Alternative Fuels Test Database Library

Project 33

Project manager: Cecilia Shaw, FAA

Lead investigator: Tonghun Lee, University of Illinois at Urbana-Champaign
Co-Investigator: Steven Zabarnick, University of Dayton Research Institute

September 26-27, 2017
Alexandria, VA

ASCENT
AVIATION SUSTAINABILITY CENTER

Project Overview

A foundational database of current and newly emerging alternative jet fuels

Year 3: 8/15/2016 to 8/14/2017

Lead PI: Tonghun Lee (University of Illinois Urbana-Champaign)

Co-PI: Steven Zabarnick (University of Dayton Research Institute)

Project Manager: Cecilia Shaw (Federal Aviation Administration)

Advisory Committee:

- Tim Edwards (Air Force Research Laboratory)
- Pamela Chu (National Institute of Standards & Technology)
- Robert Morris (Naval Research Laboratory)
- Mike Kweon (Army Research Laboratory)

Goals:

- ***Compile data*** on alternative jet fuels (AJF) in comprehensive and centralized knowledgebase
- ***Support alternative fuels research*** and fuel certification across academia, government, and industry
- ***Increase accessibility*** to AJF testing data and approval reporting

Approach

Identify available data and select sources for use

Year 1

- Collect scattered data (standardized reports, pre-existing database, research/reports from academia and industry)

Prioritize data retrieval and construct web portal

Year 2

- Determine scope and range of data registry/web portal
- Develop interactive and intuitive cataloguing system
- Seed registry/database with initial data

Optimize structure and analyze data

Year 3

- Optimize overall database vision and standardized structure
- Leverage funded efforts: FAA ASCENT, FAA ASCENT NJFCP, …
- Prepare comprehensive analysis of available data

Enhance database features

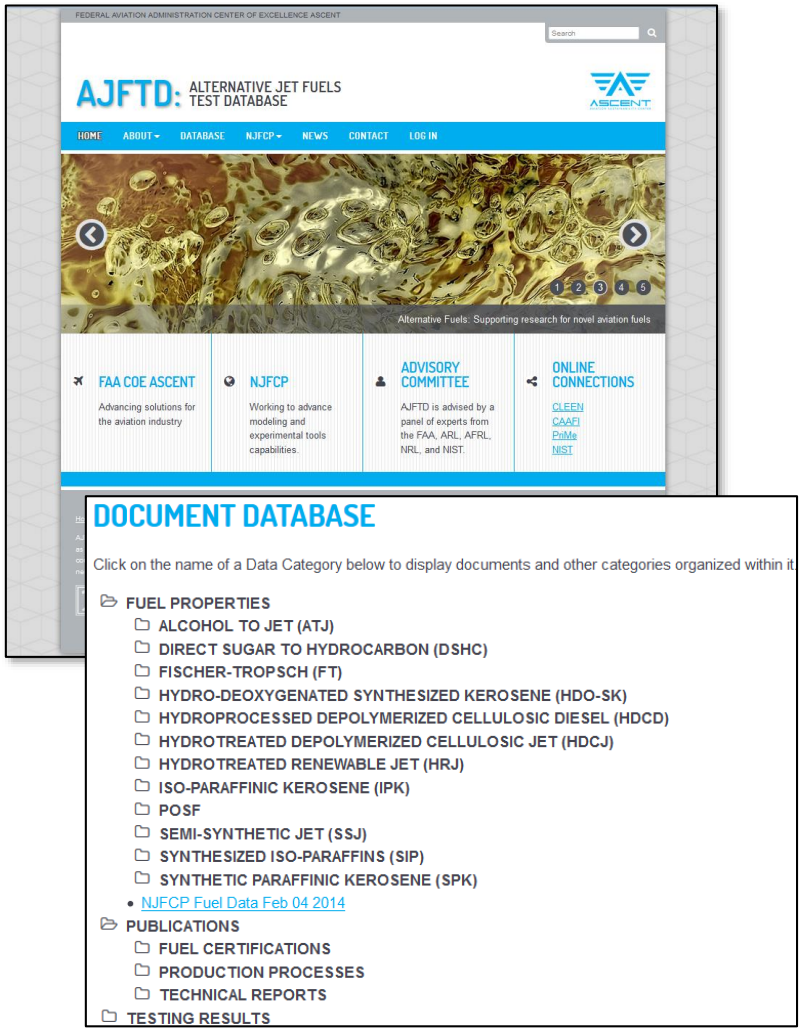
Year 4

- Provide updated AJF data via site fuel summary tool
- Evaluate fuel blending tools to support ASTM Generic Annex work
- Extend data to additional categories: GCxGC, emissions, rig testing, …

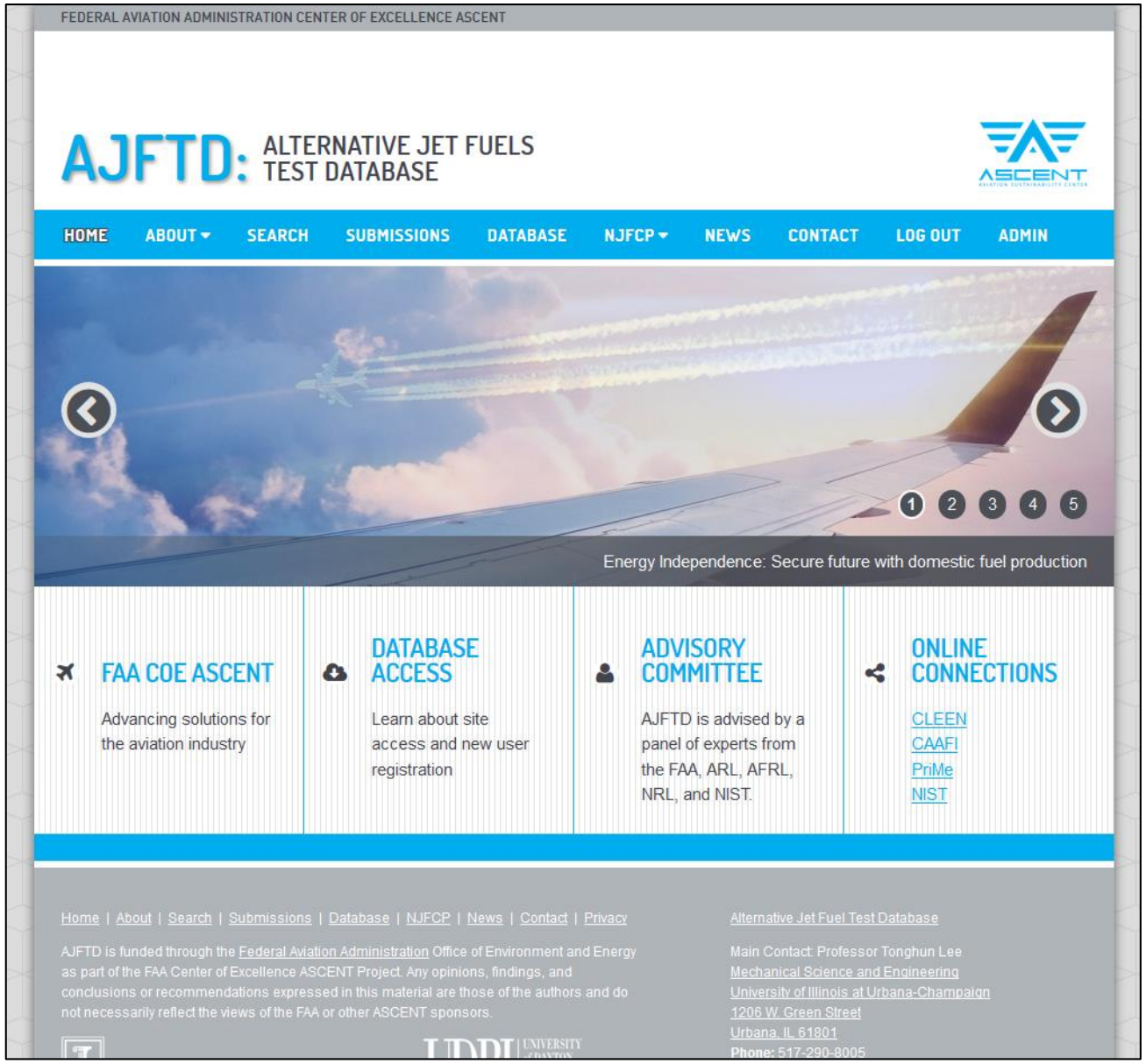
Current AJFTD Database

- Containing information on:
  - Fuel specification analyses
  - Technical papers
  - Fuel approval reports
- 400+ documents
  - Around 300 POSFs covering alt and conventional jet fuels
- Preparing fuel spec and variation analysis paper using AJFTD resources
- Looking to support ASTM Generic Annex through fuel blending tools and test data access
  - Evaluate fuel blend properties

altjetfuels.illinois.edu

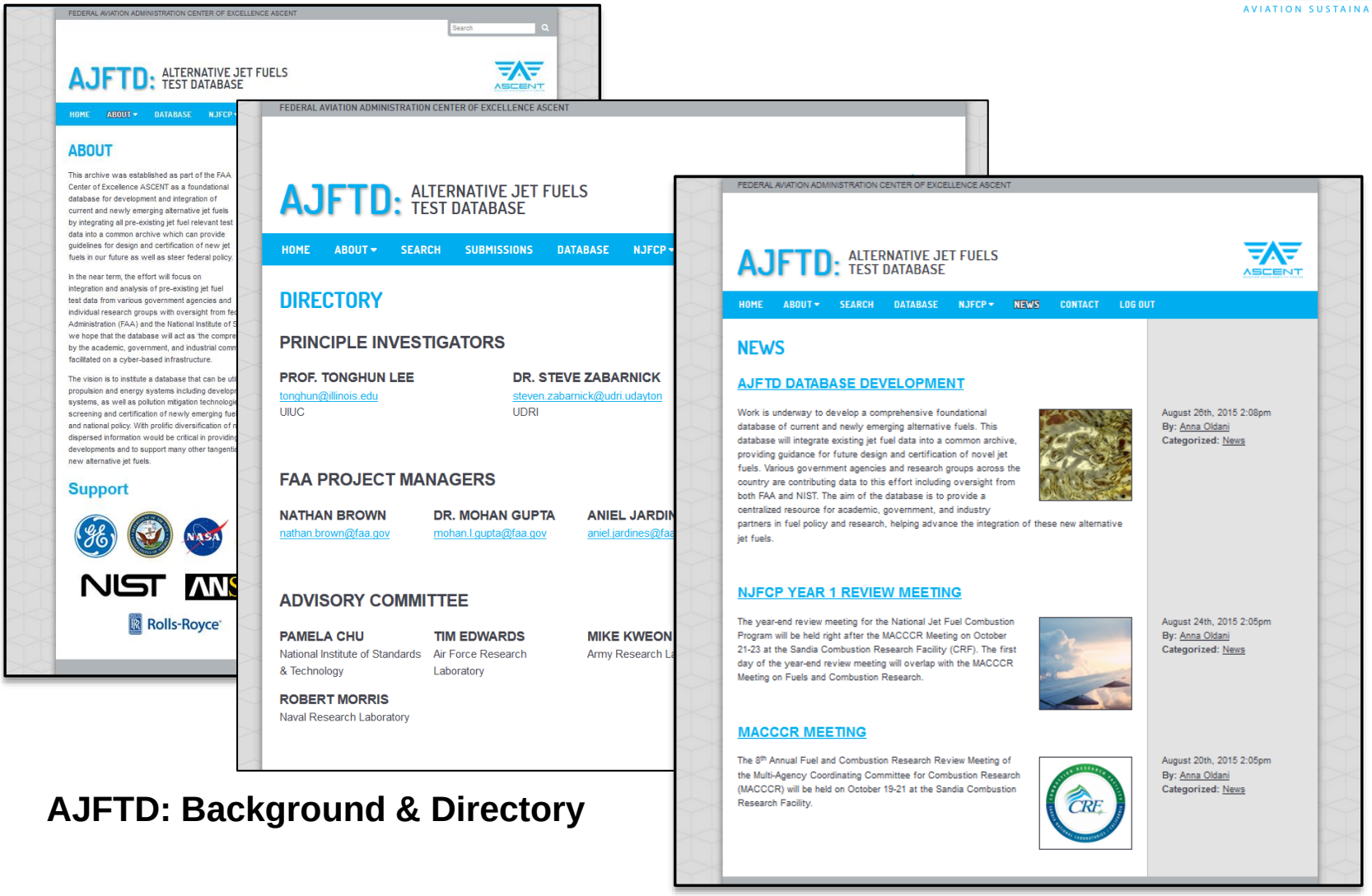


AJFTD Web Portal



- Log-in requires authorization
- **Data submission** available for users
- Improved search result accessibility
- **Comments** can be left on data (community wide screening)

AJFTD Public Access

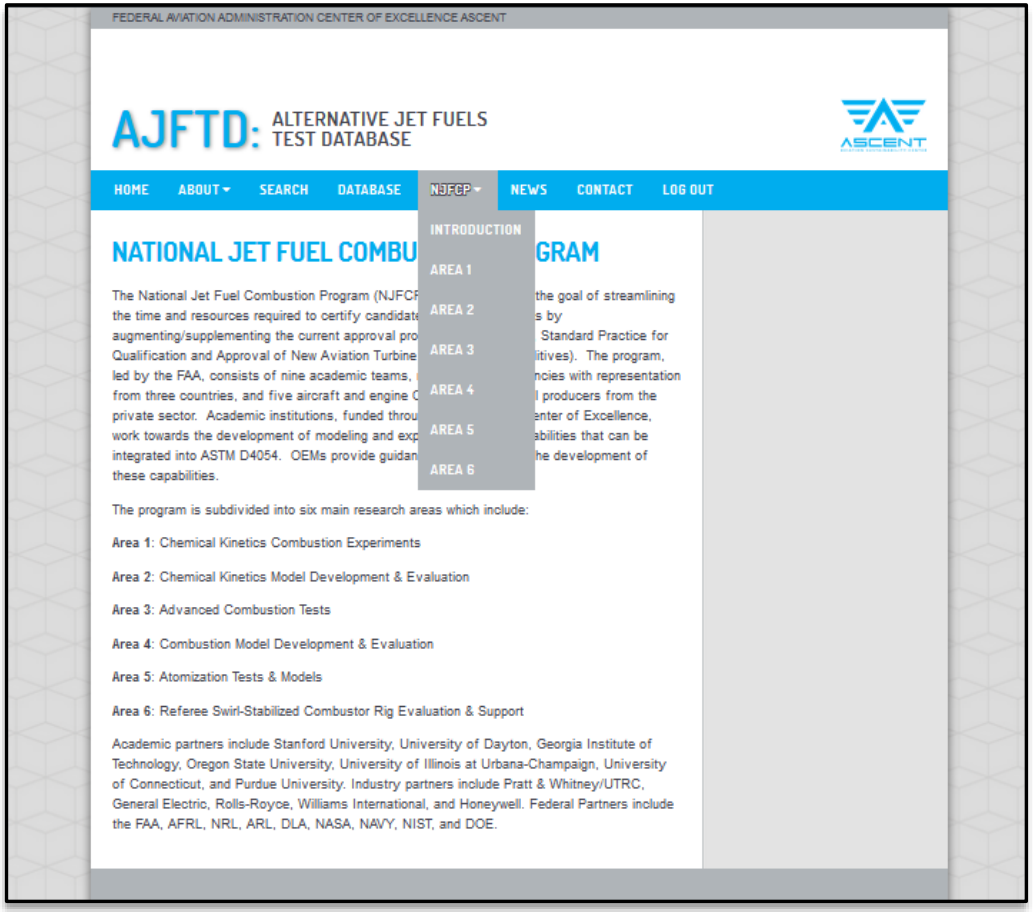


AJFTD: Background & Directory

Relevant News & Updates

AJFTD NJFCP Data Support

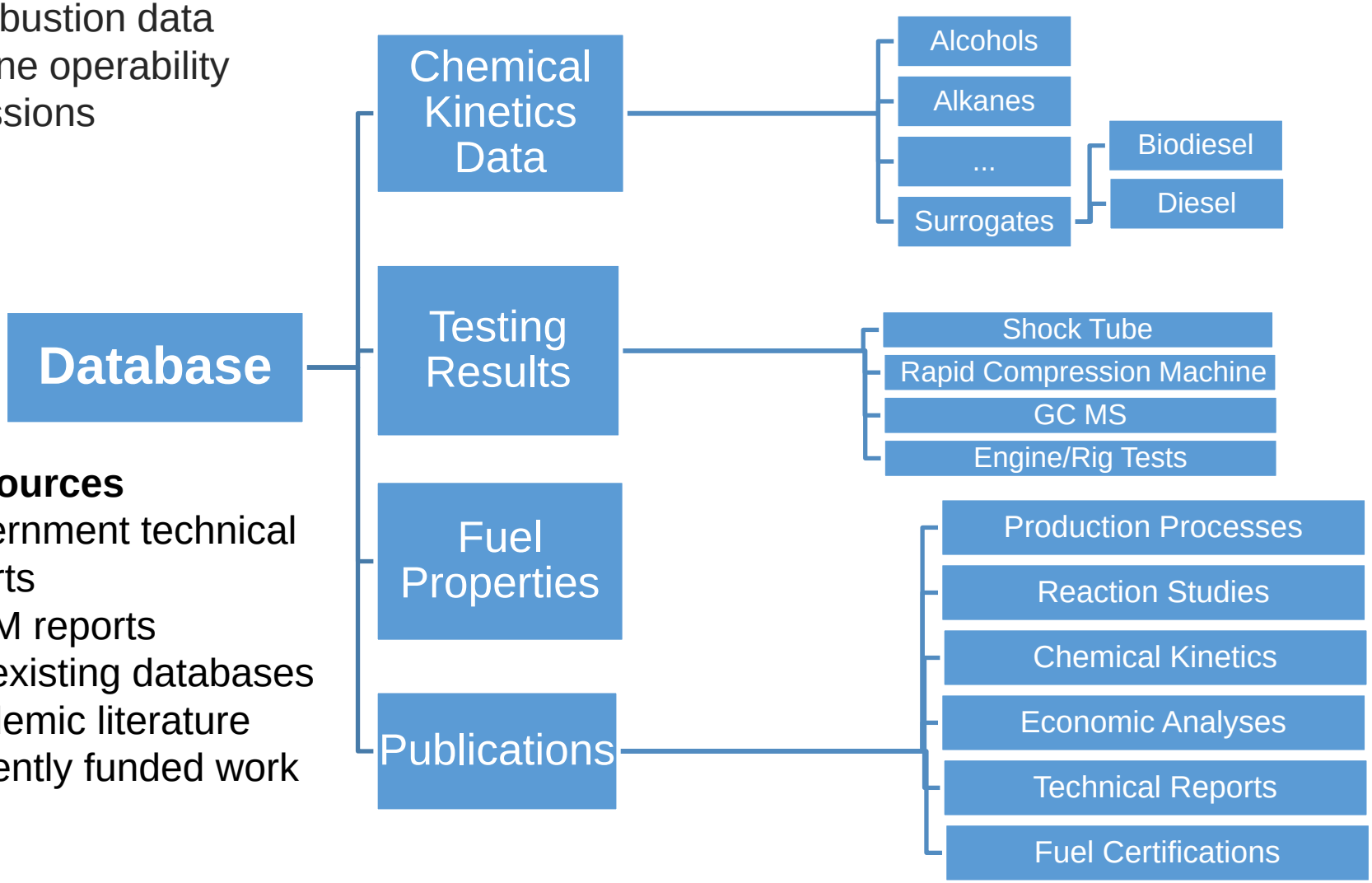
- AJFTD will provide route to make NJFCP data and documentation accessible
- Detailed under **Data Management Plan** (DMP) in compliance with Public Access Plan requirements
- To include:
  - Publications
  - Presentations
  - Data analysis results



Database Dropdown Organization

Focus areas

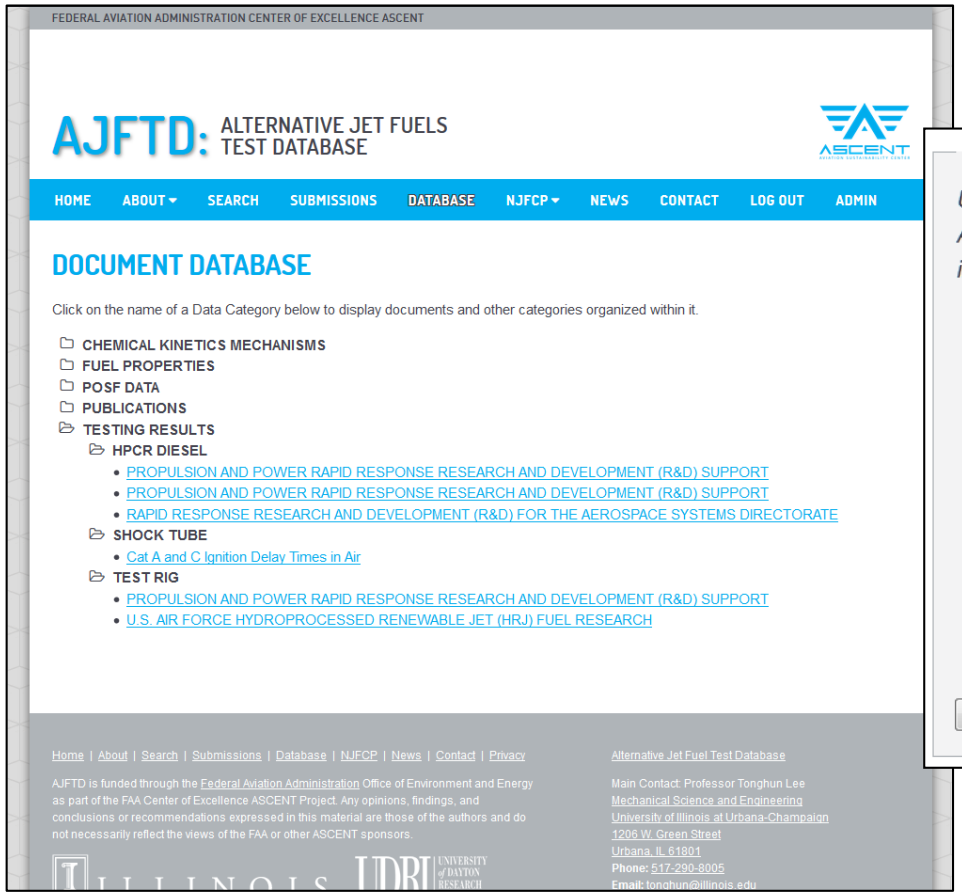
- Fuel component data
- Combustion data
- Engine operability
- Emissions

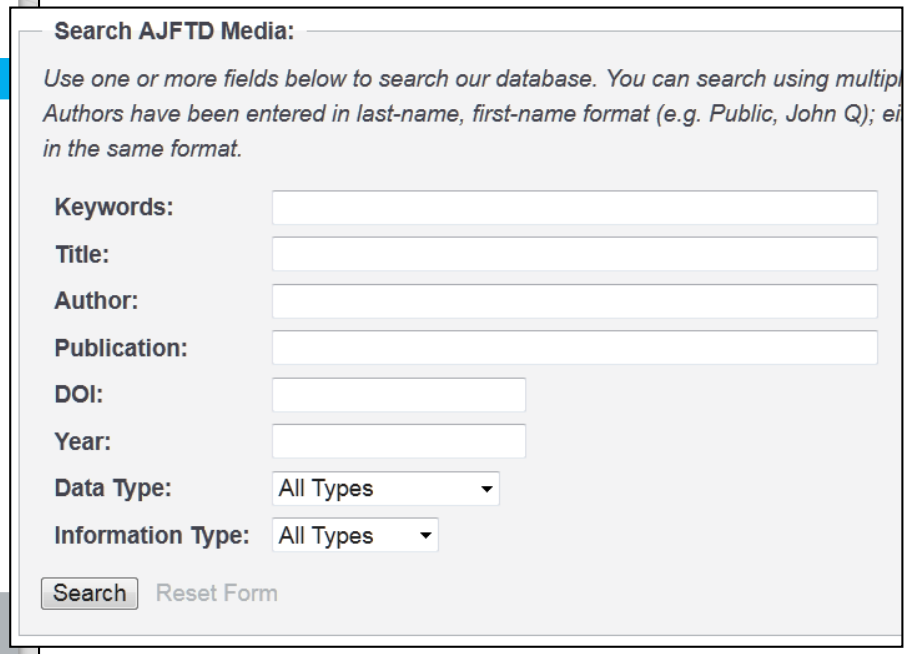


Data Sources

- Government technical reports
- ASTM reports
- Pre-existing databases
- Academic literature
- Currently funded work

Database Search Functionalities





- Familiar file folder breakdown to view all documents in relevant categories
- Database also accessible through basic or advanced search
  - Additional fields in advanced search:
    - Data Type: PDF, excel, .csv
    - Information Type: Publications, Data, Standards, Reports

Current POSF Data

DOCUMENT DATABASE

Click on the name of a Data Category below to display documents and other categories organized within it.

- CHEMICAL KINETICS MECHANISMS
- FUEL PROPERTIES
- POSF DATA
  - 12223
  - 4751
  - 4909
  - 5033
  - 5109
  - 6152
  - 6153

POSF 12223 DATA

- Received: 01/05/2015
- Fuel Type: C14:1,3,5-Trimethyl-benzene (9405:10447) Blend
- Quantity: 475 gallon(s)
- Origin:
- Description: 84/16 Blend of POSF 9405 (C14) & POSF 10447 (1,3,5-Trimethyl-benzene)

Download Data:

POSF 12223 Fuel Properties 01/07/15

POSF 12223 Fuel Properties 01/27/15

POSF 12223 Net Heat of Combustion and Hydrogen Content

AFPET LABORATORY REPORT
AFPA/PTPLA
2430 C Street
Building 70, Area B
Wright-Patterson AFB, OH 45433-7632

Lab Report No:2015LA52622001 Date Received:01/27/15 0903 hrs* Date Sampled: **
Cust Sample No:12223 Date Reported:02/13/15 1436 hrs* Protocol:FU-AVI-0019
JON: GENERAL FUND

Sample Submitter:
AFRL/RQTF
1790 Loop Road N
Bldg 490
Wright-Patterson AFB, OH 45433

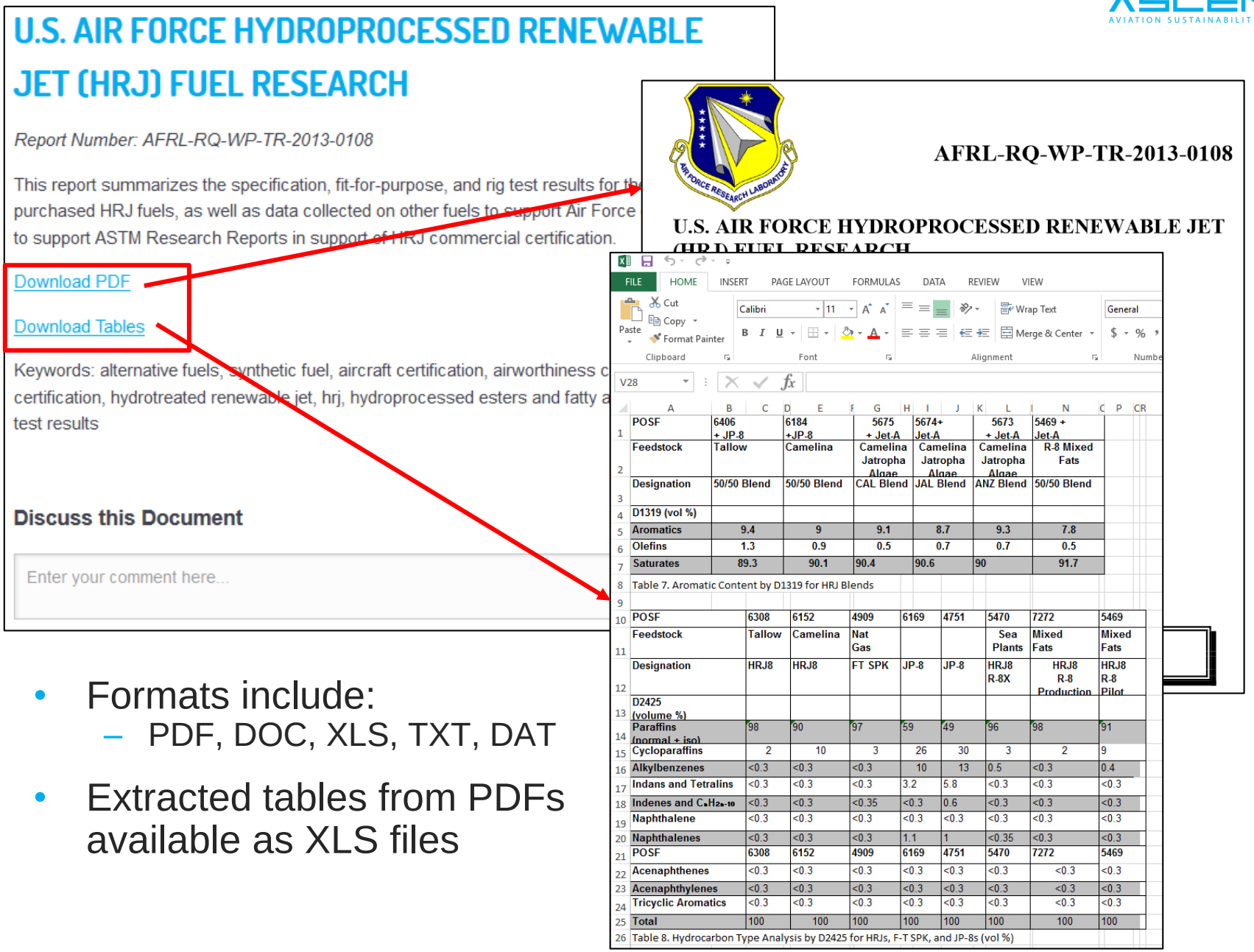
Reason for Submission: AFRL Research
Product: Aviation Turbine Fuel, Kerosene
Specification: MIL-DTL-83133H w/Amd 2 Grade:JP-8

Qty Submitted: 1 gal

Method	Test	Min	Max	Result	Fail
MIL-DTL-83133H w/Amd 2	Workmanship			Pass	
ASTM D 3242 - 11	Total Acid Number (mg KOH/g)		0.015	0.002	
ASTM D 1319 - 14	Aromatics (% vol)		25.0	17.6	
ASTM D 3227 - 13	Mercaptan Sulfur (% mass)		0.002	0.000	
ASTM D 86 - 12	Distillation				
	Initial Boiling Point (°C)			172	
	10% Recovered (°C)		205	190	
	20% Recovered (°C)			198	
	50% Recovered (°C)			224	
	90% Recovered (°C)			233	
	End Point (°C)		300	236	
	Residue (% vol)		1.5	1.1	
	Loss (% vol)		1.5	0.8	
ASTM D 93 - 13e1	Flash Point (°C)	38		58	
ASTM D 4052 - 11	Density @ 15°C (kg/L)	0.775	0.840	0.782	
ASTM D 5972 - 05e1	Freezing Point (°C)		-47	-45	X
ASTM D 976 - 06 (2011)	Cetane Index, Calculated	Report Only		61	
ASTM D 1322 - 14	Smoke Point (mm)	25.0		30.0	
ASTM D 130 - 12	Copper Strip Corrosion (2 h @ 100°C)		1 (Max)	1a	

- Fuel Types:
  - Conventional (JP-8)
  - Biojet, HEFA
  - Blends
  - IPK, SPK, F-T

Data Downloads Available



U.S. AIR FORCE HYDROPROCESSED RENEWABLE JET (HRJ) FUEL RESEARCH

Report Number: AFRL-RQ-WP-TR-2013-0108

This report summarizes the specification, fit-for-purpose, and rig test results for th purchased HRJ fuels, as well as data collected on other fuels to support Air Force to support ASTM Research Reports in support of HRJ commercial certification.

Download PDF

Download Tables

Keywords: alternative fuels, synthetic fuel, aircraft certification, airworthiness c certification, hydrotreated renewable jet, hrj, hydroprocessed esters and fatty a test results

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AFRL-RQ-WP-TR-2013-0108

U.S. AIR FORCE HYDROPROCESSED RENEWABLE JET (HRJ) FUEL RESEARCH

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	CR
1	POSF	6406 + JP-8		6184 +JP-8			5675 + Jet-A		5674+ Jet-A			5673 + Jet-A		5469 + Jet-A			
2	Feedstock	Tallow		Camelina			Camelina Jatropha Algae		Camelina Jatropha Algae			Camelina Jatropha Algae		R-8 Mixed Fats			
3	Designation	50/50 Blend		50/50 Blend			CAL Blend		JAL Blend			ANZ Blend		50/50 Blend			
4	D1319 (vol %)																
5	Aromatics	9.4		9			9.1		8.7			9.3		7.8			
6	Olefins	1.3		0.9			0.5		0.7			0.7		0.5			
7	Saturates	89.3		90.1			90.4		90.6			90		91.7			
8	Table 7. Aromatic Content by D1319 for HRJ Blends																
9																	
10	POSF	6308		6152			4909		6169			4751		5470		7272	5469
11	Feedstock	Tallow		Camelina			Nat Gas							Sea Plants		Mixed Fats	Mixed Fats
12	Designation	HRJ8		HRJ8			FT SPK		JP-8			JP-8		HRJ8 R-8X		HRJ8 R-8 Production	HRJ8 R-8 Pilot
13	D2425 (volume %)																
14	Paraffins (normal + iso)	98		90			97		59			49		96		98	91
15	Cycloparaffins	2		10			3		26			30		3		2	9
16	Alkylbenzenes	<0.3		<0.3			<0.3		10			13		0.5		<0.3	0.4
17	Indans and Tetralins	<0.3		<0.3			<0.3		3.2			5.8		<0.3		<0.3	<0.3
18	Indenes and C_nH_{2n-10}	<0.3		<0.3			<0.35		<0.3			0.6		<0.3		<0.3	<0.3
19	Naphthalene	<0.3		<0.3			<0.3		<0.3			<0.3		<0.3		<0.3	<0.3
20	Naphthalenes	<0.3		<0.3			<0.3		1.1			1		<0.35		<0.3	<0.3
21	POSF	6308		6152			4909		6169			4751		5470		7272	5469
22	Acenaphthenes	<0.3		<0.3			<0.3		<0.3			<0.3		<0.3		<0.3	<0.3
23	Acenaphthylenes	<0.3		<0.3			<0.3		<0.3			<0.3		<0.3		<0.3	<0.3
24	Tricyclic Aromatics	<0.3		<0.3			<0.3		<0.3			<0.3		<0.3		<0.3	<0.3
25	Total	100		100			100		100			100		100		100	100
26	Table 8. Hydrocarbon Type Analysis by D2425 for HRJs, F-T SPK, and JP-8s (vol %)																

- Formats include:
  - PDF, DOC, XLS, TXT, DAT
- Extracted tables from PDFs available as XLS files

Near Term AJFTD Extended Analysis

- Specification review paper
  - Provide statistical analysis of variance of AJF data provided in D4054 FFP report
  - Develop property-temperature relationships for various fuel types
    - Generate specification property values ranges
  - Extend CRC WFS 2006 report with additional AJFTD data
    - Compare conventional fuels against AJFs for various specification requirements
- Support ASTM Generic Annex work for AJF blending
  - Desire to introduce AJFs at lower blending limits to streamline approval pipeline
  - Evaluate fuel blending prediction tools to check blend properties
    - NRL FCAST chemometric software

Sample Data from D4054 FFP Report

(C. Moses, 2015)

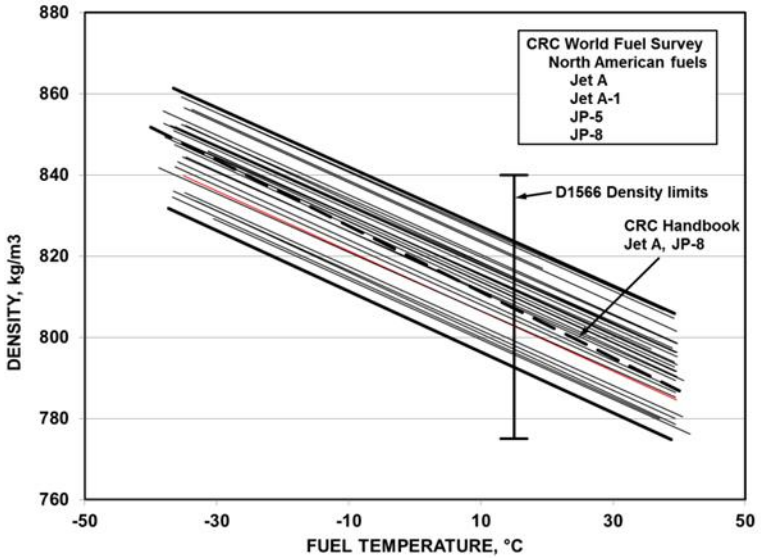


Figure 1-a. CRC World Fuel Survey

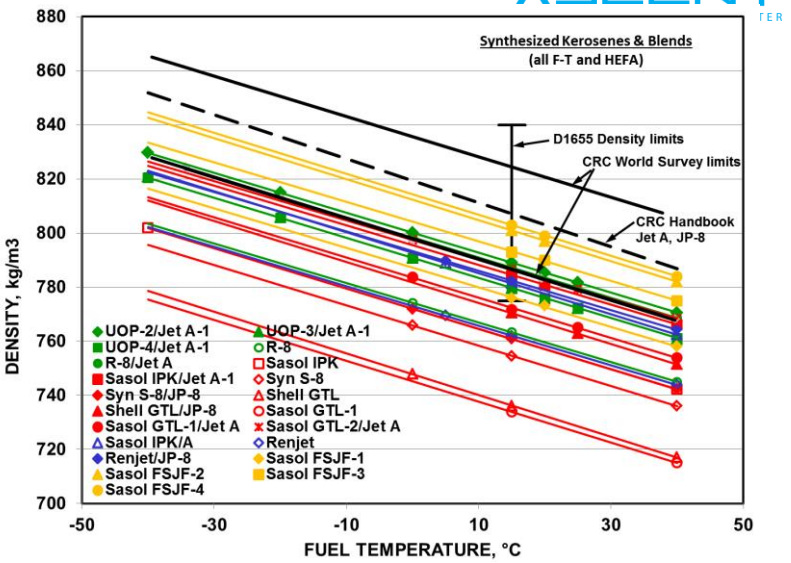


Figure 1-b. F-T and HEFA Fuels and Blends

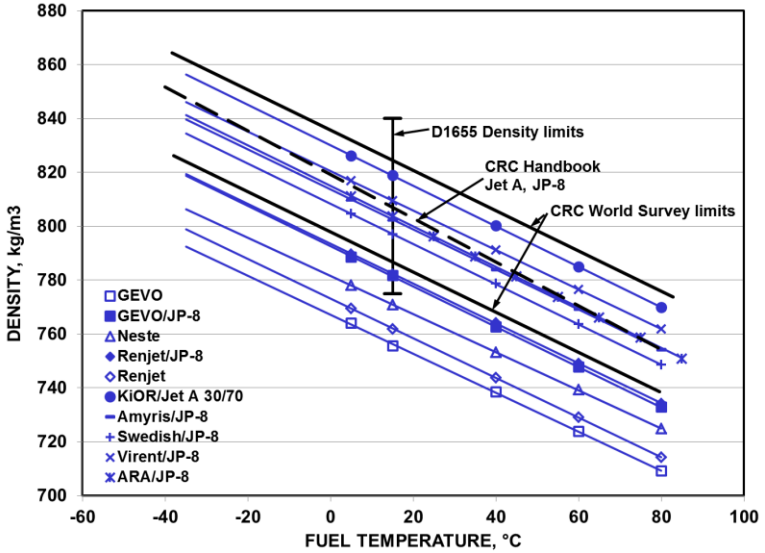


Figure 1-c. 2nd Generation Renewable Fuels and Blends

- Conclude HCs have similar temperature dependence for evaluated properties independent of processing method

Property Data Analysis

- Significant slope variance in all evaluated property categories except surface tension
  - Properties are still within allowable specification range
    - e.g. SKA density @ 15°C
      - 95% CI: 769.6 – 801.6 kg/m^3
      - Spec requirements 755 – 800 kg/m^3
- Equations can provide expected range of values for specification properties

Fuel Property	Fuel Types with Significant Variance
Density	SKA
Isentropic Bulk Modulus	HEFA, FT
Specific Heat	FT, FSJF
Speed of Sound	HEFA
Viscosity	SKA, HEFA

*No thermal conductivity data for WFS fuels

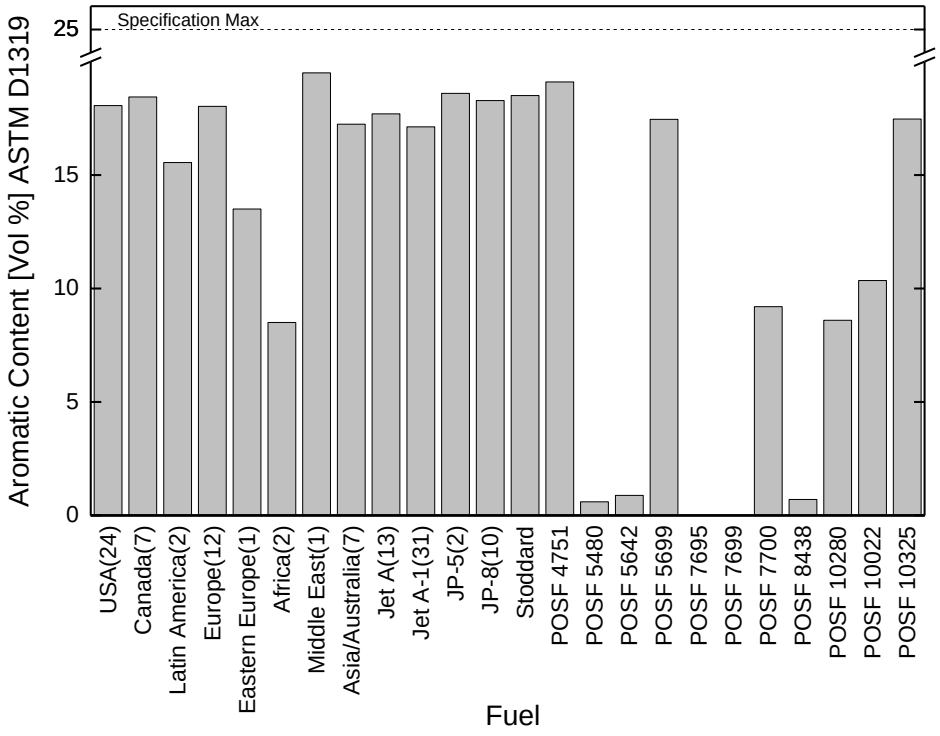
Density	Equation
WFS	y=-0.7216x +815.5
WFS w. light+heavy	y=-0.7225x +815.5
FT	y=-0.7376x +777.7
SKA	y=-0.7439x +796.8
Renewable	y=-0.7419x +796.9
HCs 1	y=-0.8881x +826.9
HCs 2	y=-0.8651x +825.5
CRC	y=-0.7723x +817.7

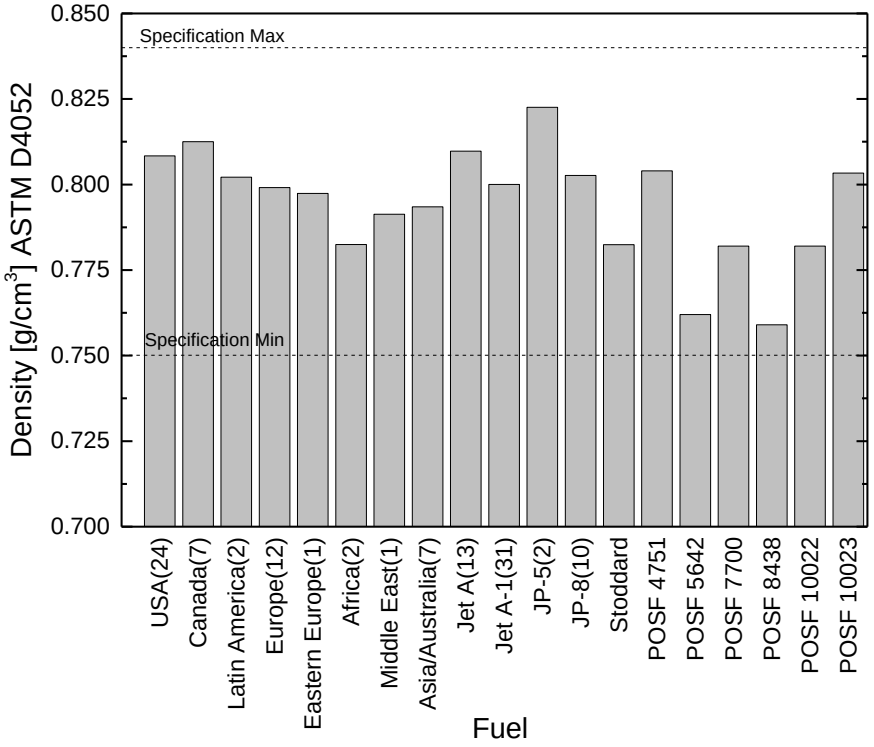
Surface Tension	Equation
WFS	y=-0.0751x +27.4
FT & HEFA	y=-0.0741x +25.9
SPK	y=-0.0800x +25.9
Renewables	y=-0.0771x +26.7
CRC	y=-0.0443x +16.0

Viscosity	Equation
FT	y=2.999*0.9758x
SKA	y=3.091*0.9815x
HEFA	y=2.894*0.9777x
WFS	y=2.849*0.9750x
2nd Gen	y=3.262*0.9708x
HCs	y=1.850*0.9890x

WFS and AJF Property Evaluation

- Utilized AJFTD data to extend results from CRC WFS 2006 report
  - Obtained data for additional AJF POSFs used in ASTM approval reports to compare conventional and AJF specification properties





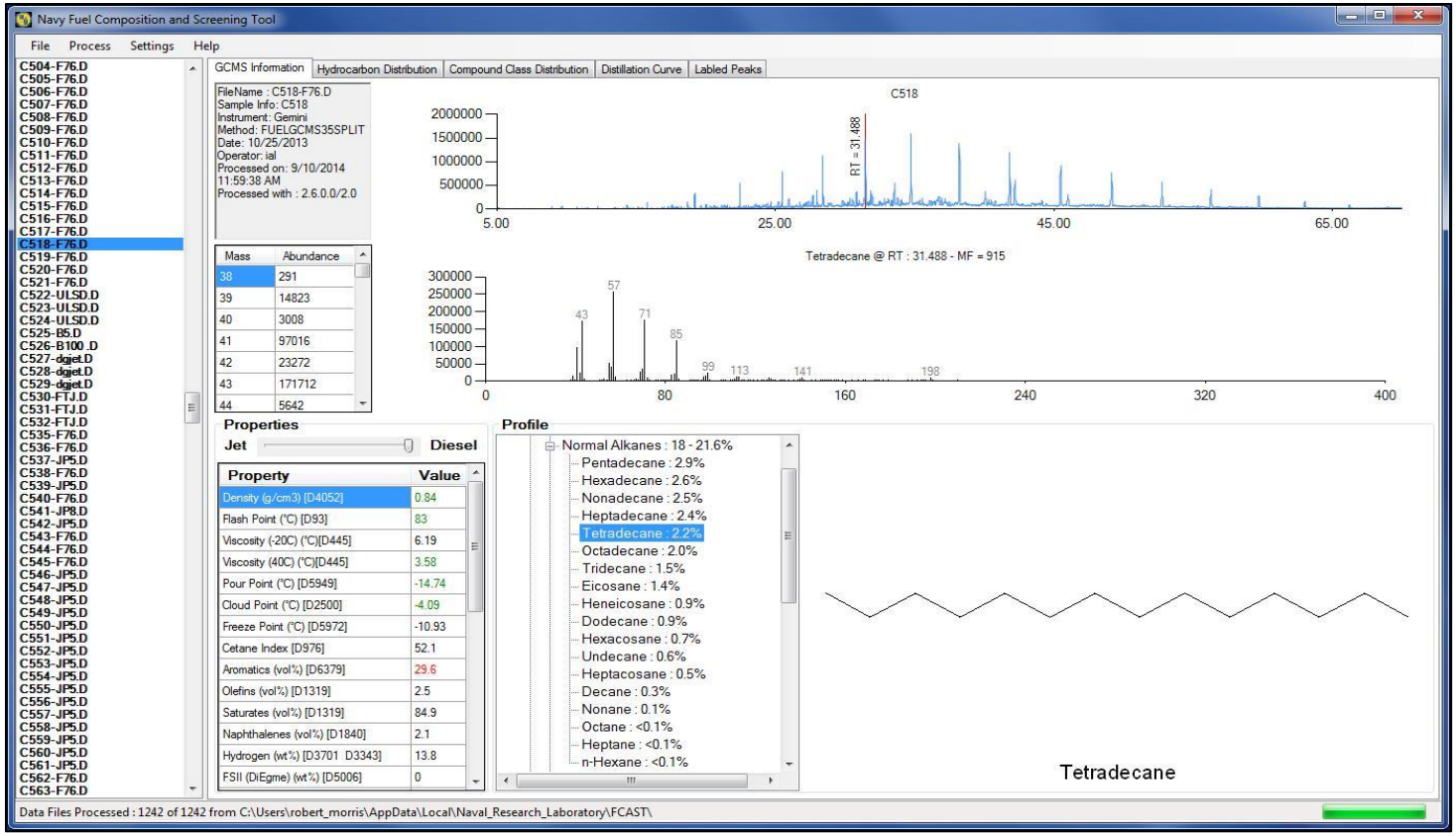
ASTM Generic Annex Proposal

- Streamline certification process independent of resource processing based on composition and final blend
  - No prototype testing
  - Sets conservative limits – AJF blend ratio (~10%)
- Provide confidence that blends are controlled on composition as compared to other annexes
  - Allows producers get closer to production much earlier and secure funding by reducing risks
  - Gives OEMs confidence new blends won't impact durability performance or safety
  - Saves time and resources for evaluating new fuels

Fuel Property Blending Tools

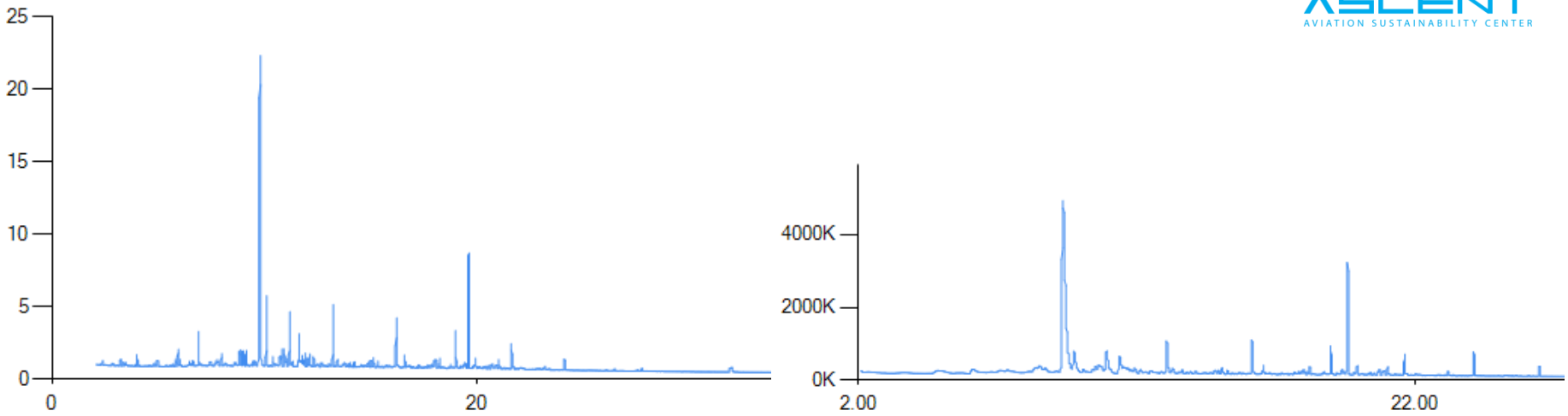
- NRL *FCAST*: Navy Fuel Composition and Screening Tool
  - Developed to pre-screen new fuels
    - Utilizes PLS Regression analysis to establish statistical relationship between composition and critical FFP fuel properties
    - Predict analyzed fuel properties from GCxMS data
    - Individual compound abundance estimates
    - Carbon distribution of total fuel with class breakdown
  - Provides route to predict fuel properties of possible fuel blends
    - Developed to preserve robustness in presence of new, uncalibrated data – important for alternative fuels
    - Future adaptation to employ other data inputs (e.g. GCxGC data)

NRL FCAST



- NRL FCAST (Fuel Composition & Screening Tool)
  - Provides GCxMS interpretation and modeling tools:
    - TICs
    - Hydrocarbon compositional profiles
    - Chemical structures of compounds present
    - Relevant ASTM fuel specification property predictions

FCAST Blend Prediction Capabilities



50:50 A1 (10264) :C1 (11498) blend
calculated TIC (L), actual TIC (R)

- Calculated blend done by proportional blending of TIC profiles
- Generally <5% difference between calculated blend and actual blend predicted spec properties
  - FCAST provides ASTM relevant spec property predictions
- Can be used to support goals of ASTM Generic Annex for fuel blends

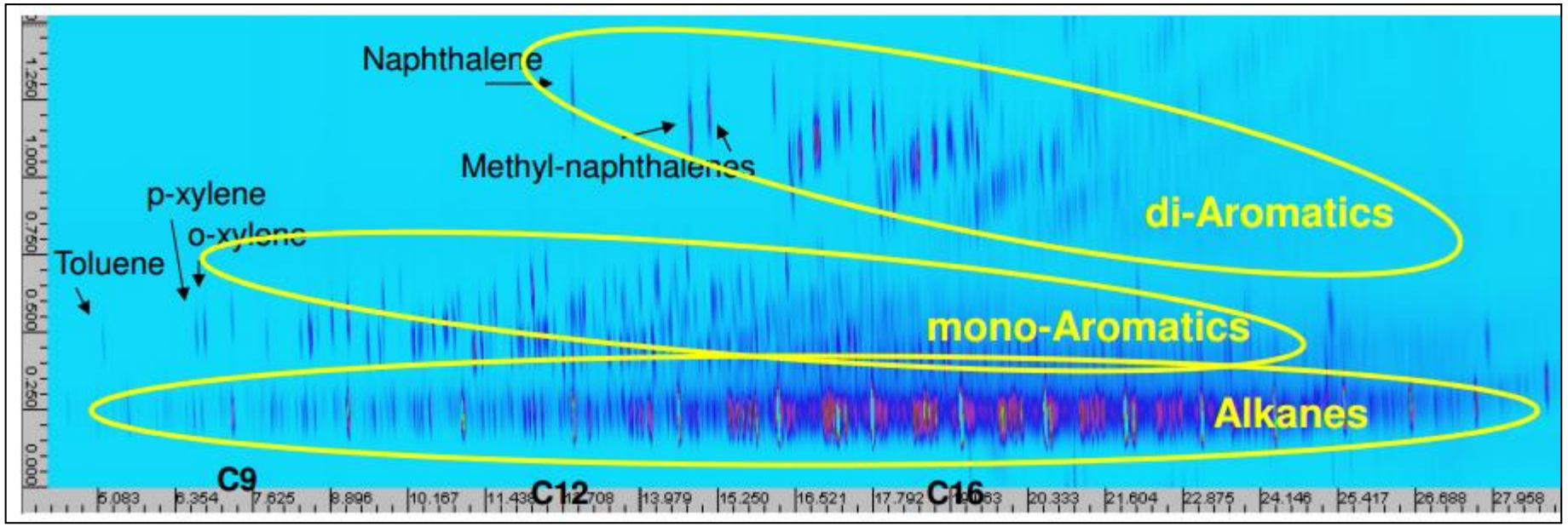
% Difference	90:10	70:30	50:50	30:70	10:90
Density (g/cm3) [D4052]	1.19%	0.48%	0.00%	0.36%	0.12%
Flash Point (°C) [D93]	4.90%	2.01%	8.79%	3.31%	2.50%
Viscosity (-20°C) [D445]	4.83%	4.09%	3.01%	3.74%	2.37%
Viscosity (40°C)[D445]	7.26%	5.06%	13.21%	8.56%	1.16%
Pour Point (°C) [D5949]	0.79%	0.30%	5.16%	2.29%	0.71%
Cloud Point (°C) [D2500]	7.56%	2.48%	3.93%	2.71%	4.72%
Freeze Point (°C) [D5972]	0.72%	0.57%	3.76%	1.67%	1.92%
Cetane Index [D976]	1.75%	0.22%	0.86%	0.22%	0.00%
Aromatics (vol%) [D6379]	5.80%	3.38%	6.22%	1.95%	0.47%

GCxGC Fuel Analysis – Year 4

- Two-dimensional gas chromatography
  - Pair of GC columns connected in series through a modulator
  - Provide more detailed fuel analysis than conventional GCxMS
- GCxGC data for AJFs supplied in ASTM approval reports for new fuels
- Efforts to formalize specification procedure to standardize methods across labs
  - Groups modify technique according to fuels tested and analytes of interest
- Generally used for HC type classification but can also be used for polar analyses and other impurities

GCxGC Fuel Analysis – Year 4

- Analysis results can be reported:
  - Molecular types indexed to n-alkanes
  - Molecular type homologous series by carbon number
  - User specified resolved compounds or molecular type groups
- Image represents:
  - X-axis: retention time from primary column
  - Y-axis: retention time from secondary column
  - Coloring: FID signal intensity



GCxGC data for 7890A diesel fuel showing boiling point distribution and hydrocarbon class clusters

Future Work

- Inclusion of new data areas
  - Emissions
  - GCxGC – evaluate existing data from AFRL and other groups
  - Rig testing
  - Etc…
- Database enhancement
  - *Fuel type summary tool* – generate updated testing results for various fuel categories
    - Increases user accessibility to view most recent AJF fuel property data
- ASTM Generic Annex support
  - FCAST and other tools for blend property predictions to support blending limits