EAR 99 - Non-Proprietary

### **National Jet Fuels Combustion Program**



### **Overview of NJFCP Program**

Vision: Develop an experimental and analytical capability to facilitate OEM's evaluation of fuel physical and chemical properties on engine operability and to streamline ASTM fuels approval process.



#### Program uniqueness:

- Integrated systemwide approach involving all stages of testing and modeling areas for identical conditions
- Real-time communication and share of info among all 6 areas (experimentalists and modelers) and OEMs
- Brings state of the art knowledge, computer capabilities, and engineering experience together

Area 7: Program interface and integration

NJFCP is relating fuel properties to combustion Figures of Merit (FOM)

### **Improved OEM Screening of Fuels with NJFCP Integration**



Benefits: Early fuel screening, targeted Tier 3 and 4 tests, and increased OEM confidence

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### **Concept to Determine Blend Margin Using NJFCP**



### **Proposed Approach to Develop Fuel Screening**

### Yr 3 & Yr 4 of NJFCP

- Mature Experimental Test Methods
- Mature Modeling
- Develop Correlation to OEM Designs
- Identify Methods with Sufficient Maturity at End of Yr 4 for Fuel Screening
  - Testing
  - Modeling
- Develop Yr 5 Plan to Mature/Refine Fuel Screening Process
  - Assess Limiting Blend Margin
  - OEM Consensus Required Regarding "Value Added"

### NJFCP: Program Budget and Contributors

	\$K										
Agency	Year-1	Year-2	Year-3	Year-4							
FAA*	2500	1353	2000	950							
NASA	_	1103	1315	1,300							
AFRL**	1971	1650	1000	1,000							
DLA Energy	750	500	500	500							
NavAir	200	200	400	0							
ARL	_	-	-	650							
Grand Total	5421	5191	5215	4400							

\*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 Contributions**

- AFOSR (in-house activities)
- DOE (in-house activities at National Labs and possible support to secure fuels for testing)
- 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)

### **Program Sponsors, Contributors, Performers & Industry Members**



A strong community of hundreds of international (JetScreen) participants from 40 entities

FAA CENTER OF EXCELLENCE FOR ALTERNATIVE JET FUELS & ENVIRONMENT

### National Jet Fuels Combustion Program (NJFCP) Projects 25-30, 34

Project manager: Cecilia Shaw, FAA

#### Meredith Colket, Contractor Joshua Heyne, University of Dayton

Sept. 26-27, 2017 Alexandria, VA

Opinions, findings, conclusions and recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of ASCENT sponsor organizations.



# **Original ASCENT Project <u>PIs</u> and Key Contributors**

- Area 1: <u>Ron Hanson</u> (Stanford), Dave Davidson (Stanford), Shock Tube and Flow Reactor Studies.
- Area 2: <u>Hai Wang</u> (Stanford), Chemical Kinetics Model Development and Evaluation.
- Area 2.5: <u>Tianfeng Lu (U. Conn)</u>, Wenting Sun (Georgia Tech), Stephen Zeppieri (UTRC), Computational Acceleration.
- Area 3: <u>Tim Lieuwen</u> (Georgia Tech), Jerry Sietzman (Georgia Tech), David Blunck (Oregon State), Tonghun Lee (Illinois Urbana-Champaign), Advanced Combustion.
- Area 4: <u>Suresh Menon</u> (Georgia Tech), Matthias Ihme (Stanford), Venkat Raman (U. Michigan), Combustion Model Development and Evaluation.
- Area 5: <u>Robert Lucht</u> (Purdue), Paul E. Sojka (Purdue), Scott Meyer (Purdue), Carson Slabaugh (Purdue), Jay Gore (Purdue), Atomization Tests and Models.
- Area 6: <u>Scott Stouffer</u> (Dayton), Steven Zabarnick (Dayton), Tonghun Lee (Illinois Urbana-Champaign), Referee Combustor.
- Area 7: <u>Josh Heyne</u> (Dayton), Med Colket (contractor), Alex Briones (Dayton), Tonghun Lee (UIUC), Coordination and UDF Development.
- FAA, NASA, AFRL, and ARL Funded Activities



STANFORD











### **Fuel Properties to Figure of Merit** (FOM) Behavior

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

- Lean Blowout
- Cold Start Ignition
- Altitude Relight

### NJFCP Topic Areas for FOM Evaluation:

- 1. Chemical Kinetics
- 2. Lean Blowout (LBO)
- 3. Ignition
- 4. Spray
- 5. Computational Fluid Dynamics (CFD) Modeling
- 6. Common Format Routine (CFR)



### **Current NJFCP Structure with Working Groups**

#### • LBO:

- AFRL/UDRI Referee Rig
- AFRL/UDRI Well-Stirred Reactor
- Ga. Tech. High Sheer Rig
- Univ. of Sheffield Tay Combustor
- Univ. of Cambridge Bluff-body Stabilized Swirl Combustor
- Honeywell Auxiliary Power Unit (APU)
- Oregon State Turbulent Flame Speed
- OEMs

### • CFD (OEM Working Group lead):

- Stanford Modeling Referee Rig
- Ga. Tech. Modeling Referee Rig
- UTRC Modeling Referee Rig and Ga. Tech. High Sheer Rig
- OEMs

#### Kinetics:

- Stanford Shock Tube ignition delays and species profiles
- Stanford HyChem kinetic modeling
- UConn Chemistry reduction
- OEMs

#### Ignition (OEM Working Group lead):

- AFRL/UDRI Referee Rig
- Ga. Tech. Forced Ignition Rig
- ARL/UIUC Altitude testing of Referee Rig Swirler/nozzle
- NRC Canada Altitude testing of Microturbo TRS-18
- Honeywell APU
- Univ. of Cambridge Bluff-body Partially Prevaporized flow rig
- University of Michigan Forced ignition modeling
- OEMs
- Common Format Routine, CFR (OEM Working Group lead):
  - UDRI
  - Stanford Flamelet Models
  - Ga. Tech LESLIE Code
  - OEMs

#### Sprays (OEM Working Group lead):

- Purdue Rules and Tools Rig with Referee Rig Swirler and nozzle
- NRC Canada Referee Rig Nozzle
- Honeywell Altitude Spray Rig
- OEMs

### Key 'Take Aways' since Spring 2017

#### • LBO:

- 7 rigs now show linear dependency of DCN on LBO
- Additional fuels have been tested at GT

### • Ignition (OEM Working Group lead):

- Facilities with cold fuel and air as well as subatmospheric capabilities have been developed
- Ignition data is being collected at cold conditions (Referee Rig, GT, and ARL)

### • CFD (OEM Working Group lead):

- Spray injection based on measured data & consistent among 3 research groups simulating Referee Rig LBO
- Referee Rig LBO simulations for A2 & C1 underway

#### Kinetics:

- Real time measurement of additional species for constraining kinetic models
- New diagnostic for aromatics under development
- Model reductions have been refined and limits defined.

### • Common Format Routine (CFR):

- Academic combustion models & GUI delivered to OEMs
- Sprays (OEM Working Group lead):
  - Data gathered for fuels at cold conditions, similar to conditions of atmospheric cold ignition experiments in Referee Rig.
  - Fuel X further refined to incorporate new test data.

### **Key Interactions:**

- OEMs are fully involved and guiding the program direction, in fact leading multiple working groups.
- Community-wide national and international participation increasing
  - Sasol/Univ. Cape Town representative is presenting at the upcoming June meeting on their alt. fuels experience.
  - Continued participation from Cambridge, DLR Germany, Sheffield, JetScreen, and NRC Canada
- Leveraging interagency and international support

### **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



300

280

A3: low H/C, high

viscosity, high flash

(within experience

C-1 and C-5 were selected for detailed study in Year 1. C-6 and C-6a not available

### **NJFCP Fuels Update**

# Several new test fuels available to explore the jet fuel property "envelope" in Year 3

- Three new Category C test fuels
   C-7 blended fuel with maximum achievable cycloparaffins (~62 vol%)
   C-8 blended fuel with maximum aromatics (25 vol%)
   C-9 modified alternative fuel that has maximum DCN (63)
- Three modified jet test fuels with constant properties but varying DCN (30, 45, 55)
- Fuel with constant fuel property but with different TSI (threshold sooting propensity) shipped to GT
- Surrogate #3 which best matches fuel boiling range available in 2017 (Surrogates 1 and 2 already tested)

# **OEM Reaffirm NJFCP Benefits**

- The historical controlling parameters for LBO proposed by Lefebvre (correlations) are incomplete.
- Chemical properties could be just as important as physical properties! Combustor operability were more evaporation controlled (pres. atomizers), influenced by physical properties, while modern combustors may be controlled by other processes such as reaction rates.
- Fuel composition impacts combustor performance.
- Referee rig developed at AFRL/UDRI could play a role in ASTM D4054 fuel approval process reducing OEM rig and engine testing.
- Spray characterization could be eliminated for some candidate fuels, reducing overall test requirements.
- Gaining confidence in role of FFP properties and how they should be used to guide fuel formulation.
- The relative importance of properties on LBO depends on the combustor geometry and the operational 
   conditions. Limited geometries tested with available resources is a program challenge.
- Pyrolysis product species spectra shows promise to bridge DCN and generic LBO correlation.
- Significant progress was made on LBO modeling tools by groups; not there yet, but marching steadily.





# **LBO Working Group**



### More fundamental

More "Product-like"





Georgia Tech



AFRL/UDRI Referee Rig



**Univ. Sheffield** 

### **Rig Conditions and Fuels Tested**

The blue shaded region is the typical flight envelop. Only LBO points are plotted.



\*Highlighted cells indicate new tests since Fall 2017 ASCENT meeting

	A-1	A-2	A-3	C-1	C-2	C-3	C-4	C-5	F-1	F-2	F-3	F-4	S-1	S-2	nC12	
GT	Х	x	x	x	x	x	x	x	x	x	x		x	x	x	'E' fuels are
Honeywell	x	X	X	X	X			X								hlandad fuals
Referee Rig	x	X	x	X	X	X	X	X	x	x	x	X	x	x	x	F-1 to 3 are
WSR		X	X	X			X	X							x	
NASA		X		X		x										C-1/A-2 Dienas,
Sheffield	х	Х	х	X		х	X	X								and F-4 is a
Oregon State		x		x				x								A-2/C-5 blend.
Cambridge		х		х				х								
Univ. Cape Town/	Crude	e-derive	ed Jet /	A-1,Jet	A-1 +	50% r	n-dode	cane,	FSJF (	certifi	icatior	n), FSJF	- (com	merci	al), FSJF	10
Sasol (via DLR Ger.)	(com) Heavy	nercial / naphi	) + 1.5 tha refi	% нСР inery s	tream	erime	ntal G	IL Ker	osene	, Synt	netic	paraffi	nic ke	rosen	е (SPK),	18

### 8 of 9 Rigs Show First Order DCN Dependency

### **Rigs that show DCN trends:**

- 1. Referee Rig AFRL/UDRI
- 2. GT High Sheer Rig
- 3. Well-Stirred Reactor (WSR)
- 4. Sheffield (Rolls-Royce Rig)
- 5. Univ. Cape Town/ Sasol via DLR Germany Standard Rig
  - Used different fuels than NJFCP
- 6. UTRC Partially Premixed Rig
  - Used different fuels than NJFCP
- 7. University of Cambridge
- 8. NASA LDI Rig
  - Emissions data show similar trends.  $\phi$ (LBO is not directly determined.

Most LBO data scales linearly with DCN.



#### Combine Feature Importance (Referee Rig, GT, Sheffield, and WSR)



 $\phi(LBO_{A2})$ 

 $\phi(LBO_i)$ 

## **Combustion Chemistry**

### Shock Tube/ Laser Measurements (Data: Hanson, Stanford

and Model: Wang, Stanford; Lu, UConn)

#### CN fuels and A2, 4%O2 in Ar, scaled to 4atm with P<sup>-0.6</sup>, Phi~1

### For range of fuels:

- Ignition delay is strong function of Derived Cetane Number -(DCN)
  - Consistent with LBO trends
- Efforts to further reduce species while reproducing combustion characteristics still challenging
  - Looking at methods to couple with CFD for online reduction



### **Combustion Chemistry: Fuel X Model**

### Shock Tube/ Laser Measurements (Data: Hanson, Stanford and Model: Wang, Stanford; Lu, UConn)

**Previously concluded:** Fuel X modeling, DCN value, and ignition delay were all strongly dependent on intermediate product species.

## New optical diagnostics for real-time measurement of pyrolysis product species.

- Measurement method for iso-butene developed. Role of interfering species in progress
  - Isobutene increases with increasing isoalkane results in lowering the DCN
- 2. Methods for other species refined for greater accuracy
  - Ethylene increases with increasing nalkane concentration and results in a higher DCN
- 3. Techniques for aromatics in progress
  - Will enable better mass balance



### **Sprays: Fuels and Test Conditions**



### Sprays: Phase Doppler Particle Analyzer (PDPA) Data



**Radial Location [mm]** 

- No significant variation in D<sub>32</sub> and axial velocity observed for varied fuel type
- Investigation of near-LBO conditions has wrapped up for the time being.
- Next goal is to measure cold fuel/ cold N<sub>2</sub>.

25

30

35

20

Radial Location [mm]

# **Sprays: Fuel X Model**

Purdue data (0)

Model accounts for fuel property effects on SMD and Velocity. Includes (for particular fuel nozzle) radial distribution of drop size and velocities

 $0.0135 (\sigma_F \mu_F)^{0.5} FAR^C (T_3/288)^{1.0}$ = drop size with same liquid surface to SMD, m = $U_{A} ((\Delta P/P)_{A}/0.02)^{0.39} (B + (A (1.5 U_{F}/U_{A})^{3} - (A (1.5 U_{F}/U_{A})^{2} + A(1.5 U_{F}/U_{A}))^{0.5} \rho^{0.0}$ volume ratio as the spray 5. Use projected boundary conditions for 1. Acquire spray characteristics ( $\overline{SMD}_{\Omega}$ , spray for CFD  $SMD_0(r)$ ,  $n_0(d,r)$ ,  $V_{0,r}$ ,  $V_{0,x}$ ) for reference 6. Confirm accuracy using cold flow fuel (A-2) with known properties simulations (no vaporization, etc) and 2. Acquire physical properties for Fuel-X compare with (cold flow) experimental 3. Compute new SMD, based on Fuel-X data property data and extend to other spray Run CFD simulations using fuel-7. properties based on correlations dependent vaporization and combustion 4. Linearly project spray characteristics back models: confirm reacting flow data with to injection location A-2 Performance Map of Air-Assist Atomizer 2000 , 1500 Injection plane • Air DP = 2% 70 Air DP = 3% 40 D [μm]  $\Delta ir DP = 4\%$ r = -15 mm Air DP = 5% 50 40 30 20 , D [µm] Air Temn = 3951 Air Press = 2 har 10 3000 2500 2000 50 100 150 200 Fuel  $\Delta P$ , psid

80

D [um]

24

# **CFD: Referee Rig LBO Simulations**

- Cold flow simulations reviewed & agreed on common boundary conditions (BCs)
- Reacting spray simulations reviewed and agreed on common injection condition (based on experimental data)
- Agreed on step-wise reduction in equivalence ratio (fuel flow rate) procedure to approach LBO
- Analyze total evaporation rate and heat release rate before next fuel flow reduction
- One set of CFD simulations has shown correct LBO trend for A2 vs C1 (but using "old" Dome Effusion cooling BC)
- Significant speed-up (5X) being pursued for GTech/UTRC teams with new grid and domain decomposition





Non-reacting time-averaged velocity



Time-avg Temperature at near LBO<sub>25</sub>

## **CFD Modeling: Next Steps**

- Demonstration of CFD predicting correct trends in LBO fuel sensitivity for Referee Rig
- Continue development of CFD simulations of prevaporized ignition experiments
- Support of Common Format Routine efforts

## **Ignition Working Group**

### **Working Group Contributors**

 Areas 3 and 6, Univ. of Cambridge, NRC, ARL, and Honeywell



### More fundamental

More 'Product-like'



Spray Georgia Tech



ARL



Honeywell

### **Ignition Fuels and Test Conditions**



# **Ignition Working Group Update**

Execute forced ignition experiments of select fuels to highlight the impact of fuel property variation on ignition in gas turbine combustors

- Flow and thermodynamic conditions relevant to product engine combustors
  - special focus on cold conditions (high altitude, low P and ground starts)
  - fuel conditioning (controlled fuel Temperature, spray, vaporized, etc.)
- Understand ignition characteristics as a function of fuel properties (physical and chemical)
- Collect data to support future modelling work
  - Validation data (final and intermediate)
  - Model input (spray, plasma, etc.)

Initial results suggest that a lower BP aids in combustion, e.g. the C-5 fuel.



- PA-Pressure Atomizer
- AB-Air Blast Atomizer
- PV-Prevaporized
- LDI- Lean Direct Injection

#### **Rig Geometry:**

- GT-Georgia Tech
- RR-Referee Rig
- Sheff- Univ. Sheffield
- HON Honeywell (3% DP) 29

### **Statistical Analysis of Ignition Data**



# **CFR Development Update**

#### GUI, below, develops flamelet lookup tables for Fuel X Chemistry inputs that OEMs can utilize.

Thermo-Chemical-Transport Data PreTabulator - Version 1.0.6372.24645



- Flamelet/Progress Variable with complete S-curve Common Format Routines (CFR) development is nearly complete.
- GUI's have been enhanced and bugs have been corrected.
- Tuning of the commercial software numerics for coupling CFR/LES/FPV model is underway.
- Statistics collection algorithms and software were developed
- Task is less than a year into development. Modeling comparison of CFR team and industry models.



#### Industry code result

CFR/LES/FPV (current status, numerical tuning required)

#### Python script messages displayed here. FPV and FPI flamelet generation GUI for laminar and turbulent flames Model Boundary Conditions Numerics Table Generator Output Model Selection Heat Transfe Transport Mode Flow EPI Laminar Adiabatic Unity Lewis Number O Turbulent ○ FPV Non-Adiabatic Mixture Average Diff MultiComponent Diff Cantera Chemistry File Path (.cti) C:\Users\Lab\Documents\CodeDevelopment\Table\_Generation\_Codes\FPV\gri30.xml Browse Chemkin2cti About Settinas Theory User Guide Restor Ok Enhanced Storage Dialog **Resolved Scale Simulation GUI Turbulence** Parameters Compute Ymean (URANS, SAS, DES, and LES) Fluent Variable: Variable Enabled RMS Species Enabled Average RMS Average 1 1 1 1 V H20 V 1 [ CMEAN co 1 1 **EVAR** V 1 CO2 100 V 1 1 LAMBDA 1 V TEMPERATURE FMEAN SOURCE V 1 1 CMEAN SOURCE Statistics (RMS, Average) Collection Start Time Schmidt Parameters Time to start collection 0.000004 Fmean 0.9 Fyar 0.9

Cmean 0.9

Ok

### Overall NJFCP Accomplishments (Expected and Completed) Spring 2017

- Created and demonstrated capability to measure fuel-dependent LBO limits in 'real' combustor hardware outside of OEM facility
- Demonstrated correlations with DCN, a chemical marker of the fuel
- Created and demonstrated capability to measure fuel-dependent ignition limits in 'real' combustor hardware with cold fuel and cold air outside of OEM facility
- Created and demonstrated techniques to measure several of the dominant species from fuel pyrolysis
- Hybrid Chemistry (HyChem) models (and their reduction to ~35 species) created and demonstrated for petroleum fuels and several NJFCP test fuels.
- Fuel-X modeling approaches (including blends) developed for chemistry and fuel nozzle spray parameters (drop size, velocity)
- Developed CFD models to predict fuel-dependent LBO limit trends

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# Year 4 Objectives

- LBO:
  - Alternative Geometries
  - Additional fuels
- Ignition
  - Complete fuel screening
  - Analyze data from screening
- Sprays
  - Complete screening of fuels at ignition conditions
- CFD
  - Capture fuel sensitivity trends
- Kinetics
  - Complete ignition testing for new fuels
  - Measure additional species concentrations
- CFR
  - Develop additional CFR capabilities

# Challenges

### **Programmatic:**

- Generating sufficient experimental data at extreme conditions to enable fuel sensitivity evaluation
- Balancing experimental resources to maximize impact of NJFCP program
- Integration, coordination, and scheduling of activities with year end goals considered
- Implementing validated models into Common Format Routines (CFRs)
- Sustained Federal support

### **Technical:**

### **Experimental:**

 Collecting, documenting, and analyzing data to support streamlining fuel approvals

### Modeling:

- Validation of CFD simulations
- Validating Fuel X approach for sprays and kinetics

## **OUTSIDE ENGAGEMENTS**

#### • Conference Proceedings/Presentations: 103

- Area 1 (Stanford): 17 presentations (2 peer reviewed)
- Area 2 (Stanford): 8 presentations
- Area 2.5 (Uconn & Georgia Tech): 8 presentations
- Area 3 (Georgia Tech, Oregon St.): 15 presentations
- Area 4 (Georgia Tech): 11 presentations
- Area 4/5 (Stanford): 10 presentations
- Area 5 (Purdue): 5 presentations
- Area 6 (Dayton): 8 presentations
- Area 7 (Dayton): 16 presentations
- UIUC (Related non-NJFCP Funded): 3 presentations
- Surrogates: 2 presentations
- Peer Reviewed Journal Publications: 15
  - Area 1 (Stanford): 1 paper
  - Area 2.5 (Uconn & Georgia Tech): 1 paper
  - Area 3: (GaTech): 6 papers
  - Area 4/5 (Stanford): 4 papers
  - Area 3/6 (UIUC): 1 paper
  - Area 6: 2 papers
  - Area 7: 1 paper

#### **RECENT:**

• JetScreen meeting in Rome

## **OUTSIDE ENGAGEMENTS**

#### **UPCOMING: AIAA Scitech**

#### • Mon, Jan 8, 2018

#### 11:30 AM - 12:00 PM

Correlation of Alternative Jet Fuel Physical Properties to Engine Ignition at Altitude Conditions Pervez Canteenwalla; Andrew Corber; Wajid A. Chishty

#### 12:00 PM - 12:30 PM

Near Lean Blowout Simulations of Non-premixed and Premixed Swirling Methane Flames Jeffrey Labahn; Peter C. Ma; Hao Wu; Matthias Ihme • Thursday, Jan 11

#### 9:30 AM - 10:00 AM

Year 3 of the National Jet Fuels Combustion Program: Practical and Scientific Impacts of Alternative Jet Fuel Research Joshua S. Heyne; Erin Peiffer; Meredith B. Colket; Aniel Jardines; Cecilia Shaw; Jeffrey P. Moder; William M. Roquemore; James T. Edwards; Chiping Li; Mark Rumizen; Mohan Gupta • Friday, Jan 12

#### 10:00 AM - 10:30 AM

Spray Characteristics at Lean Blowout and Cold Start Conditions using Phase Doppler Anemometry Andrew Bokhart; Dongyun Shin; Neil S. Rodrigues; Paul Sojka; Jay P. Gore; Robert P. Lucht

#### 10:30 AM - 11:00 AM

Fuel Sensitivity of Lean Blowout in a RQL Gas Turbine Combustor Changju T. Wey

(Also on Friday, will conduct Year 2 Review of NASA Combustion Modeling Grants, 8-5, at SciTech)

- 1. Davidson, D. F., Tugestke, A., Zhu, Y., Wang, S., Hanson, R. K., "Species time-history measurements during jet fuel pyrolysis," 30th International Symposium on Shock Waves, Paper 179, Tel Aviv, Israel, July 2015. (Conference Papers)
- 2. Zhu, Y., Wang, S., Davidson, D. F., Hanson, R. K., "Shock tube measurements of species time-histories during jet fuel pyrolysis and oxidation," 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, Paper 262, Leeds, UK, August 2015. (Conference Papers)
- **3. D. Hernandez, D. Llanos, S. Banerjee and C. T. Bowman,** Flow Reactor Study of Combustion Characteristics of Jet and Rocket Fuels, presented at the 9th US National Combustion Meeting, 2015, Cincinnati, OH.
- **4. Rock, N., Chterev, I., Smith, T., Ek, H., Emerson, B., Noble, D., Seitzman, J., Lieuwen, T.** "Reacting Pressurized Spray Combustor Dynamics, Part 1. Fuel Sensitivities and Blowoff Characterization" *Proceedings of the ASME Turbo Expo 2016, Seoul, South Korea*, 2016, *GT2016-56346*
- 5. Chterev, I., Rock, N., Ek, H., Smith, T., Emerson, B., Noble, D., E. Mayhew, T. Lee, N. Jiang, S. Roy, Seitzman, J., Lieuwen, T. "Reacting Pressurized Spray Combustor Dynamics, Part 2. High Speed Planar Measurements" *Proceedings of the ASME Turbo Expo 2016, Seoul, South Korea*, 2016, GT2016-56345
- 6. Fillo, A., Blunck, D., "Effects of Fuel Chemistry and Turbulence Intensity on Turbulent Consumption Speed for Large Hydrocarbon Fuels," Western States Section of the Combustion Institute, Fall 2015.

- 7. Chterev, I., N. Rock, H. Ek, T. Smith, B. Emerson, D.R. Noble, E. Mayhew, T. Lee, N. Jiang, S. Roy, J. Seitzman, T. Lieuwen, Simultaneous High Speed (5 kHz) OH-PLIF and Stereo PIV Imaging of Pressurized Swirl-Stabilized Flames using Liquid Fuels, Int. Symp. on Combustion 2016: Seoul, South Korea. In Review.
- 8. Sforzo, B., Dao, H., Wei, S. & Seitzman, J. "Liquid Fuel Composition Effects on Forced, Non-Premixed Ignition" Proceedings of the ASME Turbo Expo 2016, Seoul, South Korea, 2016, GT2016-56163
- **9. A. Fillo, D. Blunck,** "Effects of Fuel Chemistry and Turbulene Intensity on Turbulent Consumption Speed for Large Hydrocarbon Fuels," Western States Section Meeting of the Combustion Institute, Provo, UT (2015).
- **10.** J. Bonebrake, A. Fillo, D. Blunck, "Effect of Turbulent Fluctuations on Radiation Emissions from a Premixed Flame," Western States Section Meeting of the Combustion Institute, Provo, UT (2015).
- **11. E. Zeuthen, D. Blunck,** "Radiation emissions from Turbulent Diffusion Flames Burning Large Hydrocarbon Fuels," Western States Section Meeting of the Combustion Institute, Provo, UT (2015).
- **12. E. Zeuthen, D. Blunck,** "Radiation Characteristics of Turbulent Diffusion Flames Burning Alternative Aviation Fuels," 9th US Combustion Meeting, Cincinnati, OH (2015).

- **13.** Ranjan, R., Hannebique, G., Panchal A., and Menon, S., "Towards Numerical Prediction of Jet Fuels Sensitivity of Flame Dynamics in a Swirl Spray Combustion System", Accepted for presentation at the 2016 AIAA Propulsion and Energy Forum and Exposition, Salt Lake City, Utah, 25-27 July, 2016.
- 14. Hannebique, G., Akiki, M., Ranjan, R., and Menon, S., "A Hybrid Eulerian-Eulerian/Eulerian-Lagrangian Method for Dense-to-Dilute Dispersed Multiphase Reacting Flows ", Accepted for presentation at the 2016 AIAA Propulsion and Energy Forum and Exposition, Salt Lake City, Utah, 25-27 July, 2016.
- **15.** Yang, S., Ranjan, R., Yang, V., Menon, S., and Sun, W., "Parallel on-the-fly adaptive kinetics in direct numerical simulation of turbulent premixed flame", Accepted for presentation at the 36<sup>th</sup> Combustion Symposium, Seoul, Korea, July 31- August 5, 2016.
- **16.** Esclapez, L., Nik, M.B., Ma, P.C., Carbajal, S., and Ihme, M., "LES of combustion dynamics near blowout in a realistic gas-turbine combustor." presentation at APS-DFD, Nov. 22-24, 2015, Boston.
- **17.** Ma, P.C., Esclapez, L., and Ihme, M., "Analysis of Fuel Injection and Atomization of a Hybrid Air-Blast Atomizer" presentation at APS-DFD, Nov. 22-24, 2015, Boston.
- **18.** Ma, P.C., Nik, M.B., Carbajal, S., Ihme, M., Buschhagen, T., Naik, S.V., Gore, J.P., Lucht, R.P., "Large-Eddy Simulations of Fuel Injection and Atomization of a Hybrid Air-Blast Atomizer" Presented at AIAA SciTech Meeting, San Diego, 2016.

- **19.** Nik, M.B., Ma, P.C., Carbajal, S., and Ihme, M., "Characterization of Fuel Efects on Lean Blowout in Gas Turbine Combustors." Presented at AIAA SciTech Meeting, San Diego, 2016.
- **20.** Govindaraju, P., Wang, Q., Ihme, M., "Multicomponent Droplet Evaporation Using Group Contribution Methods" Presented at 9th US National Combustion Meeting, 2015, Cincinnati, OH.
- 21. Stagni, A., Esclapez, L., Govindaraju, P., Cuoci, A., Favarelli, T., and Ihme, M., "The role of preferential evaporation on the ignition of multicomponent fuels in a homogeneous spray/air mixture." Accepted for presentation at Int. Symp. Combust, Seoul, 2016.
- 22. T. Buschhagen, R. Z. Zhang, S. V. Naik, C. D. Slabaugh, S. E. Meyer, J. P. Gore, and R. P. Lucht, "Effect of Aviation Fuel Type and Fuel Injection Conditions on Non-reacting Spray Characteristics of Hybrid Air Blast Fuel Injector," Presented at AIAA SciTech Meeting, San Diego, CA, 4-8 January 2016.
- 23. P. C. May, M. B. Nik, S. E. Carbajal, S. Naik, J. P. Gore, R. P. Lucht, and M. Ihme, "Large-Eddy Simulations of Fuel Injection and Atomization of a Hybrid Air-Blast Atomizer," Presented at AIAA SciTech Meeting, San Diego, CA, 4-8 January 2016.

- 24. E. Corporan, T. Edwards, C. Neuroth, D. Shouse, S. Stouffer, T. Hendershott, C. Klingshirn, M. DeWitt, S. Zabarnick, J. Diemer, "Initial Studies of Fuel Impacts on Combustor Operability and Emissions at AFRL", Poster Presentation at IASH 2015, 14th International Symposium on Stability, Handling and Use of Liquid Fuels Charleston, South Carolina USA 4-8 October 2015.
- **25.** Stouffer, S.D., Hendershott, T.H., Monfort, J.R., Corporan, E., Combustion Characteristics in a Single Cup Combustor Using Jet A and Research Fuels Paper for Central States Section of the Combustion Institute, Knoxville, Tennessee, May 15-17, 2016.
- **26.** J. S. Heyne, F. L. Dryer, S. H. Won, F. M. Haas, "Reactivity Comparisons of Conventional and Alternative Jet Fuels in a Variable Pressure Flow Reactor" presented at 9th US National Combustion Meeting, 2015, Cincinnati, OH.
- 27. J. S. Heyne, M. Colket, "National Jet Fuels Combustion Program: Overall Program Integration and Analysis," CRC Aviation Committee Meetings, Nashville, TN, 6 May 2015.
- 28. M. Colket, J. S. Heyne, M. Rumizen, J. T. Edwards, M. Gupta, W. M. Roquemore, J. P. Moder, J. M. Tishkoff, C. Li, et al., "An Overview of the National Jet Fuels Combustion Program," Presented at AIAA SciTech Meeting, San Diego, 2016.

## **Presentations (cont.)**

- 29. Stachler, R.D., Heyne, J.S., Miller, J.D., Stouffer, S.D., Zeppieri, S.P., Colket,
   M.B., Roquemore, W.M "Well Stirred Reactor Emission Studies of Fuel Surrogates", Paper for
   Central States Section of the Combustion Institute, Knoxville, Tennessee, May 15-17, 2016.
- **30.** Bell, D., Heyne, J. S., Dryer, F. L., Won, S. H., Haas, F. M., Dooley, S., "On the development of fuel surrogates to match chemical, physical, and distillate properties," ASME DESS, Dayton, OH, November 2016.
- **31. Stachler, R.D., Heyne, J.S., Miller, J.D., Stouffer, S.D., Roquemore, W.M** "Cross-Experiment Analysis of a Well-Stirred Reactor and other Gas Turbine Experiments", ASME DESS, Dayton, OH, November 2016.
- **32.** Carson, J., Heyne, J. S., Hendershot, T., Stouffer, S., Corporan, E., "Predicting LBO based on Random Forest Modeling," ASME DESS, Dayton, OH, November 2016.
- **33.** Lee, T., *Alternative Jet Fuel Database*, Federal Aviation Agency AEC Roadmap Meeting, Washington DC, May (2016).
- 34. Xu, R., Chen, D., Wang H. "Hybrid approach to combustion chemistry of jet fuels," poster presentation at the 36th International Symposium on Combustion, Seoul, Korea, July 31-August 5, 2016.
- **35.** Wang, H., "Key phenomena enabling direct simulation of real fuel combustion chemistry," 2015 PacifcChem Conference, Honolulu, Hawaii, December 18, 2015.

## **Presentations (cont.)**

- **36.** Davidson, D. F., Zhu, Y., Wang, SJ., Parise, T., Sur, R., Hanson, R. K., "Shock Tube Measurements of Jet and Rocket Fuels," AIAA 2016-0178, *54th AIAA Aerospace Sciences Meeting*, San Diego CA, American Institute of Aeronautics and Astronautics, January 2016.
- **37.** Aaron Fillo, Jonathan Bonebrake, David Blunck, "Sensitivity of jet fuel global consumption speed to fuel chemistry and turbulent intensity," 4P088 poster presentation at the 36th International Symposium on Combustion, Seoul, Korea, July 31-August 5, 2016.
- 38. Chterev, I., Rock, N., Ek, H., Emerson B., Seitzman J., Jiang, N., Roy, S., Lee, T., Gord, T., and Lieuwen, T. 2017. Simultaneous Imaging of Fuel, OH, and Three Component Velocity Fields in High Pressure, Liquid Fueled, Swirl Stabilized Flames at 5 kHz. Combustion and Flame. 186, pp. 150-165.
- **39.** Rock, N., Chterev, I., Emerson, B., Seitzman, J., and Lieuwen, T., Blowout Sensitivities in a Liquid Fueled Combustor: Fuel Composition and Preheat Temperature Effects. 2017. In ASME Turbo Expo 2017. GT2017-63305. Emerson managed the project.
- **40. Wei, S., Sforzo, B. and Seitzman, J.** "High Speed Imaging of Forced Ignition Kernels in Non-Uniform Jet Fuel/Air Mixtures," 2017. Accepted for publication in Journal of Engineering for Gas Turbines and Power.

### AIAA SciTech Presentations and Paper Submissions

- 41. A. J. Bokhart, D. Shin, R. M. Gejji, P. E. Sojka, J. P. Gore, R. P. Lucht, S. V. Naik, and T. Buschhagen, "Spray Measurements at Elevated Pressures and Temperatures Using Phase Doppler Anemometry," Paper 2017-0828, presented at the 55nd Aerospace Sciences Meeting, Grapevine, TX, 9-13 January, 2017.
- **42.** Govindaraju, P., Esclapez, L., and Ihme, M., "Construction of Physical Fuel Surrogates using Computational Techniques," *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.
- **43.** Esclapez, L., Ma, P. C., Mayhew, E., Xu, R., Stouffer, S.D., Lee, T., Wang, H., and M. Ihme, M., "Large-Eddy Simulations of Fuel Effects on Gas Turbine Lean Blow-out", AIAA Paper AIAA-2017-1955, AIAA SciTech Conference Jan 9-13, 2017.

- **44.** Davidson, D. F., Shao, J., Parise, T., and Hanson, R. K., "Shock Tube / Laser Absorption Measurements of Jet and Rocket Fuel Oxidation and Pyrolysis," *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.
- **45.** Allison, P. M., Sidney, J. A. M., and Mastorakos, E., "Forced Response of Kerosene Flames in a Bluff-body Stabilised Combustor," *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.
- **46.** Sidney, J. A. M., Allison, P. M., and Mastorakos, E., "The effect of fuel composition on swirling kerosene flames," *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.
- **47. Canteenwalla, P., and Chishty, W. A.,** "Investigation of Engine Performance at Altitude Using Selected Alternative Fuels for the National Jet Fuels Combustion Program," *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.

- 48. Chtev, I., Rock, N., Ek, H., Smith, T., Emerson, B., Nobel, D. R., Seitzman, J., Lieuwen, T., Mayhew, E., Lee, T., Jiang, N., and Roy, S., "Simultaneous High Speed (5 kHz) Fuel-PLIE, OH-PLIF and Stereo PIV Imaging of Pressurized Swirl-Stabilized Flames using Liquid Fuels," 55th AIAA Aerospace Sciences Meeting, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.
- **49. Edwards, J. T.,** "Reference Jet Fuels for Combustion Testing," *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.
- **50.** Stouffer, S.D., Hendershott, T.H., Monfort, J.R., Diemer, J. Edwin Corporan, E., Wrzesinski, P.J., Caswell, A., "Blowout and Ignition Characteristics of Conventional and Surrogate Fuels Measured in a Swirl Stabilized Combustor", AIAA Paper AIAA-2017-1954, AIAA SciTech Conference Jan 9-13, 2017.

- **51. Sforzo, B., Wei, S., & Seitzman, J.** "Ignition of Alternative Liquid Jet Fuels in a Stratified Flow" 2017 AIAA Science and Technology Forum and Exposition, Grapevine, TX, 2017, AIAA-2017-0147
- **52.** Stachler, R. D., Heyne, J. S., Stouffer, S. D., Miller, J. D., and Roquemore, W. M., "Investigation of Combustion Emissions from Conventional and Alternative Aviation Fuels in a Well-Stirred Reactor," *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.
- **53. Temme, J., Kurman, M. S., and Kweon, C.-B. M.,** "Characterization of Alternative Jet Fuel Spray and Combustion at Engine Relevant Ambient Conditions," *52nd AIAA/SAE/ASEE Joint Propulsion Conference*, Salt Lake City, UT: American Institute of Aeronautics and Astronautics, 2016.
- **54. Temme, J., Colburn, V. D., and Kweon, C.-B. M.,** "High-speed chemiluminescence measurements of alternative jet fuels at engine relevant ambient conditions," *Submitted to the 55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.

- **55.** Yang, S., Ranjan, R., Yang, V., Menon, S., and Sun, W., "Parallel on-the-fly adaptive kinetics in direct numerical simulation of turbulent premixed flame," *Submitted to the 55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.
- **56.** Mayhew, E., Mitsingas, C., Mcgann, B., Hendershott, T. H., and Stouffer, S. D., "Spray Characteristics and Flame Structure of Jet A and Alternative Jet Fuels," AIAA Paper AIAA-2017-0148, *55th AIAA Aerospace Sciences Meeting*, American Institute of Aeronautics and Astronautics, 2017.
- **57.** Xu, R., Chen, D., Wang, K., and Wang, H., "A Comparative Study of Combustion Chemistry of Conventional and Alternative Jet Fuels with Hybrid Chemistry Approach," *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.
- **58.** Bell, D., Heyne, J. S., Won, S. H., Dryer, F. L., Haas, F. M., and Dooley, S., "On the Development of General Surrogate Composition Calculations for Chemical and Physical Properties," *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.

- 59. **Podboy, D. P., Chang, C., and Moder, J. P.,** "Lean Blowout Fuel Sensitivity for a Lean Direction Injection Combustor," *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX: American Institute of Aeronautics and Astronautics, 2017.
- 60. Monfort, J.R., Stouffer, S.D., Hendershott, T.H., Wrzesinski, P.J., Foley, W.S., "Evaluating Combustion Instability in a Swirl-Stabilized Combustor Using Simultaneous Pressure, Temperature, and Chemiluminescence Measurements at High Repetition Rates," AIAA Paper AIAA 2017-1101, AIAA SciTech Conference Jan 9-13, 2017.

# **ASME Turbo Expo 2017**

- 61. "Blowout Sensitivities in a Liquid Fueled Combustor: Fuel Composition and Preheat Temperature Effects." Proceedings of the ASME Turbo Expo GT2017-63305
- 62. "Reacting Pressurized Spray Combustor Dynamics, Part 1. Fuel Sensitivities and Blowoff Characterization." Proceedings of the ASME Turbo Expo GT2016-56346
- 63. "Reacting Pressurized Spray Combustor Dynamics, Part 2. High Speed Planar Videos." Proceedings of the ASME Turbo Expo GT2016-56345
- **64. S. Wei, B. Sforzo and J. Seitzman,** "High Speed Imaging of Forced Ignition Kernels in Non-Uniform Jet Fuel/Air Mixtures," GT2017-63300, Proceedings of the ASME/IGTI Turbo Expo 2017.

### Peer Reviewed Archival Publications

- 1. X. Gao, S. Yang, W. Sun, "A global pathway selection algorithm for the reduction of detailed chemical kinetic mechanisms" Combustion and Flames, 2016 (doi:10.1016/j.combustflame.2016.02.007)
- 2. D. Valco, K. Min, A. Oldani, T. Edwards, T. Lee, Low Temperature Autoignition of Conventional Jet Fuels and Surrogate Jet Fuels with Targeted Properties in a Rapid Compression Machine, Proc. Comb. Symp. accepted (2016)
- **3. Davidson, D. F., Zhu, Y., Shao, J., Hanson, R. K.,** "Ignition Delay Time Correlations for Distillate Fuels," Fuel 187 (2017) 26-32, DOI: 10.1016/j.fuel.2016.09.047P. Govindaraju and M. Ihme, Group contribution method for multicomponent evaporation with application to transportation fuels, Int. J. Heat & Mass Transfer, 2016, 102, 833-845
- **4. A. Stagni, L. Esclapez, P. Govindaraju, A. Cuici, T. Favarelli, M Ihme,** The role of preferential evaporation on the ignition of multicomponent fuels in a homogeneous spray/air mixture, Proc. Comb. Inst., 2016
- 5. H. Wu, M. Ihme, Compliance of combustion models for turbulent reacting flow simulations, submitted to Fuel, 2016
- 6. M. Colket, J. S. Heyne, M. Rumizen, J. T. Edwards, M. Gupta, W. M. Roquemore, J. P. Moder, J. M. Tishkoff, C. Li, et al., "An Overview of the National Jet Fuels Combustion Program," AIAA Journal, DOI: 10.2514/1.J055361.
- 7. Escalpez,L., M, P.C., Xu, R., Stouffer, S.D. Lee, T., Wang, H., Imhe, M., "Fuel Effects on Lean Blow-out in a Realistic Gas Turbine Combustor, Accepted for Combustion and Flame (2017).
- 8. Briones, A.M., Stouffer, S.D., Vogiatzis, K., Rein, K., Rankin, B.A., Effects of Effusion and Film Cooling Jet Momenta on Combustor Flow Fields, To be published in J. Eng. Gas Turbines & Power, 2017.

- 1. A. Panchal, R. Ranjan, S. Menon, "Subgrid Mixing and Evaporation Modeling in Large Eddy Simulation of Two-Phase Reacting Flows," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- 2. M. E. Feyz, Razi Nalim, J. P. Gore, Ali Tarraf, "Analytical study on near-field entrainment in a transient turbulent free jet," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- **3.** Yujie Tao, Gregory P. Smith, Hai Wang, "Uncertainty of a Foundational Fuel Chemistry Model," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- 4. Chao Xu, Muhsin M. Ameen, Sibendu Som, Jacqueline H. Chen, Tianfeng Lu, "Dynamic adaptive combustion modeling of diesel spray flames based on chemical explosive mode analysis," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- 5. Robert D. Stachler, Joseph K. Lefkowitz, Timothy M. Ombrello, Scott D. Stouffer, Joshua S. Heyne, Joseph D. Miller, "The effect of residence time on the ignitability of ethylene and air mixtures in a toroidal jet-stirred reactor," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.

- 6. Ji-Woong Park, Tianfeng Lu, "Chemical explosive mode analysis on extinction of 1-D premixed counterflow flames," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- 7. Karla Dussan, Frederick L. Dryer, Sang Hee Won, Stephen Dooley, "Predicting Real Transportation Fuel Combustion Properties: Distinct Chemical Functionalities in Hydrocarbon Laminar Burning Velocities," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- 8. Martin Rieth, Reetesh Ranjan, Suresh Menon, Andreas Kempf, "On the Comparison of Finite-Rate Kinetics and Flamelet Base Subgrid Models for LES of Turbulent Premixed Flame," 10th US National Combustion Meeting, Maryland, April 23–26, 2017.
- **9.** Shengkai Wang, Thomas Parise, David F. Davidson, Ronald K. Hanson, "A New Diagnostic for Hydrocarbon Fuels using 3.41-μm Diode Laser Absorption," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **10.** Michael Halloran, Nicholas Traina, Tonghun Lee, Jihyung Yoo, "Measurements of low concentration hydrocarbons at elevated temperatures and pressures using supercontinuum laser absorption spectroscopy," 10th US National Combustion Meeting, Maryland, April 23-26, 2017.

- **11.** Jiankun Shao, Yangye Zhu, Shengkai Wang, David F. Davidson, Ronald K. Hanson, "Shock Tube Study of Jet Fuel Pyrolysis and Ignition at Elevated Pressure," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **12.** Alison M. Ferris, David F. Davidson, Ronald K. Hanson, "Combined Laser Absorption and Gas Chromatography (GC) Speciation in a Shock Tube: Validation and Application to Ethylene Pyrolysis," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **13.** Aaron W. Skiba, Campbell D. Carter, Stephen D. Hammack, Tonghun Lee, "A simplified approach to multi-scalar imaging for turbulent premixed flames," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- 14. A.M. Tulgestke, D.F. Davidson, R.K. Hanson, "Laser absorption measurements of ethylene and carbon monoxide time-histories during *n*-heptane oxidation at low temperatures behind reflected shock waves," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **15. R. Xu, H. Wang, D. F. Davidson, R. K. Hanson, C. T. Bowman, F. N. Egolfopoulos,** "Evidence Supporting a Simplified Approach to Modeling High-Temperature Combustion Chemistry," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.

16.	R. Xu, D. Chen, K. Wang, Y. Tao, J. K. Shao, T. Parise, Y. Zhu, S. Wang, R. Zhao, D.
	J. Lee, F. N. Egolfopoulos, D. F. Davidson, R. K. Hanson, C. T. Bowman, H. Wang,
	"HyChem Model: Application to Petroleum-Derived Jet Fuels," 10th US National
	Combustion Meeting, College Park, Maryland, April 23-26, 2017.

- **17. Pavan B. Govindaraju, Matthias Ihme,** "Sensitivity to Experimental Uncertainty in Surrogate Descriptions of Aviation Fuels," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **18. Yang Gao, Tianfeng Lu,** "Reduced HyChem Models for Jet Fuel Combustion," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **19. K. Wang, R. Xu, T. Parise, J. K. Shao, D. J. Lee, A. Movaghar, D. F. Davidson, R. K. Hanson, H. Wang, C. T. Bowman, F. N. Egolfopoulos,** "Combustion Kinetics of Conventional and Alternative Jet Fuels using a Hybrid Chemistry (HyChem) Approach" 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- 20. K. Wang, R. Xu, T. Parise, J.K. Shao, D. F. Davidson, R. K. Hanson, H. Wang, C. T. Bowman, "Evaluation of a Hybrid Chemistry Approach for Combustion of Blended Petroleum and Bio-derived Jet Fuels," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017

- **21. Chao Xu, Tianfeng Lu,** "An iterative uncoupled quasi-steady-state method for dynamic chemical stiffness removal," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- **22.** Xiang Gao, Wenting Sun, "Using Global Pathway to Understand Chemical Kinetics," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- **23.** Alex Krisman, Tianfeng Lu, Jacqueline H. Chen, "A direct numerical simulation study of the quenching of jet fuel flame kernels subject to intense isotropic turbulence," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- **24. Giulio Borghesi, Jacqueline H. Chen, Alexander Krisman, Tianfeng Lu,** "Direct Numerical Simulation of a Turbulent Autoigniting-Dodecane Jet at Low- Temperature Diesel Conditions, 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- 25. Jeffrey Labahn, Peter C Ma, Lucas Esclapez, Mattias Ihme, "Investigation of initial droplet distribution and importance of secondary breakup model on lean blowout predictions of a model gas turbine combustor," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.

- 26. **Sang Hee Won, Francis M. Haas, Stephen Dooley, Frederick L. Dryer,** "Chemical Functional Group Descriptor for Jet Fuel Surrogate," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- 27. Jeffrey R. Monfort, Scott D. Stouffer, Tyler H. Hendershott, Edwin Corporan, Andrew Caswell, "Experimental Characterization of Fuel-Dependent Resonance in a Representative Swirl Combustor," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- 28. Robert Zhang1, Andrew C. Pratt, Robert P. Lucht, Carson D. Slabaugh, "Investigation of the Pilot Stagnation Region in a High Power Liquid-Fueled C Combustor," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- **29. R. Ranjan, A. Panchal, B. Muralidharan, S. Menon**, "Simulation of the Evolution of Premixed Flame Kernels in a Turbulent Channel Flow," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.
- **30.** Chiara Saggese1, Ajay V. Singh, Joaquin Camacho, Hai Wang, "Effect of Distillate Fraction of Real Jet Fuel on Sooting Propensity Part 1: Nascent Soot Formation in Premixed Stretch-Stabilized Flames," 10<sup>th</sup> US National Combustion Meeting, College Park, MD, April 23-26, 2017.

- **31.** Giacomo Flora, Moshan S. P. Kahandawala1, Matthew DeWitt, Edwin Corporan, "Ignition Delay Measurements for Alternative Jet Fuels at Mid to Low Temperatures," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **32.** Kyungwook Min, Daniel Valco, Anna Oldani, Tonghun Lee, "Autoignition Behavior of Jet Fuel Relevant Pure Hydrocarbon Components in a Rapid Compression Machine," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **33.** Utsav Jain, Chao Han, Haifeng Wang, "Characteristics and Parameterization of Spray Combustion in Laminar Counter-flow Jet Flames," 10th US National Combustion Meeting, Maryland, April 23–26, 2017.
- 34. Aaron J. Fillo1, Jonathan M. Bonebrake1, David L. Blunck, "Impact of fuel chemistry and stretch rate on the global consumption speed of large hydrocarbon fuel/air flames," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **35.** Suo Yang1, Reetesh Ranjan, Vigor Yang, Wenting Sun, Suresh Menon, "Sensitivity to Chemical Kinetics Models in Time-Evolving Turbulent Non-Premixed Flames," 10th US National Combustion Meeting, Maryland, April 23-26, 2017.
- **36. Debolina Dasgupta, Wenting Sun, Marc Day, Tim Lieuwen,** "Sensitivity of chemical pathways to reaction mechanisms for *n*dodecane," 10th US National Combustion Meeting, Maryland, April 23-26, 2017.

- **37.** Jacob Sebastian, Benjamin Emerson, Timothy Lieuwen, "Stability Analysis of Multiple Reacting Wakes 10th US National Combustion Meeting," 10<sup>th</sup> US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **38.** Jeffrey O'Brien, Friedrich Bake, Matthias Ihme, "Modal Analysis of Direct Core Noise in a Model Combustor," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **39.** Xin Xue, Chih-Jen Sung, Hai Wang, "Effect of Distillate Fraction of Real Jet Fuel on Sooting Propensity Part 2: Soot Formation in Nonpremixed Counterflow Flames," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **40.** John Palmore Jr., Olivier Desjardins, "Simulations of Vaporizing Droplets in Turbulence," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.
- **41.** Gerald Mairinger, Alessio Frassoldati, Alberto Cuoci, Ernst Pucher, Kalyanasundaram Seshadri, "Autoignition of Jet Fuels and Surrogates in Nonpremixed Flows at Elevated Pressures," 10th US National Combustion Meeting, College Park, Maryland, April 23-26, 2017.





- All data including DLR (323K 6g/s airflow config. B, best R^2 for several different points checked at different temps and airflow rates) and only GT 2017 data with lines formatted to be the same length
- Data with only A, C, and nc12 fuels (S2 for RR and S1/S2 for GT were pretty far from the line of fit)
- 3. Only lines





# LBO Working Group Update

 Older correlations from Lefebvre did not include explicit kinetic or autoignition dependencies



Mellor, and later by Burger, described the process as a function of time scales.

$$\phi_{LBO_{i}} \sim \left[ \left( \frac{1}{\tau_{evap_{i}}} + \frac{1}{\tau_{mix_{i}}} + \frac{1}{\tau_{chem_{i}}} \right) \right]^{-1} \tau_{chem_{i}}$$

$$\tau_{chem_{i}}$$

$$\tau_{chem_{i}}$$

$$\tau_{chem_{i}}$$

$$\tau_{chem_{i}}$$

$$\tau_{chem_{i}}$$

$$\tau_{chem_{i}}$$

$$\tau_{chem_{i}}$$

$$\tau_{chem_{i}}$$

$$\tau_{chem_{i}}$$





### Current Dominant LBO 'Path': Referee Rig, GT, Sheffield, Sasol, and WSR



\*Arrows represent relative sensitivity path to FOM. \*\*Referee Rig shows some sensitivity to the dist. curve. 64 EAR 99 – Non-Proprietary

### HON Rig Shows No Significant Dependence on DCN

The 'worst' behaving category C fuel, C-1, behaved the 'best' at NJFCP LBO conditions.

Actual Values

-15

-20 -20

0.06

-15

0.08

-10

0.10

**Relative Importance** 

-5

Predicted Values

0.12

DCN

0.04

0.02

 $R^2 = 0.924$ 

5

0.14

10

0.16

0.18

Combustor Pressure, Pa Surface Tension (-10 °C), mN/m

> Air Temperature, °C 20% Recovered, °C 50% Recovered, °C Density (15 °C), kg/m3 Total Aromatics 10% Recovered. °C

MW\_Average, g/mole 90% Recovered, °C

Hydrogen Content, % Mass

Viscosity (-20 °C), mm<sup>2</sup>/s

Flash Point. °C

Freezing Point, °C

Smoke Point, mm End Point, °C  $\Delta$ H C, MJ/kg

Total iso-Paraffins

Total n-Paraffins

Total Cycloparaffins

Initial boiling point, °C

Radical Index

TSI

DCN

0.00



Thermo and physical properties dominate the HON regression.

## **Current HON LBO 'Path'**



\*Arrows represent relative sensitivity path to FOM.

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# **NJFCP: Major Impacts**

Collectively, technical advances will help streamline the ASTM alt. fuel certification process by reducing fuel, time, and cost required consistent with the OEM documented benefits of the program.

- Need for setting DCN limits for new fuels in ASTM approval
- Recommendation for a new test procedure (tbd) for measuring intermediate (pyrolysis) product species; ethylene is first priority.
- Method of recommending blending ratios of new fuel and petroleum fuels (still needs to be quantified)
- Greater understanding of the various chemical groups on combustion behavior – better ability to tailor new fuels that may not qualify initially
- Creation of new rig and spray test facilities available for ASTM testing
- Once matured, the CFD codes will allow fuel sensitive predictions with OEM hardware, further streamlining the process.