National Jet Fuels Combustion Program

Low Volume Evaluation of Alternative Jet Fuels and Data Library

Med Colket
Retired Senior Fellow
United Technologies Research Center

Josh Heyne
University of Dayton

Tonghun Lee
University of Illinois - UC

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

Marriott Metro Center,
Washington D.C.

5 December 2018

Parker Aerospace
United Technologies Research Center
Rolls-Royce
Honeywell
Williams International
ANSYS
CONVERGENT SCIENCE
Canada
NRC-CNRC
NAVAIR
NIST
National Institute of Standards and Technology
U.S. Department of Commerce

Georgia Institute of Technology
Stanford
PRINCETON UNIVERSITY
PURDUE UNIVERSITY
UCONN
Oregon State UNIVERSITY
UNIVERSITY of DAYTON
ILLINOIS
UNIVERSITY OF CAMBRIDGE
USC University of Southern California

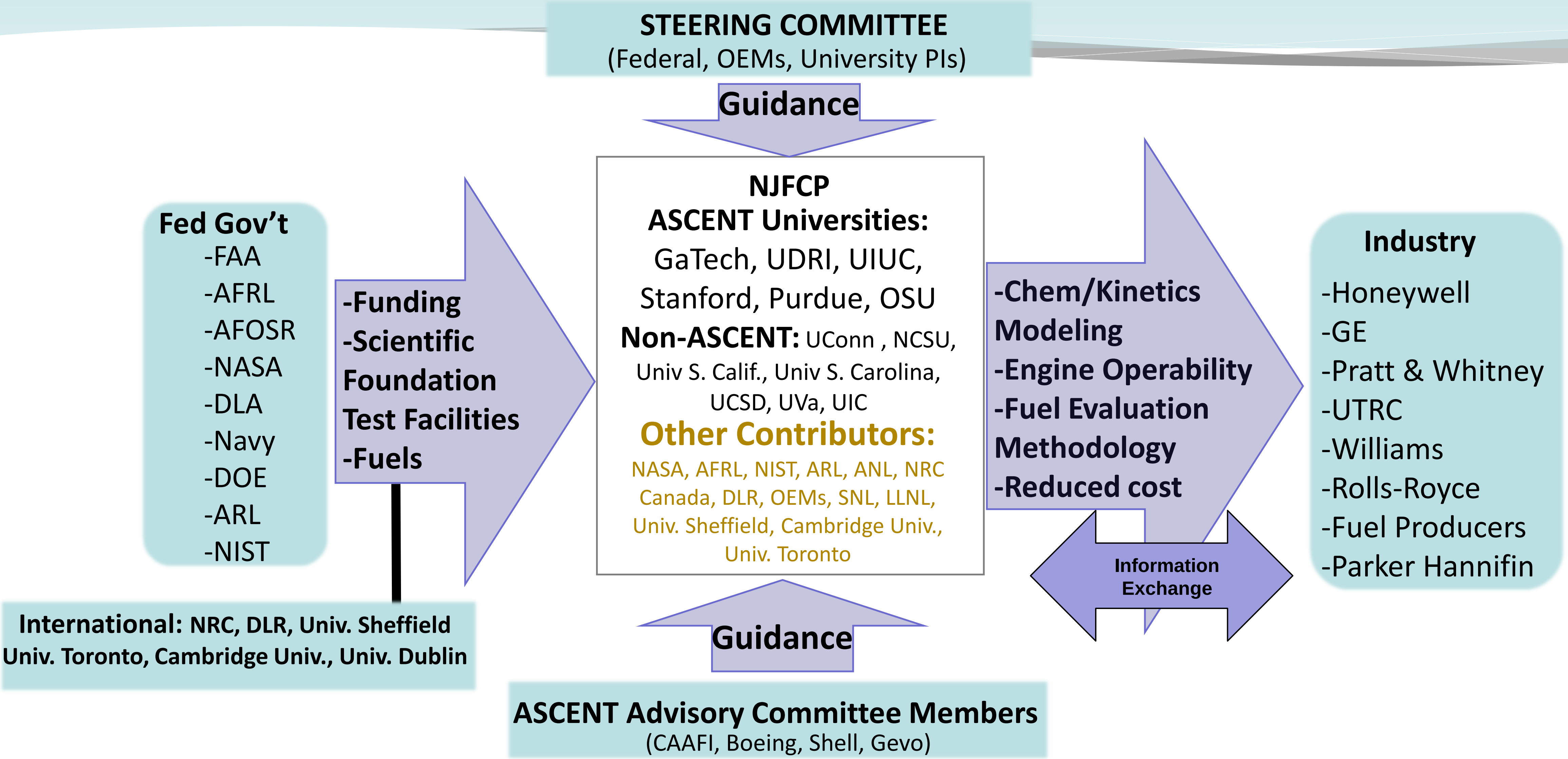
Argonne NATIONAL LABORATORY
ARL
ASCENT
AVIATION SUSTAINABILITY CENTER
The University Of Sheffield.
Trinity College Dublin
The University of Dublin
FEDERAL AVIATION ADMINISTRATION
NASA
DEPARTMENT OF ENERGY UNITED STATES OF AMERICA
AIR FORCE OFFICE OF SCIENTIFIC RESEARCH UNITED STATES AIR FORCE
AIR FORCE RESEARCH LABORATORY
DEFENSE LOGISTICS AGENCY
DLR
PRATT & WHITNEY DEPENDABLE ENGINES
UNIVERSITY OF MICHIGAN

Alternative Jet Fuels Evaluation: Problems, NJFCP Objectives and Achievements

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

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

NJFCP Community and Acknowledgements: Program Sponsors, Contributors, Performers & Industry Members



STEERING COMMITTEE
(Federal, OEMs, University PIs)

Guidance

NJFCP
ASCENT Universities:
GaTech, UDRI, UIUC, Stanford, Purdue, OSU
Non-ASCENT: UConn , NCSU, Univ S. Calif., Univ S. Carolina, UCSD, UVa, UIC
Other Contributors:
NASA, AFRL, NIST, ARL, ANL, NRC Canada, DLR, OEMs, SNL, LLNL, Univ. Sheffield, Cambridge Univ., Univ. Toronto

Fed Gov't
- -FAA
- -AFRL
- -AFOSR
- -NASA
- -DLA
- -Navy
- -DOE
- -ARL
- -NIST

-Funding
-Scientific Foundation Test Facilities
-Fuels

International: **NRC, DLR, Univ. Sheffield Univ. Toronto, Cambridge Univ., Univ. Dublin**

-Chem/Kinetics Modeling
-Engine Operability
-Fuel Evaluation Methodology
-Reduced cost

Information Exchange

Industry
- -Honeywell
- -GE
- -Pratt & Whitney
- -UTRC
- -Williams
- -Rolls-Royce
- -Fuel Producers
- -Parker Hannifin

Guidance

ASCENT Advisory Committee Members
(CAAFI, Boeing, Shell, Gevo)

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

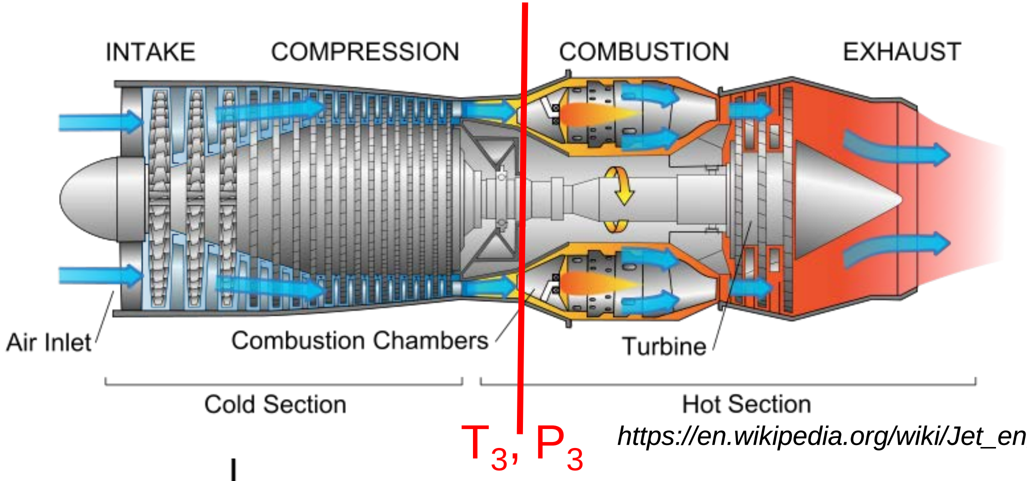
Six Critical Fuel Properties that impact FOMs

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

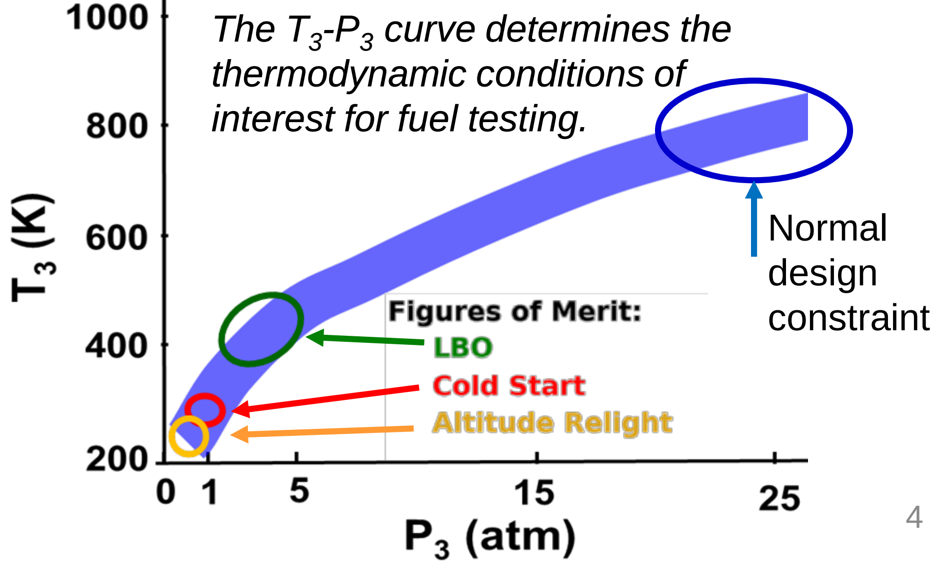
* Novel NJFCP Contributions

Relative importance changes, depending on operating conditions and combustor design

Gas Turbine Engine Schematic



https://en.wikipedia.org/wiki/Jet_engine#



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)

then	now
Geometry Variation	
Can a generic rig capture OEM product trends?	*All rigs show condition consistent trends* *(HON APU, GE TAPS, Referee Rig, and research reactors)*
Fuel Property Sensitivity	
Chemistry… important at all?	Chemistry *is* important
Surface tension… important at all?	More important than previously thought
Viscosity… how important?	Dominant property leading to ignition
Distillation curve… how important?	Dominant property in some circumstances
Model Applicability	Models can predict some FOM behavior, additional work is still needed

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

Potential ASTM FastTrack Applicability

Low fuel requirement promoted by DOE

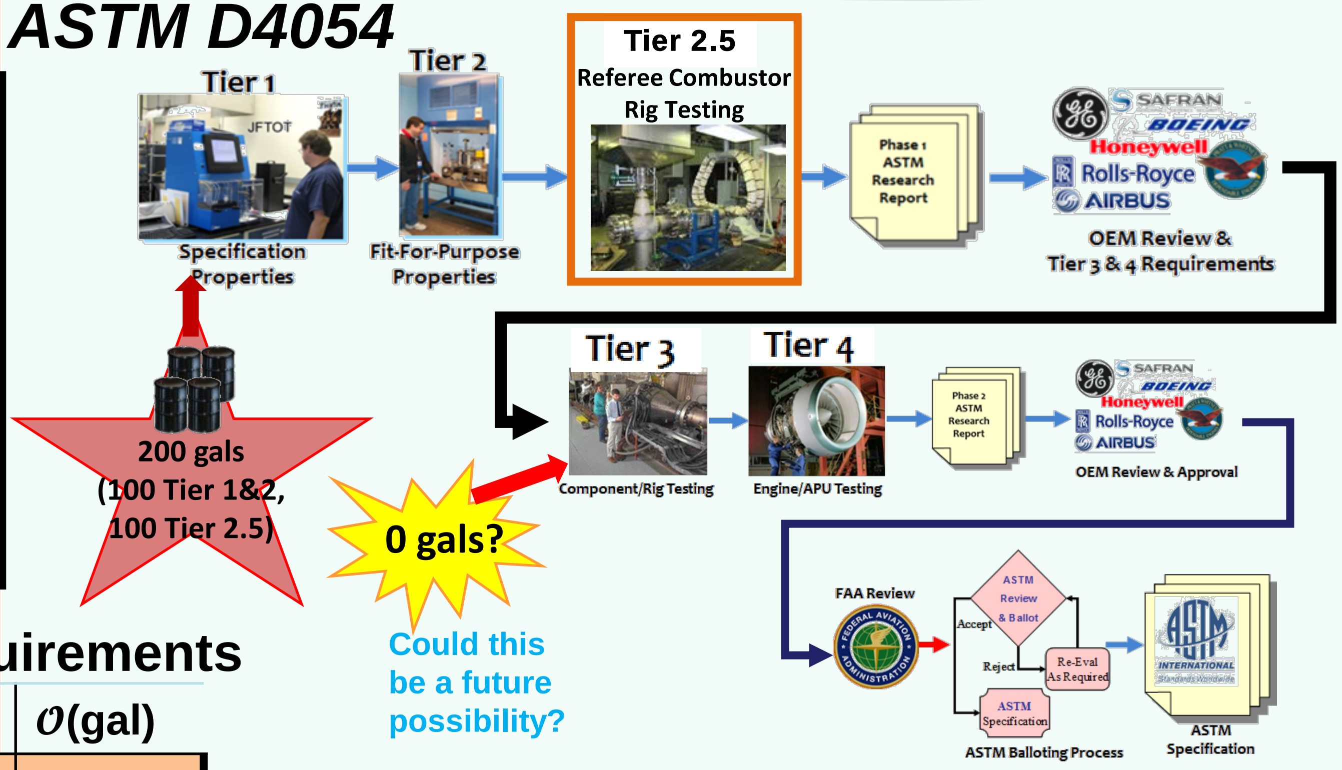
Tier 'ZERO'

~1 liter

Critical Properties & Blend Limits

- DCN
- Density
- Distillation Curve
- Viscosity
- Surface Tension

ASTM D4054



Could this be a future possibility?

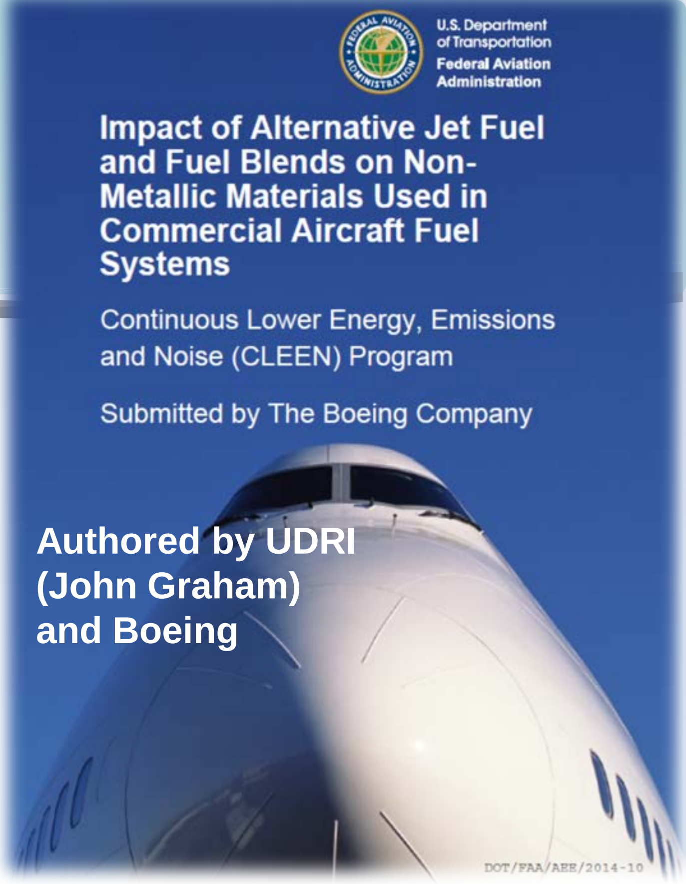
Fuel Requirements

Tier	$\mathcal{O}$(gal)
α	~10^{-2}
'ZERO'	~10^{-1}
1 & 2	~10^{2}
2.5	~10^{2}
3 & 4	~10^{3}

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)



U.S. Department of Transportation
Federal Aviation Administration

Impact of Alternative Jet Fuel and Fuel Blends on Non-Metallic Materials Used in Commercial Aircraft Fuel Systems

Continuous Lower Energy, Emissions and Noise (CLEEN) Program

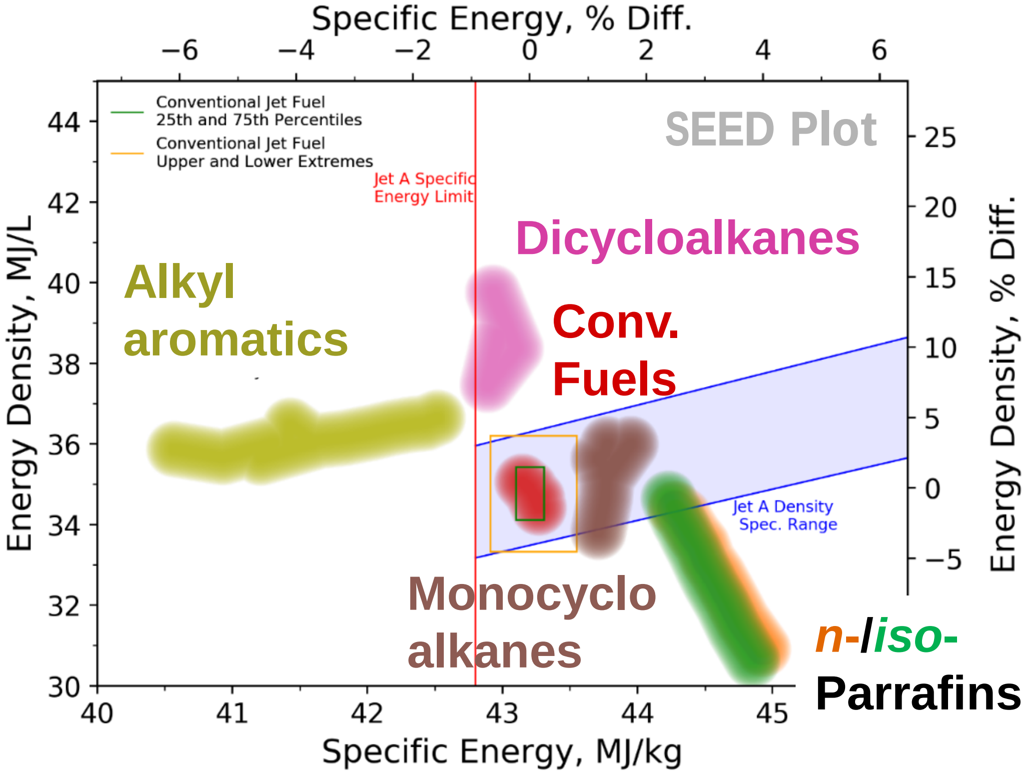
Submitted by The Boeing Company

DOT/FAA/AEE/2014-10

Authored by UDRI
(John Graham)
and Boeing

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).

NJFCP: Practical Applications

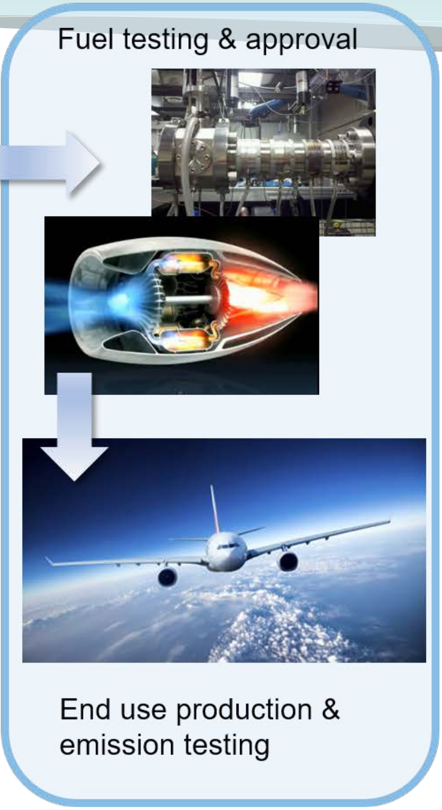
- 3 Fuel Prescreening Tools for low fuel volume costs to help streamline ASTM process:
  - Tier α, Tier ‘ZERO,’ and Tier 2.5
    - Tier ‘ZERO’ and Tier 2.5 are requirements for currently selected DOE proposals on alternative jet fuels (“100 gallons, $100K concept”)
  - Far-term impact on currently pursued 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)

Feedstock development, production & logistics

Fuel conversion, scale-up & production



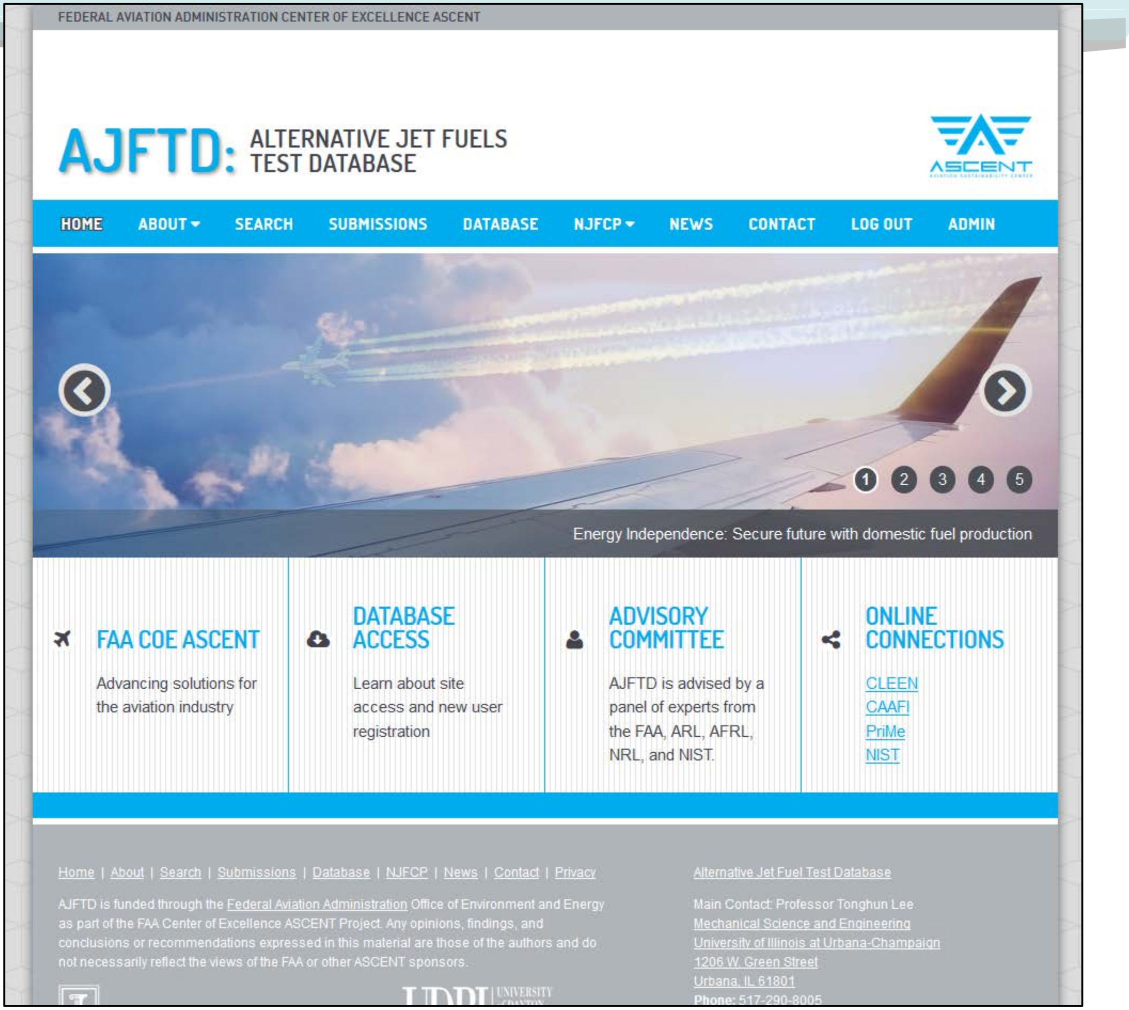
Fuel testing & approval

End use production & emission testing

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.



Energy Independence: Secure future with domestic fuel production

Advancing solutions for the aviation industry

Learn about site access and new user registration

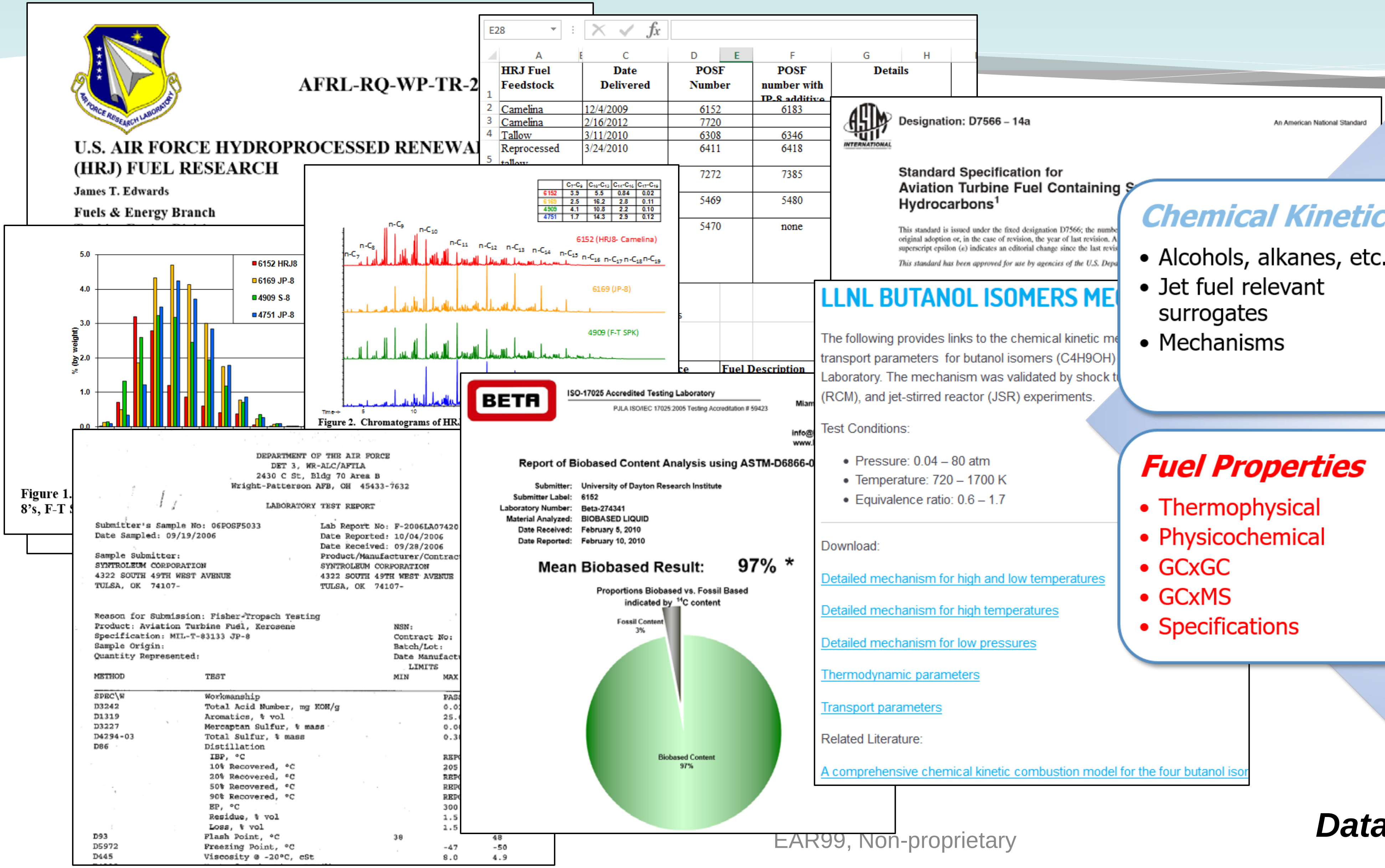
AJFTD is advised by a panel of experts from the FAA, ARL, AFRL, NRL, and NIST.

AJFTD is funded through the Federal Aviation Administration Office of Environment and Energy as part of the FAA Center of Excellence ASCENT Project. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the FAA or other ASCENT sponsors.

Main Contact: Professor Tonghun Lee
Mechanical Science and Engineering
University of Illinois at Urbana-Champaign
1206 W. Green Street
Urbana, IL 61801
Phone: 517-290-8005

altjetfuels.illinois.edu

Phase I: Information Repository



AFRL-RQ-WP-TR-2

U.S. AIR FORCE HYDROPROCESSED RENEWA
(HRJ) FUEL RESEARCH

James T. Edwards

Fuels & Energy Branch

Figure 1.
8's, F-T

E28

	HRJ Fuel Feedstock	Date Delivered	POSF Number	POSF number with JP-8 additive	Details
1					
2	Camelina	12/4/2009	6152	6183	
3	Camelina	2/16/2012	7720		
4	Tallow	3/11/2010	6308	6346	
5	Reprocessed tallow	3/24/2010	6411	6418	
			7272	7385	
			5469	5480	
			5470	none	

Fuel Description

	C_7-C_9	C_{10}-C_{13}	C_{14}-C_{16}	C_{17}-C_{19}
6152	3.9	5.5	0.84	0.02
6169	2.5	16.2	2.8	0.11
4909	4.1	10.8	2.2	0.10
4751	1.7	14.3	2.9	0.12

Figure 2. Chromatograms of HRJ

Designation: D7566 – 14a

An American National Standard

Standard Specification for
Aviation Turbine Fuel Containing S
Hydrocarbons[1]

This standard is issued under the fixed designation D7566; the numbe
original adoption or, in the case of revision, the year of last revision. A
superscript epsilon (ε) indicates an editorial change since the last revis

This standard has been approved for use by agencies of the U.S. Depa

LLNL BUTANOL ISOMERS MEC

The following provides links to the chemical kinetic me
transport parameters for butanol isomers (C4H9OH)
Laboratory. The mechanism was validated by shock t
(RCM), and jet-stirred reactor (JSR) experiments.

Test Conditions:

- Pressure: 0.04 – 80 atm
- Temperature: 720 – 1700 K
- Equivalence ratio: 0.6 – 1.7

Download:

Detailed mechanism for high and low temperatures

Detailed mechanism for high temperatures

Detailed mechanism for low pressures

Thermodynamic parameters

Transport parameters

Related Literature:

A comprehensive chemical kinetic combustion model for the four butanol isor

DEPARTMENT OF THE AIR FORCE
DET 3, WR-ALC/AFTLA
2430 C St, Bldg 70 Area B
Wright-Patterson AFB, OH 45433-7632

LABORATORY TEST REPORT

Submitter's Sample No: 06POSF5033
Date Sampled: 09/19/2006

Lab Report No: F-2006LA07420
Date Reported: 10/04/2006
Date Received: 09/28/2006

Sample Submitter:
SYNTROLEUM CORPORATION
4322 SOUTH 49TH WEST AVENUE
TULSA, OK 74107-

Product/Manufacturer/Contract
SYNTROLEUM CORPORATION
4322 SOUTH 49TH WEST AVENUE
TULSA, OK 74107-

Reason for Submission: Fisher-Tropsch Testing
Product: Aviation Turbine Fuel, Kerosene
Specification: MIL-T-83133 JP-8
Sample Origin:
Quantity Represented:

NSN:
Contract No:
Batch/Lot:
Date Manufact

METHOD	TEST	LIMITS MIN	MAX		
SPEC\W	Workmanship		PASS		
D3242	Total Acid Number, mg KOH/g		0.0		
D1319	Aromatics, % vol		25.		
D3227	Mercaptan Sulfur, % mass		0.00		
D4294-03	Total Sulfur, % mass		0.3		
D86	Distillation				
	IBP, °C		REP		
	10% Recovered, °C		205		
	20% Recovered, °C		REP		
	50% Recovered, °C		REP		
	90% Recovered, °C		REP		
	EP, °C		300		
	Residue, % vol		1.5		
	Loss, % vol		1.5		
D93	Flash Point, °C	38		48	
D5972	Freezing Point, °C		-47	-50	
D445	Viscosity @ -20°C, cSt		8.0	4.9	

BETA

ISO-17025 Accredited Testing Laboratory

PJLA ISO/IEC 17025:2005 Testing Accreditation # 59423

Miam

info@
www.

Report of Biobased Content Analysis using ASTM-D6866-0

Submitter: University of Dayton Research Institute
Submitter Label: 6152
Laboratory Number: Beta-274341
Material Analyzed: BIOBASED LIQUID
Date Received: February 5, 2010
Date Reported: February 10, 2010

Mean Biobased Result: 97% *

Proportions Biobased vs. Fossil Based
indicated by ^{14}C content

Chemical Kinetics

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

Testing Results

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

Fuel Properties

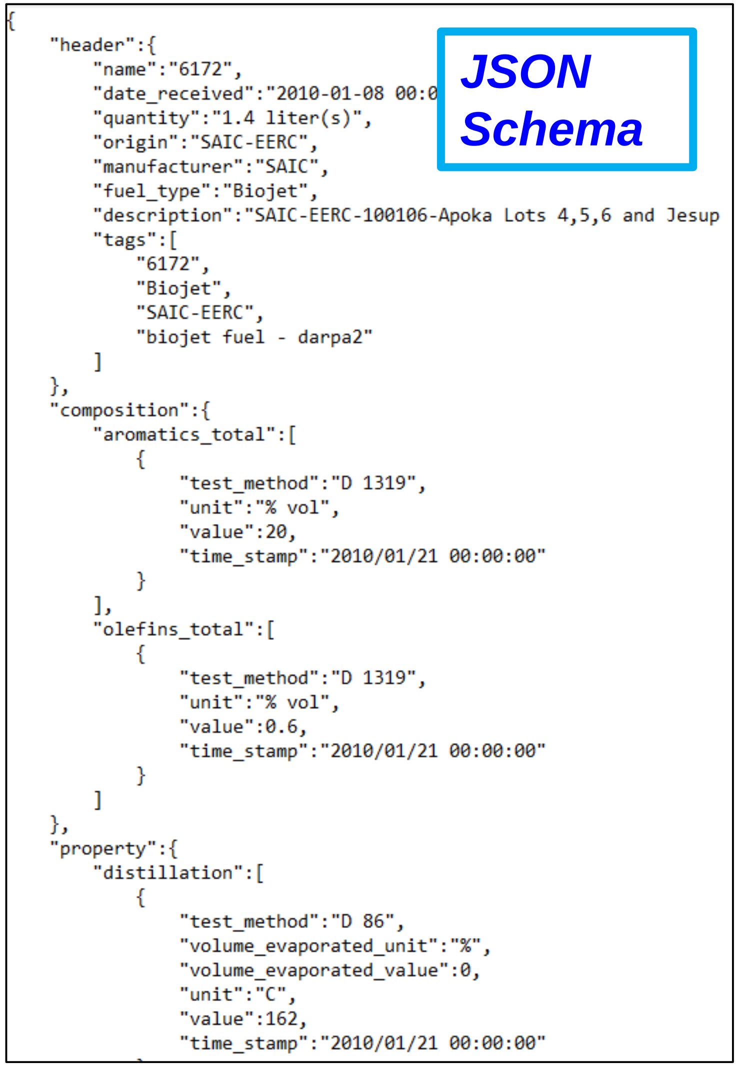
- Thermophysical
- Physicochemical
- GCxGC
- GCxMS
- Specifications

Publications

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

Database Structure

Phase II: Conversion to NoSQL



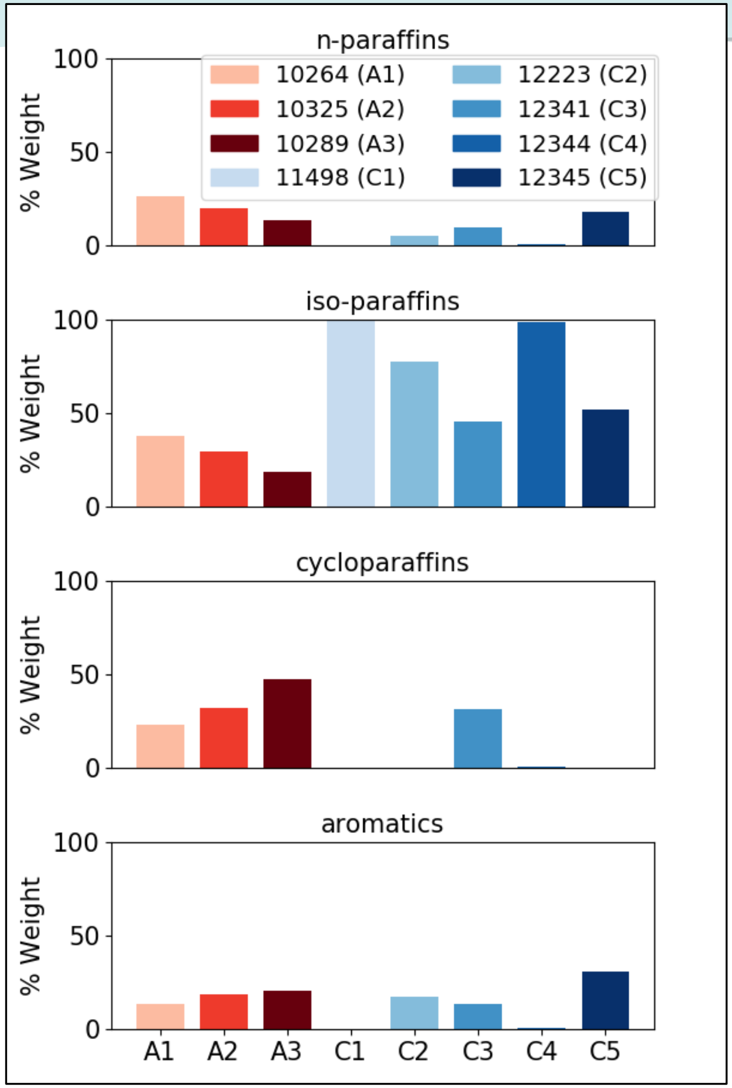
JSON Schema

```
{
    "header":{
        "name":"6172",
        "date_received":"2010-01-08 00:0
        "quantity":"1.4 liter(s)",
        "origin":"SAIC-EERC",
        "manufacturer":"SAIC",
        "fuel_type":"Biojet",
        "description":"SAIC-EERC-100106-Apoka Lots 4,5,6 and Jesup
        "tags":[
            "6172",
            "Biojet",
            "SAIC-EERC",
            "biojet fuel - darpa2"
        ]
    },
    "composition":{
        "aromatics_total":[
            {
                "test_method":"D 1319",
                "unit":"% vol",
                "value":20,
                "time_stamp":"2010/01/21 00:00:00"
            }
        ],
        "olefins_total":[
            {
                "test_method":"D 1319",
                "unit":"% vol",
                "value":0.6,
                "time_stamp":"2010/01/21 00:00:00"
            }
        ]
    },
    "property":{
        "distillation":[
            {
                "test_method":"D 86",
                "volume_evaporated_unit":"%",
                "volume_evaporated_value":0,
                "unit":"C",
                "value":162,
                "time_stamp":"2010/01/21 00:00:00"
```

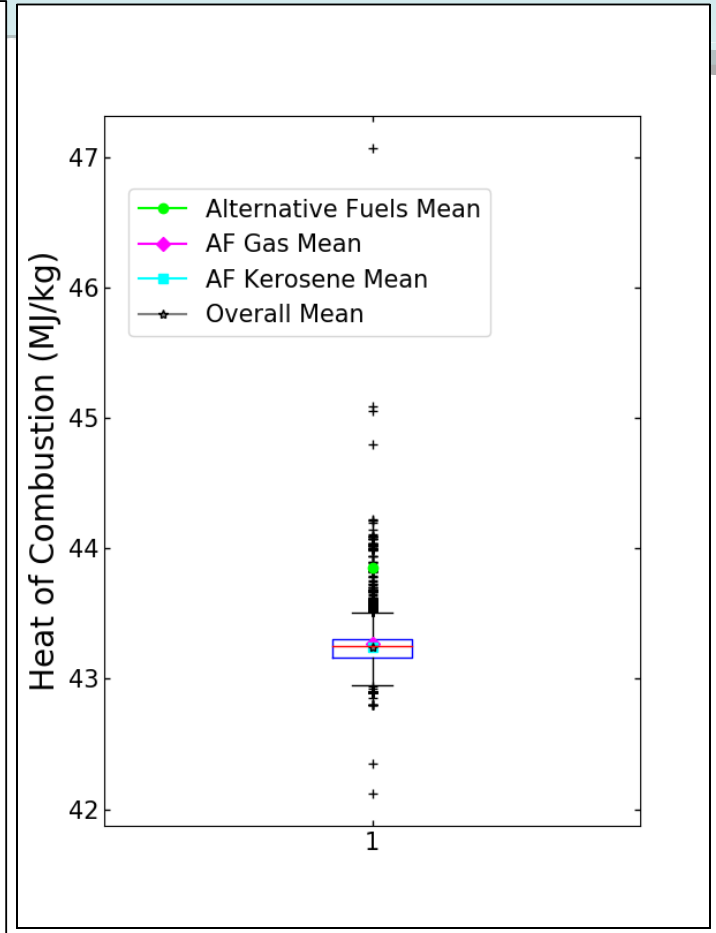
Non-Relational (NoSQL)	*Relational (SQL)*
Highly scalable	**Less scalable**
Flexible schema - data can be inserted/altered anytime without issue	**Structured schema** - data has to fit into predefined tables
Does not support JOIN operations	Supports JOIN operations
Does not use SQL as query language	Mainly uses SQL as query language

- Conversion to flexible schema (*JSON*)
  - Electronically accessible large sets of data
  - Flexible analysis: web interface (Phase II)
- Integration of AJFTD with JETSCREEN (Europe)
  - JETSCREEN uses MongoDB, a NoSQL database
  - AJFTD using ***DynamoDB*** structure

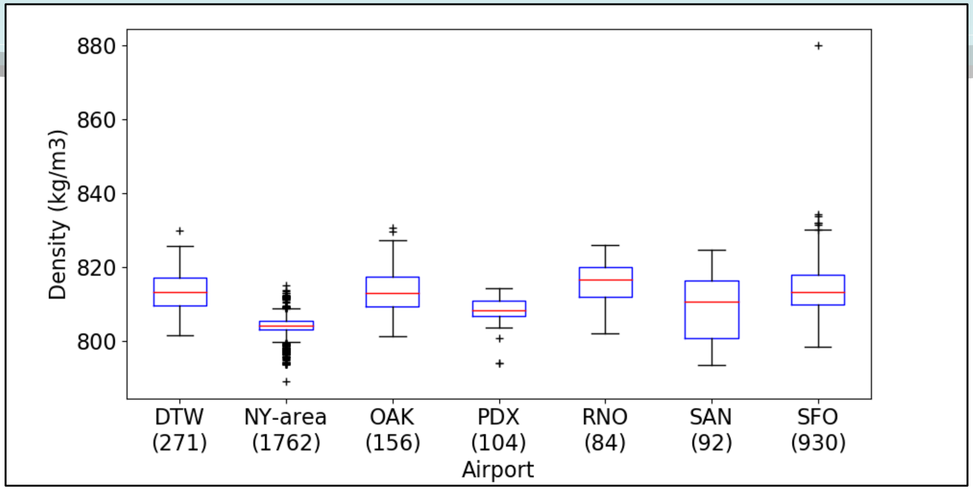
Data Processing

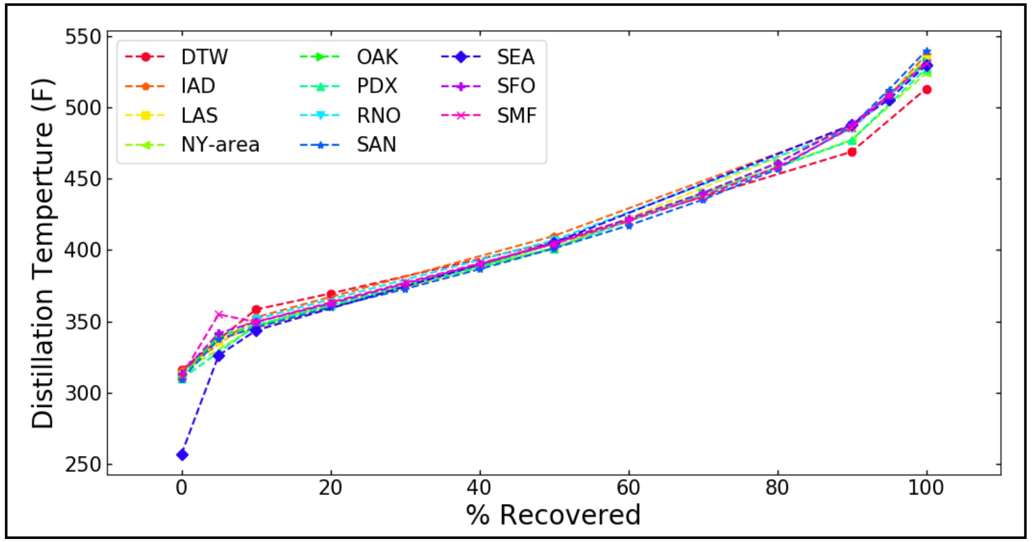


Composition breakdown for NJFCP Cat. A and C fuels



Data: PQIS





Data: Metron Aviation

Thank you

Contact Information

Med Colket	Joshua Heyne	Tonghun Lee
860-748-6612	937-609-0207	217-300-7107
med@colket.org	jheyne1@udayton.edu	Tonghun@Illinois.edu

Back-up

OEM perspective on state-of-the-art: NJFCP then & now

OEMs place high value on insights gained and broadened understanding of fuel effects on combustion – NJFCP insights <u>could help new fuel approvals</u> as well as <u>engine & combustor design efforts</u>:

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

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.

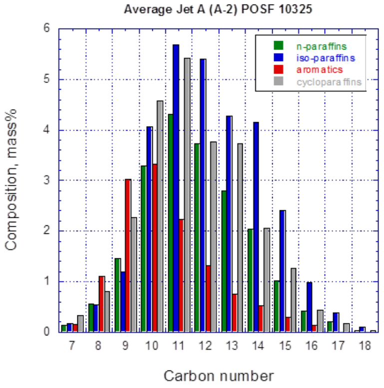
FAA, NASA, and AFRL Funded Activities

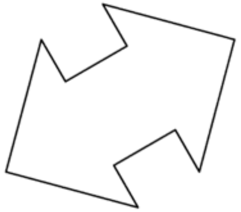
Fuel Candidates and Screening

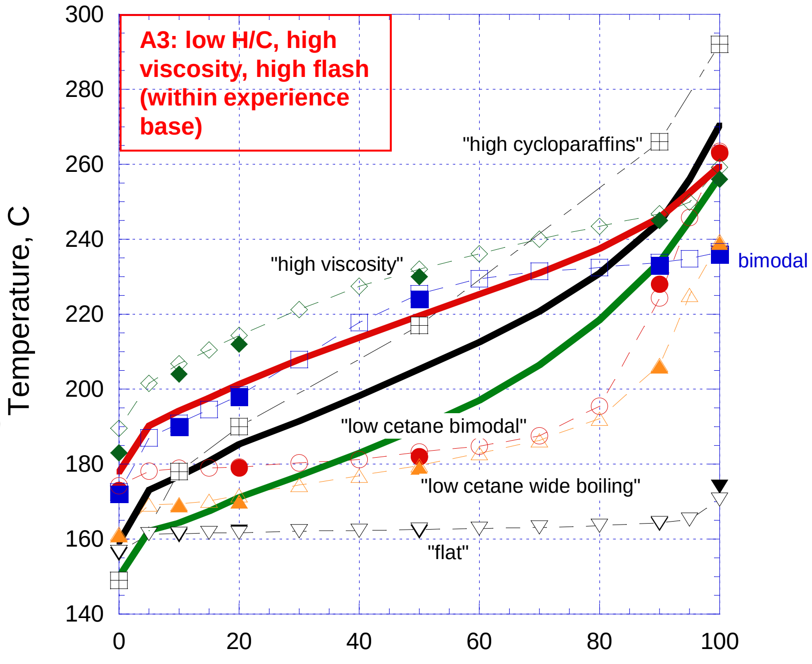
- Reference Fuels Required to Characterize Rig and Engine Fuel Response
- Category A: Three Conventional (Petroleum) Fuels

  --“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 #**

Wide range in boiling pt. and chemical character







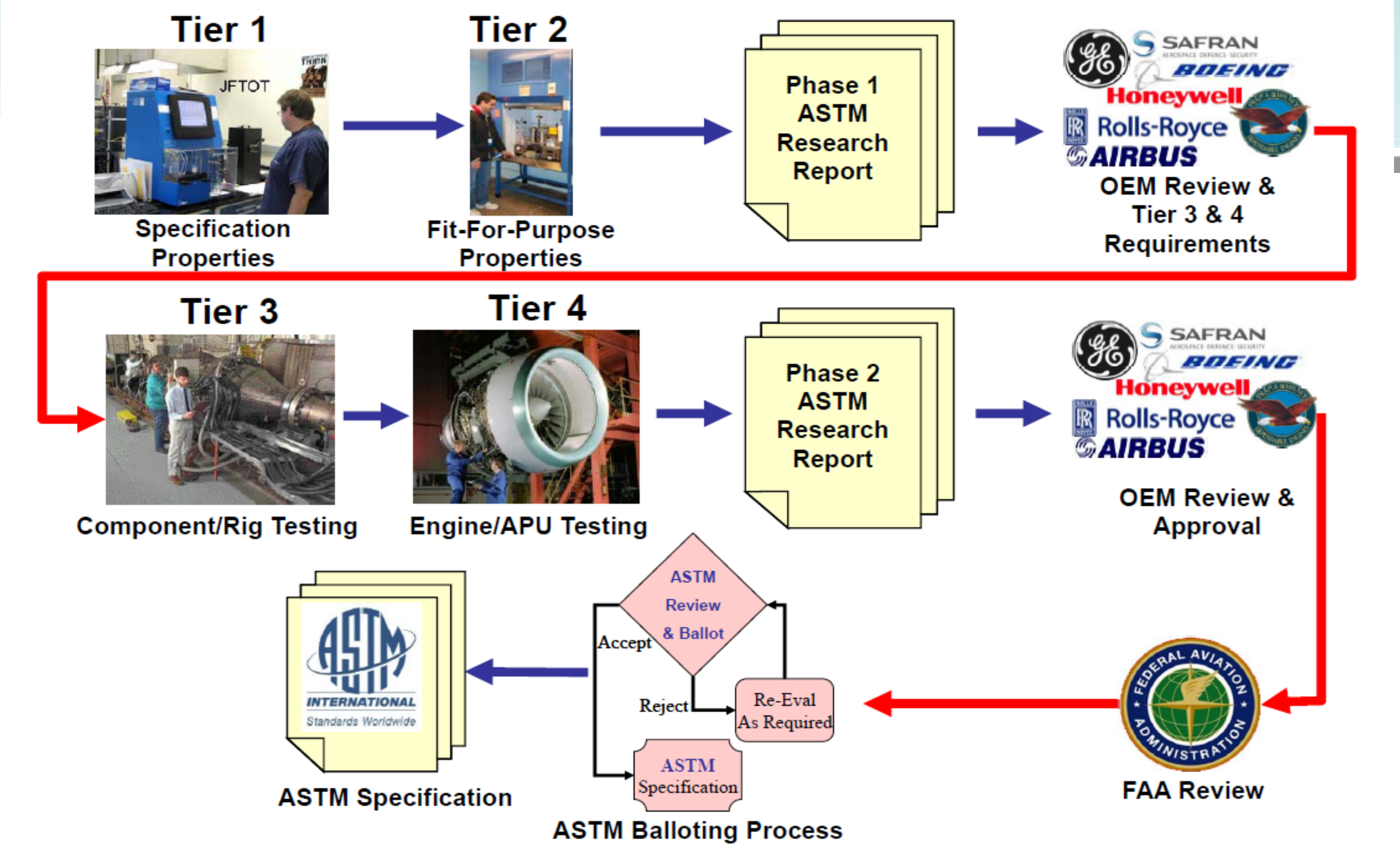
Boiling range plot

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

Current ASTM Fuel Approval Process and Intensive Resource Requirement



Tier 1

Specification Properties

Tier 2

Fit-For-Purpose Properties

Phase 1 ASTM Research Report

OEM Review & Tier 3 & 4 Requirements

Tier 3

Component/Rig Testing

Tier 4

Engine/APU Testing

Phase 2 ASTM Research Report

OEM Review & Approval

FAA Review

ASTM Review & Ballot

Accept

Reject

Re-Eval As Required

ASTM Specification

ASTM Balloting Process

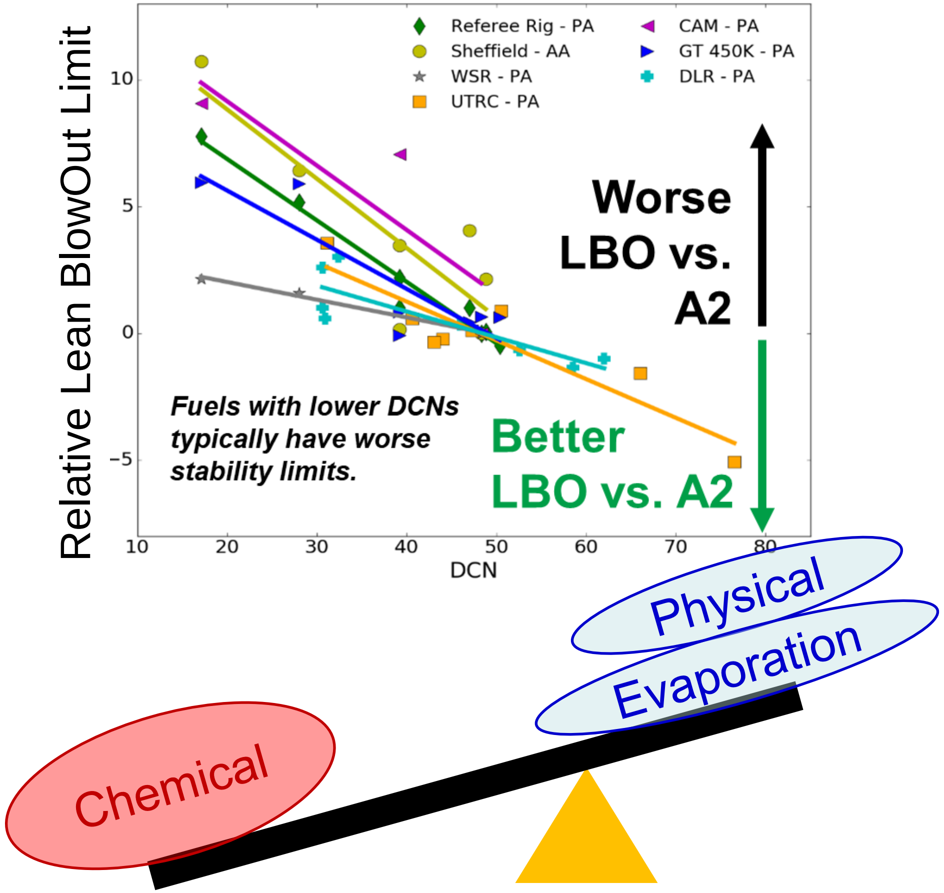
ASTM Specification

- **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)



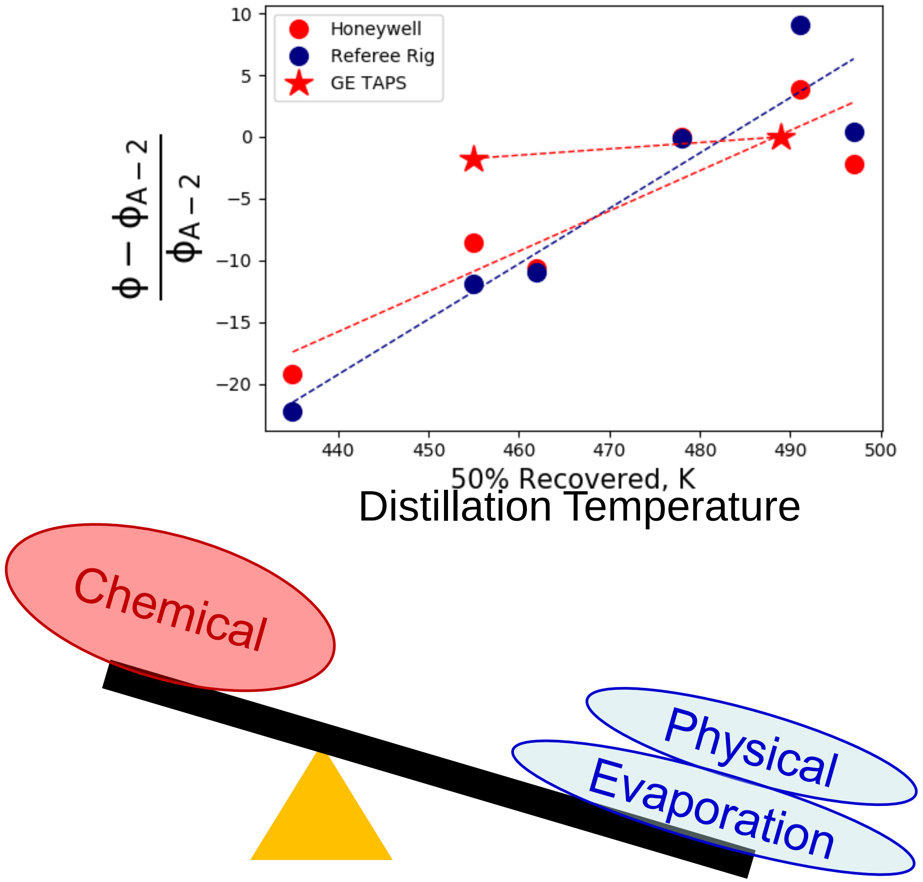
Worse LBO vs. A2

Fuels with lower DCNs typically have worse stability limits.

Better LBO vs. A2

Physically Limited

- Distillation curve dominance (for 3 rigs)



NJFCP: Program Budget and Contributors

	$K				
Agency	**Year-1**	**Year-2**	**Year-3**	**Year-4**	**Year-5**
FAA*	2500	1353	2000	950	843
NASA	-	1103	1315	1,300	560
AFRL**	1971	1650	1000	1,000	500
DLA Energy	750	500	500	500	tbd
NavAir	200	200	400	200	200
ARL				650	tbd
Grand Total	**5421**	**5191**	**5215**	**4600**	

*OEMs are supporting program through cost-share.
**AFRL spends additional funds (that are not included here) to procure/distribute fuels and develop/maintain rig.

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)