>
<tr>
<th>Tier</th>
<th>0(gal)</th>
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<tbody>
<tr>
<td>α</td>
<td>~10^-2</td>
</tr>
<tr>
<td>‘ZERO’</td>
<td>~10^-1</td>
</tr>
<tr>
<td>1 &amp; 2</td>
<td>~10^2</td>
</tr>
<tr>
<td>2.5</td>
<td>~10^2</td>
</tr>
<tr>
<td>3 &amp; 4</td>
<td>~10^3</td>
</tr>
</tbody>
</table>

- **ASTM D4054**
  - Referee Combustor Rig Testing
  - Tier 2.5
  - Phase 1 ASTM Research Report

- **Early prescreening and Tier 2.5 tests should reduce (or replace) Tier 3 and 4 testing**
Aromatic Free Jet Fuel
( Doe Funded Program Leveraging NJFCP)

Issues with the removing aromatics:

1. Loss of swelling characteristics and fuel leakage
2. Energy per gallon of fuel purchased goes down

2. Aromatic free fuels can increase:
   i. mission range,
   ii. payload, and
   iii. fuel savings while
   iv. minimizing emissions;

iso-alkane and cycloalkane fuels can meet spec

1. Select cycloalkanes reproduce the minimum swelling characteristics of Jet-A (in a 30%v blend with an IPK swell within the Jet-A range).
3 Fuel Prescreening Tools for low fuel volume costs to help streamline ASTM process:

• Tier $\alpha$, Tier ‘ZERO,’ and Tier 2.5
  • Tier ‘ZERO’ and Tier 2.5 are requirements for currently selected DOE proposals on alternative jet fuels (“100 gallons, $100K concept”)

• Far-term impact on currently pursued FastTrack approval routes

• Evaluation of Shell IH$^2$ fuel (primarily cycloalkanes) – in parallel and coordination with ASTM tiered evaluation
Alternative Jet Fuel Test Database (Project 33)

Database focus on final stages:
- Gather existing data from completed testing
- Establish database web portal
- Develop data schema to structure database
- Provide comprehensive jet fuel analysis
- Support ASTM jet fuel approval

Goal: to establish a foundational database of current and newly emerging alternative jet fuels into a common archive which can provide guidelines for design and certification of new jet fuels in our future.

altjetfuels.illinois.edu
Phase I: Information Repository

AFRL-RQ-WP-TR-3

U.S. AIR FORCE HYDROPROCESSED RENEWABLE (H2R) FUEL RESEARCH
James T. Edwards
Fuels & Energy Branch

Phase 1: Information Repository

EAR99, Non-proprietary

Database Structure

Chemical Kinetics
- Alcohols, alkanes, etc.
- Jet fuel relevant surrogates
- Mechanisms

Testing Results
- Shock Tube
- Rapid Compression Machine
- Engine/Rig Tests

Fuel Properties
- Thermophysical
- Physicochemical
- GCxGC
- GCxMS
- Specifications

Publications
- Production Processes
- Chemical Kinetics
- Economic Analyses
- Technical Reports
- Fuel Certifications

Figure 1: Chromatogram of H2R Fuel

Designation: D7666 - 14a

Fuel Description

LLNL BUTANOL ISOMERS ME

The following provides links to the chemical kinetic transport parameters for butanol isomers (C4H8OH) Laboratory. The mechanism was validated by shock tube (RCL), and jet-stirred reactor (JSR) experiments.

Test Conditions:
- Pressure: 0.04 – 80 atm
- Temperature: 720 – 1700 K
- Equivalence ratio: 0.5 – 1.7

Download:
Detailed mechanism for high and low temperatures
Detailed mechanism for low temperatures
Detailed mechanism for high temperatures
Detailed mechanism for high temperatures
Thermodynamic parameters
Transport parameters
Related Literature:
A comprehensive chemical kinetic combustion model for the four butanol iso.
Phase II: Conversion to NoSQL

### Non-Relational (NoSQL) vs. Relational (SQL)

<table>
<thead>
<tr>
<th>Highly scalable</th>
<th>Less scalable</th>
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<tbody>
<tr>
<td>Flexible schema - data can be inserted/altered anytime without issue</td>
<td>Structured schema - data has to fit into predefined tables</td>
</tr>
<tr>
<td>Does not support JOIN operations</td>
<td>Supports JOIN operations</td>
</tr>
<tr>
<td>Does not use SQL as query language</td>
<td>Mainly uses SQL as query language</td>
</tr>
</tbody>
</table>

#### Conversion to flexible schema (JSON)
- Electronically accessible large sets of data
- Flexible analysis: web interface (Phase II)

#### Integration of AJ FTD with JETSCREEN (Europe)
- JETSCREEN uses MongoDB, a NoSQL database
- AJ FTD using DynamoDB structure
Data Processing

Composition breakdown for NJ FCP Cat. A and C fuels

Data: Metron Aviation

Data: PQIS
Thank you

<table>
<thead>
<tr>
<th>Contact Information</th>
<th>Med Colket</th>
<th>Joshua Heyne</th>
<th>Tonghun Lee</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>860-748-6612</td>
<td>937-609-0207</td>
<td>217-300-7107</td>
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<td></td>
<td><a href="mailto:med@colket.org">med@colket.org</a></td>
<td><a href="mailto:jheyne1@udayton.edu">jheyne1@udayton.edu</a></td>
<td><a href="mailto:Tonghun@Illinois.edu">Tonghun@Illinois.edu</a></td>
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</table>
Back-up
OEMs place high value on insights gained and broadened understanding of fuel effects on combustion – NJFCP insights could help new fuel approvals as well as engine & combustor design efforts:

<table>
<thead>
<tr>
<th>then</th>
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<tbody>
<tr>
<td>Don’t know if generic design rigs could capture operability fuel trends compared to actual product rigs.</td>
<td>Generic combustor rigs (e.g., the referee rig) could capture operability trends with good confidence, and be used in fuel screening.</td>
</tr>
<tr>
<td>Ignition might depend on derived Cetane # (DCN).</td>
<td>Instead, LBO strongly depends on DCN. Could be used as an early predictor.</td>
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<tr>
<td>Don’t know what pyrolysis yields are, and if they correlate to combustor operability.</td>
<td>Know the pyrolysis products. Yields can be used to build chemical models. Yields seem to correlate to combustor operability and might even be used to directly predict performance.</td>
</tr>
<tr>
<td>Ignition’s dependence to properties is not clearly understood.</td>
<td>Ignition at altitude &amp; low temperature depends primarily on viscosity.</td>
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<tr>
<td>Don’t know if volatility or spray size variations has more effect?</td>
<td>Volatility affects operability more.</td>
</tr>
<tr>
<td>Don’t know if unusual fuel compositions would lead to fuel effects when blended with jet if the carbon distribution is within kerosene range.</td>
<td>They could lead to behavior outside of conventional fuel experience even if carbon distribution is within kerosene range.</td>
</tr>
<tr>
<td>Sprays thought to likely be quite distinct for different fuels when using state-of-the-art air-blast injectors at room temperature.</td>
<td>Sprays are nearly identical.</td>
</tr>
<tr>
<td>Don’t know if the conventional component washes-out the effects of an unusual blend component.</td>
<td>Blending &quot;averages&quot; the effects of the conventional and the unusual blend component.</td>
</tr>
<tr>
<td>Don’t know if LES modeling could be used to predict LBO.</td>
<td>LES is capable of achieving LBO near experimental values, but very sensitive to boundary conditions. LES modeling of LBO is very slow.</td>
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<tr>
<td>No prior knowledge on IR absorption ratio relevance to combustion behavior.</td>
<td>IR absorption ratio correlates well with DCN &amp; ignition delay time, and possibly with operability behavior.</td>
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<tr>
<td>Surface tension’s role for ignition is minimal to none.</td>
<td>Surface tension might be a stronger player than originally thought.</td>
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</tbody>
</table>
ASCENT Project PIs and Key Contributors

- **Area 1**: Ron Hanson (Stanford), Tom Bowman (Stanford), Dave Davidson (Stanford), Shock Tube and Flow Reactor Studies.
- **Area 2**: Hai Wang (Stanford), Chemical Kinetics Model Development and Evaluation.
- **Area 2.5**: Tianfeng Lu (Uconn), Wenting Sun (Georgia Tech), Stephen Zeppieri (UTRC), Computational Acceleration.
- **Area 3**: Tim Lieuwen (Georgia Tech), Jerry Sietzman (Georgia Tech), David Blunck (Oregon State), Fred Dryer (Princeton), Tonghun Lee (Illinois Urbana-Champaign), Advanced Combustion.
- **Area 4**: Suresh Menon (Georgia Tech), Matthias Ihme (Stanford), Combustion Model Development and Evaluation.
- **Area 5**: Robert Lucht (Purdue), Paul E. Sojka (Purdue), Scott Meyer (Purdue), Carson Slabaugh (Purdue), Jay Gore (Purdue), Atomization Tests and Models.
- **Area 6**: Scott Stouffer (Dayton), Steven Zabarnick (Dayton), Tonghun Lee (Illinois Urbana-Champaign), Referee Combustor.
- **Area 7**: Josh Heyne (Dayton), Med Colket (contractor), Alex Briones (Dayton), Coordination.

FAA, NASA, and AFRL Funded Activities
Fuel Candidates and Screening

- Reference Fuels Required to Characterize Rig and Engine Fuel Response
- Category A: Three Conventional (Petroleum) Fuels
  -- “Best” case (A-1)  -- “Average” (A-2)  -- “Worst” case (A-3)
- Category C: Six “Test Fluids” With Unusual Properties
  - C-1: low cetane, narrow boiling (downselected)
  - C-2: bimodal boiling, aromatic front end
  - C-3: high viscosity
  - C-4: low cetane, wide boiling
  - C-5: narrow boiling, full fuel (downselected)
  - C-6 and C-6a: high cycloparaffins
  - C-7 high cycloalkane
  - C-8 high aromatics
  - C-9 high cetane #

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<table>
<thead>
<tr>
<th>Temperature, °C</th>
<th>D86 % Distilled</th>
<th>C1</th>
<th>C2</th>
<th>C3</th>
<th>C4</th>
<th>C5</th>
<th>C6</th>
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C-1 and C-5 were selected for detailed study in Year 1.
C-6 and C-6a no longer available

Fuel supply courtesy of Tim Edwards
Most fuels approved to date have chemical compositions similar to petroleum based jet fuel
  - HEFA, FT, ATJ and DSHC (at 10% blend) fuels performed as expected.
  - DSHC at 20% exhibited unacceptable performance and was not approved.

**Resource Requirement: Fuel volume, time and cost**
  - Highest in Tier 3 and 4 testing
  - New generation of candidate fuels have different chemical composition (e.g., cycloalkanes) and will demand more testing and resources
NJFCP: Relating Fuel Properties to Jet Combustion Operability (Lean Blowout)

Chemically Limited
- DCN (chemical) dominance (for 7 rigs)

Physically Limited
- Distillation curve dominance (for 3 rigs)
Additional Synergies:

- **DOE** (in-house activities at National Labs, $12 million announced in jet fuel programs, & possible planned activities)
- **AFOSR** (in-house activities)
- **NASA** (in-house activities)
- **NIST** (in-house activities)
- **NRC Canada** (in-house activities)
- **DLR** (in-house activities, JetScreen Program)
- **Univ. Sheffield** (in-house activities, JetScreen Program)
- **Cambridge Univ.** (in-house activities)
- **Univ. South Carolina** (Supported by AFRL and NASA)
- **Univ. of Toronto** (in-house activities)
- **Univ. of Dublin** (in-house activities)

*OEMs are supporting program through cost-share.

**AFRL** spends additional funds (that are not included here) to procure/distribute fuels and develop/maintain rig.