Use of Hydrocarbon-based Alternative Fuels in Gas Turbine Applications

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USAF SBIR Contract # FA8650-09-C-2009
USAF SBIR Contract #

ISSI Subcontract # SB05010 in support of
Prime Air Force Contract # F33615-03-D-2329 DO 0002

14th ISRAELI SYMPOSIUM ON JET ENGINES & GAS TURBINES
NOVEMBER 5 2015

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Background and Motivation

- Alternatives to petroleum-based fuels are of interest to the aviation and power generation industry , adding another layer of complexity from a combustion behavior and fuel modeling standpoint.
- Alternative jet fuels need to be “drop-in” ready – i.e. function without modifications to the engine components while not affecting engine performance (emissions, stability etc.)
- Alternative fuels for power generation should not affect pollutant emissions (NOx, CO, particulates) while not greatly affecting engine maintenance schedules
- Examples of alternative jet fuels include:
  - Hydrotreated Renewable Jet Fuel (HRJ)
  - Fischer-Tropsch Fuels (F-T Fuels)
    - E.g. SPK, IPK, S-8

Background and Motivation

- A more complete method to test the combustion and ignition of alternative fuels is to examine the behavior of the fuels across a range of oxidizer conditions.
- Jet fuel injected into turbine exhaust of aircraft engines results in combustion at vitiated conditions which represent more complex combustion regimes compared to standard air.
- Exhaust gas recirculation (EGR) is being examined as a way to control emissions in power generation applications
- Vitiated air in this study is defined as:
  - oxidizer stream with reduced O_2 concentrations typically due to EGR or operation as secondary combustion devices
  - O_2 concentrations as low as 12 – 18 vol% as well as the presence of combustion products including H_2O, CO_2, CO, and NO_x

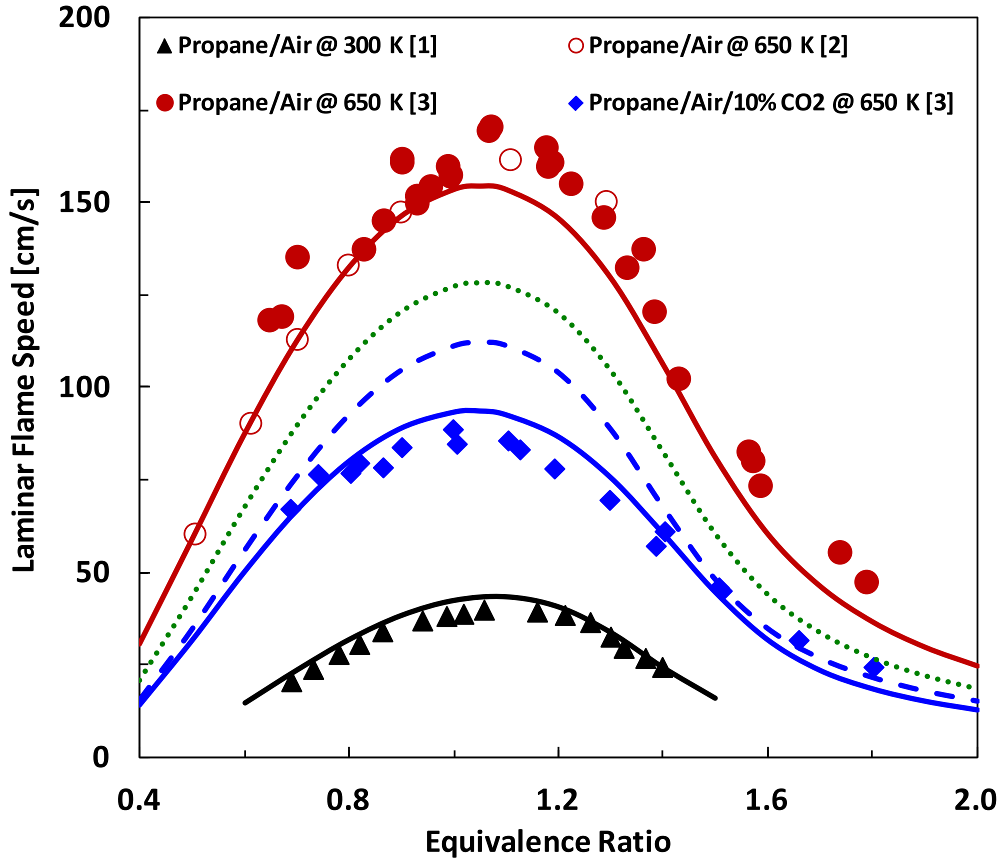
Background and Motivation

- Experimental work has shown that vitiation causes significant variations to combustion processes including
  - flame propagation
  - ignition
  - extinction
  - emissions
- There are limited experimental data available for combustion of liquid hydrocarbon fuels under vitiated conditions
- The focus of this effort is on the ignition behavior of petroleum based JP-8 and its alternatives at low-pressure vitiated conditions.
- The data obtained from this effort will be used to further develop kinetic models for surrogate fuels under normal air and vitiated combustion conditions.

Effect of Vitiation on Flame Speed

- Vitiation has been shown to have significant effects on flame propagation.
- Effects have been found to be based on the thermodynamics and the kinetics of the diluent species present in vitiated air.
- In the case of CO_2, its presence in propane/air flames reduced flame speed to a greater degree than would be expected based solely on its thermodynamic properties.

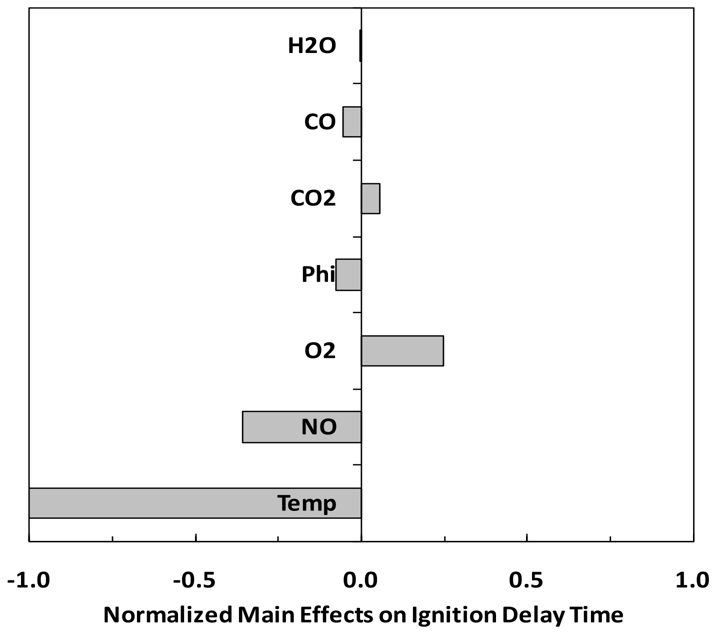
Figure adapted from Gokulakrishnan et al. 2014

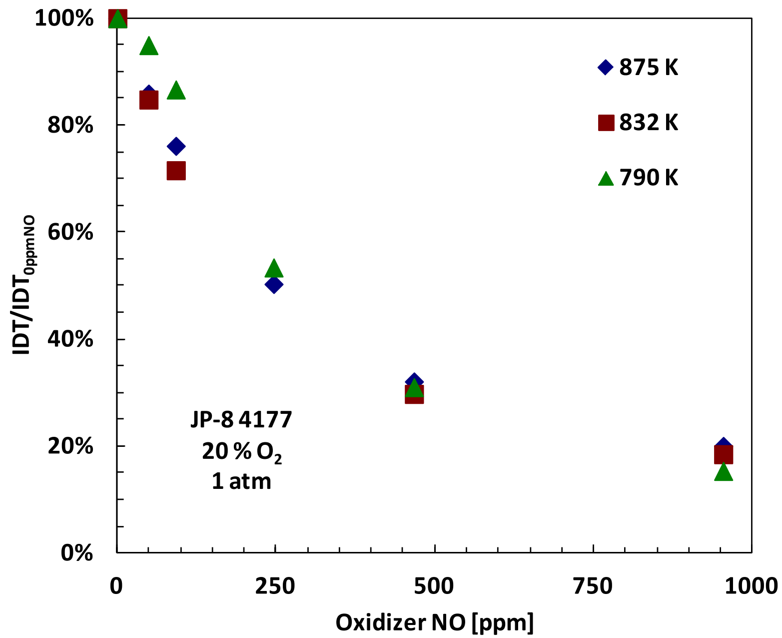


Solid Lines: Full Kinetic Model
Dashed Line: Kinetically inert CO_2 added to vitiated air
Dotted Line: 10% N_2 dilution

[1] Zhao et al. (2004); [2] Vagelopoulos and Egolfopoulos (1998); [3] Fuller et al. (2012)

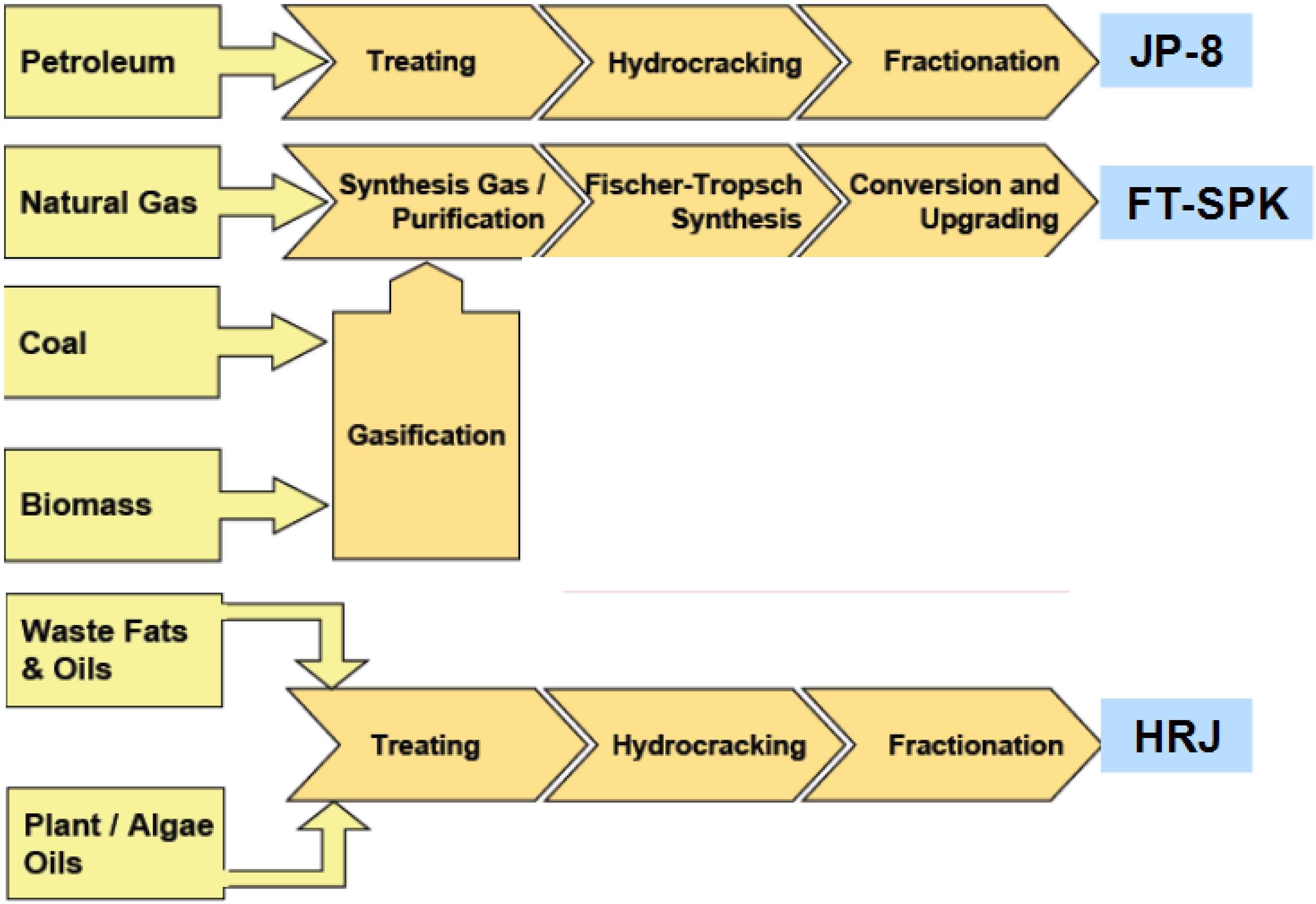
Effect of Vitiation on Ignition



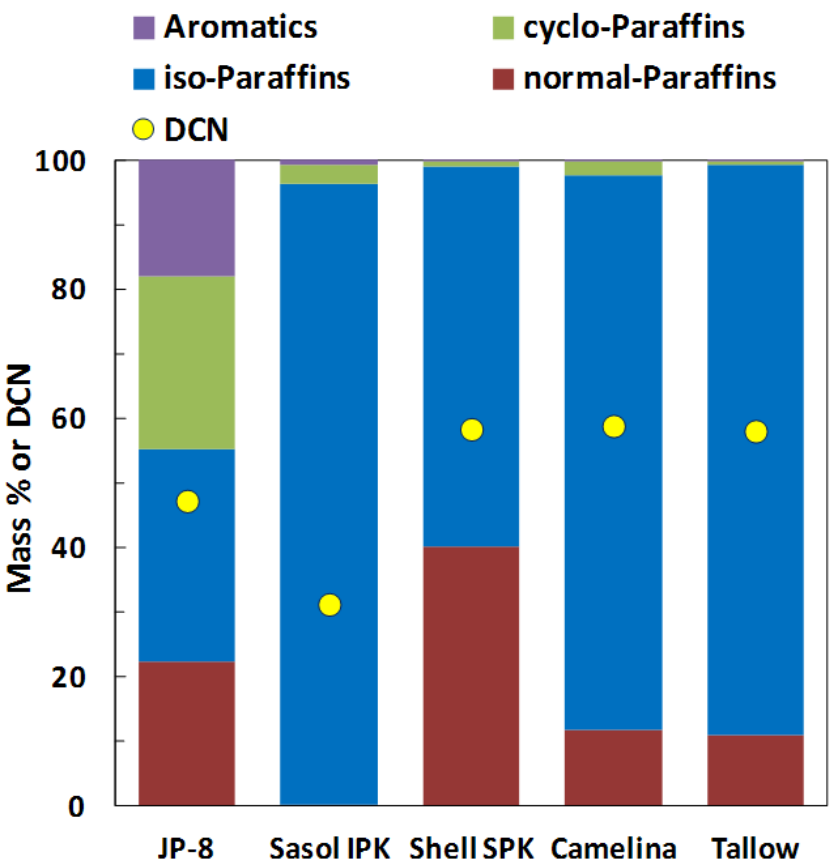


- Previous effort [Fuller et al. 2011] examined the effects of vitiation on ignition delay time of JP-8
- Temperature, O_2 and NO_x were found to have significant effect on the induction chemistry of jet fuels.
- Presence of NO_x specifically reduces ignition delay time quite significantly when it is introduced to the oxidizer stream in relatively small quantities (50 - 1000 ppm)

Alternative Jet Fuels: FT-SPK and HRJ



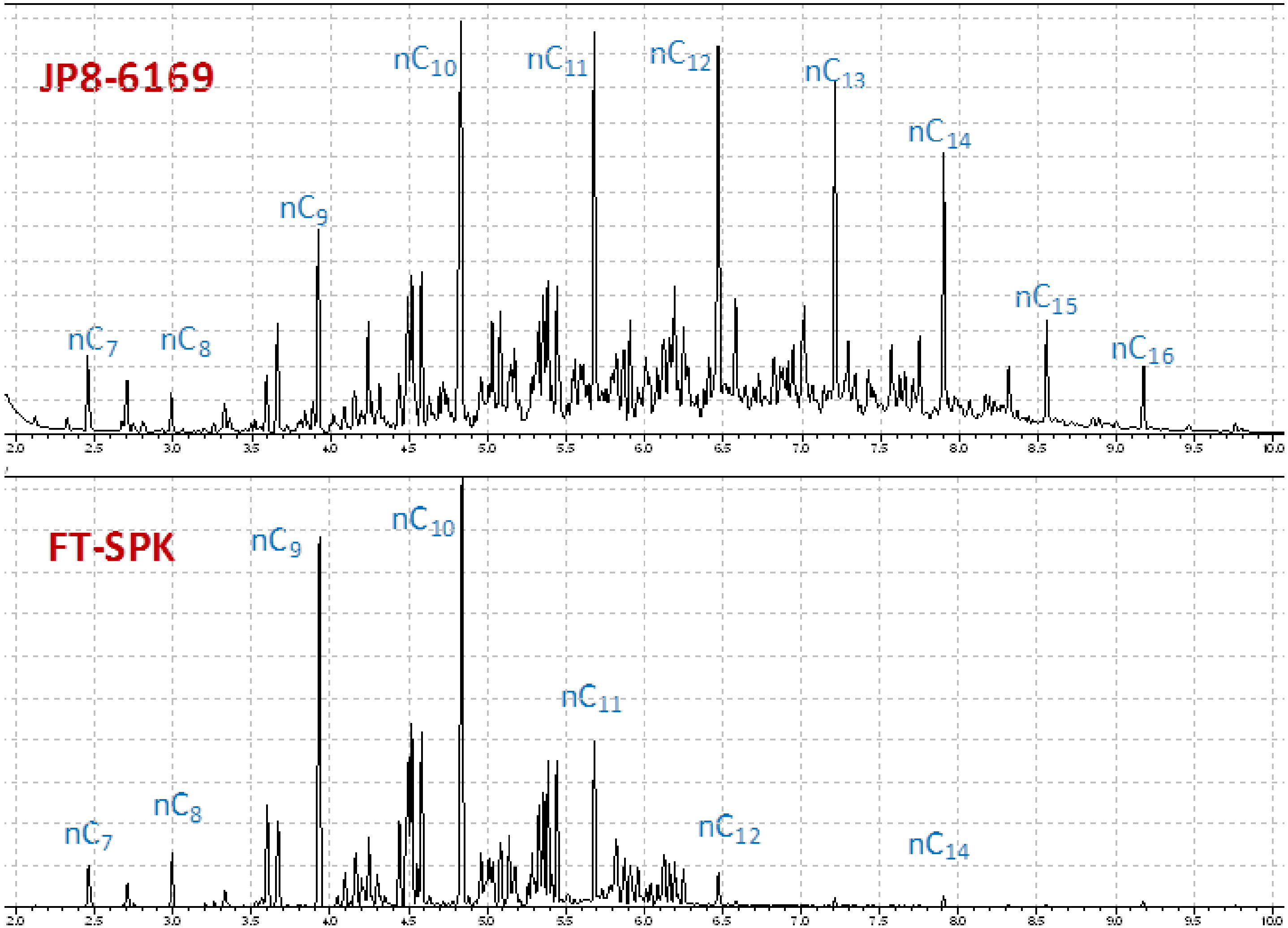
Alternative Jet Fuels



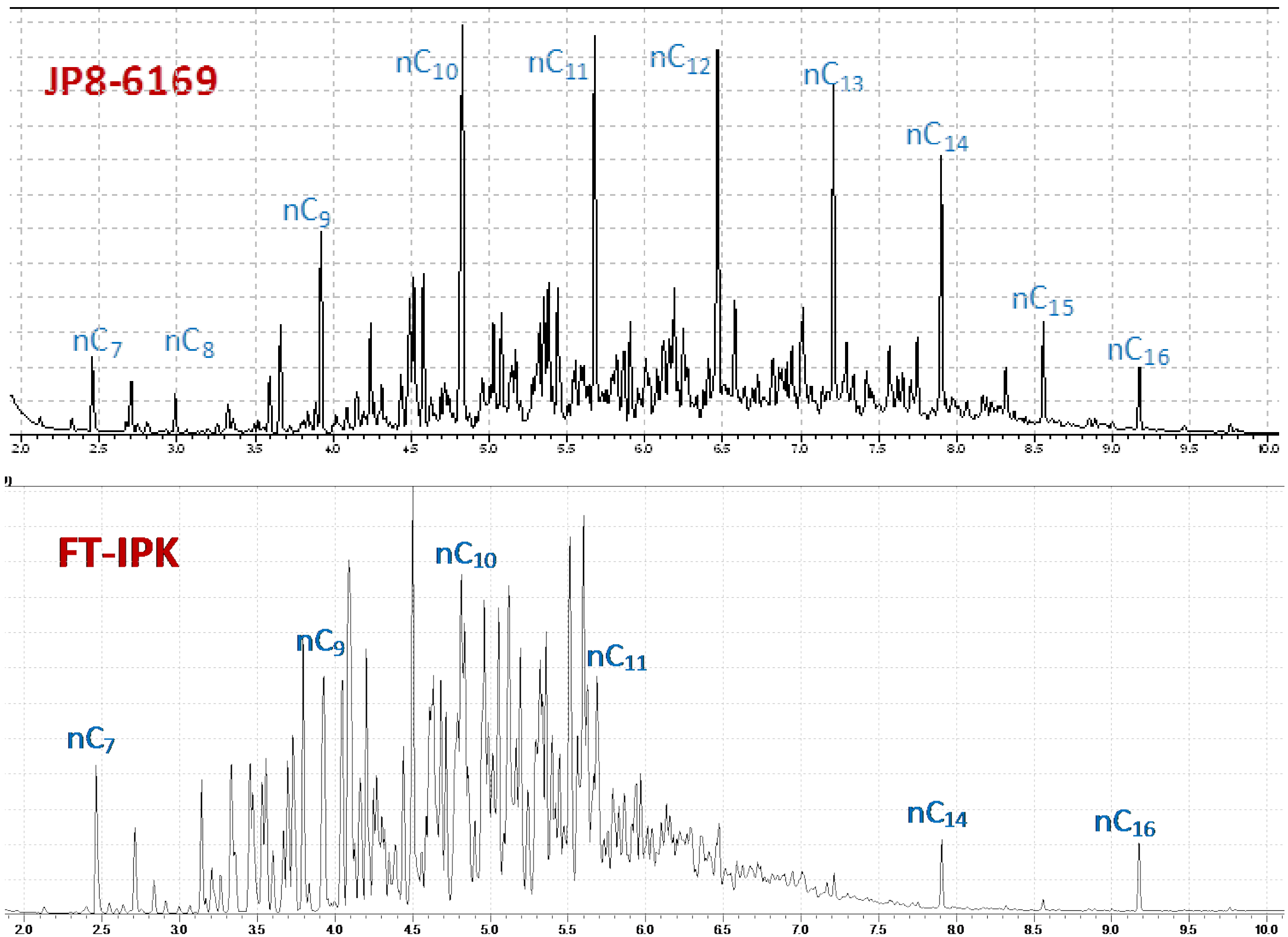
- Current study examined 5 separate fuels:
  - JP-8 6169
  - F-T: Sasol IPK 7629
  - Shell SPK 5729
  - HRJ: Camelina 7720
  - Tallow 6308
- Compositions and combustion characteristics of the fuel properties varied significantly.
- Alternative fuels lack aromatic and cyclo-paraffinic content found in JP-8 but are comprised of larger quantities of iso-paraffins

Fuel data provided by Tim Edwards (AFRL) and Won et al. (AIAA 2013-0156)

GC-MS Chromatography: JP8 vs FT Fuels



GC-MS Chromatography: JP8 vs FT Fuels



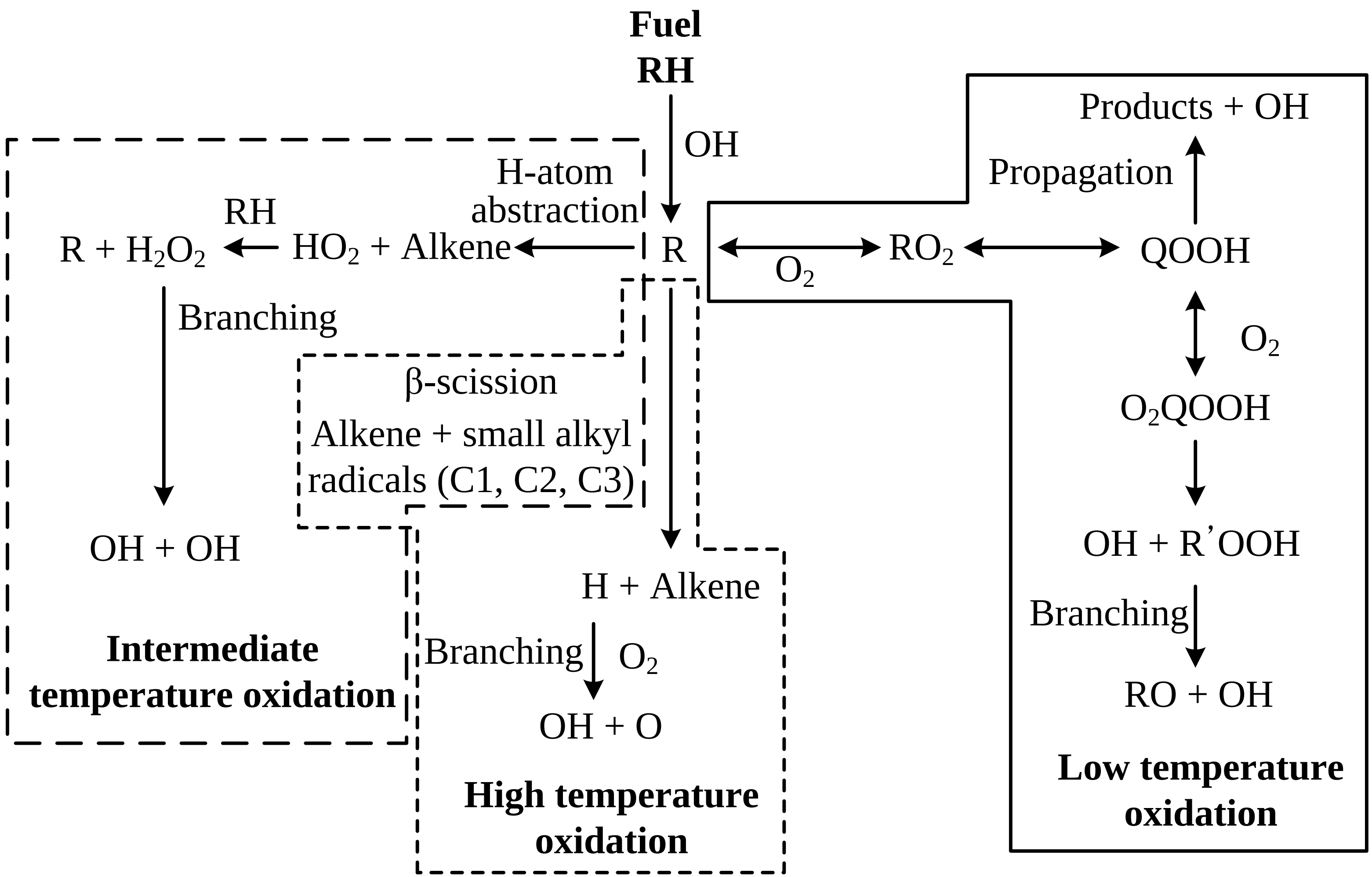
Jet Fuel Surrogate Kinetic Model

- CSE detailed surrogate kinetic model consists of four components to represent chemical groups found in jet fuels
  - n-paraffins: n-Dodecane/n-Decane
  - Iso-paraffins: iso-Octane
  - Aromatics: n-propyl-Benzene
- The surrogate model was validated for a wide range of conditions using kinetic experimental data for ignition delay time, flame speed and species profiles
- The kinetic mechanism also includes detailed nitrogen chemistry for vitiation and NOx emission predictions
- Surrogate mixture formulation is based on three target criteria:
  - Hydrogen-Carbon Ratio (H/C)
  - Derived Cetane Number (DCN)
  - Threshold Sooting Index (TSI)

Alternative JP-8 Surrogate Mixtures

Surrogate	**JP-8 6169**	**IPK 7629**	**SPK 5729**	**Tal 6308**	**Cam 7720**
n-Dodecane	0.382	0.160	0.045	0.595	0.611
n-Decane	0.000	0.000	0.746	0.000	0.000
iso-Octane	0.372	0.647	0.122	0.315	0.292
propyl-Benzene	0.246	0.193	0.087	0.090	0.096
Surrogate Mixture Properties (CSE Calculations)					
DCN	48.1	31.8	58.2	59.0	60.0
TSI	18.25	15.74	9.11	11.09	11.38
H-C Ratio	2.003	2.052	2.134	2.122	2.117
MW	137.1	124.3	138.2	148.1	149.1
Target Fuel Properties (Princeton Measurements)					
DCN	47.3	31.3	58.4	58.1	58.9
TSI	19.29	17.28	9.11	11.58	11.99
H-C Ratio	2.017	2.195	2.237	2.176	2.202
MW	153.9	149.2	136.7	161.0	165.0

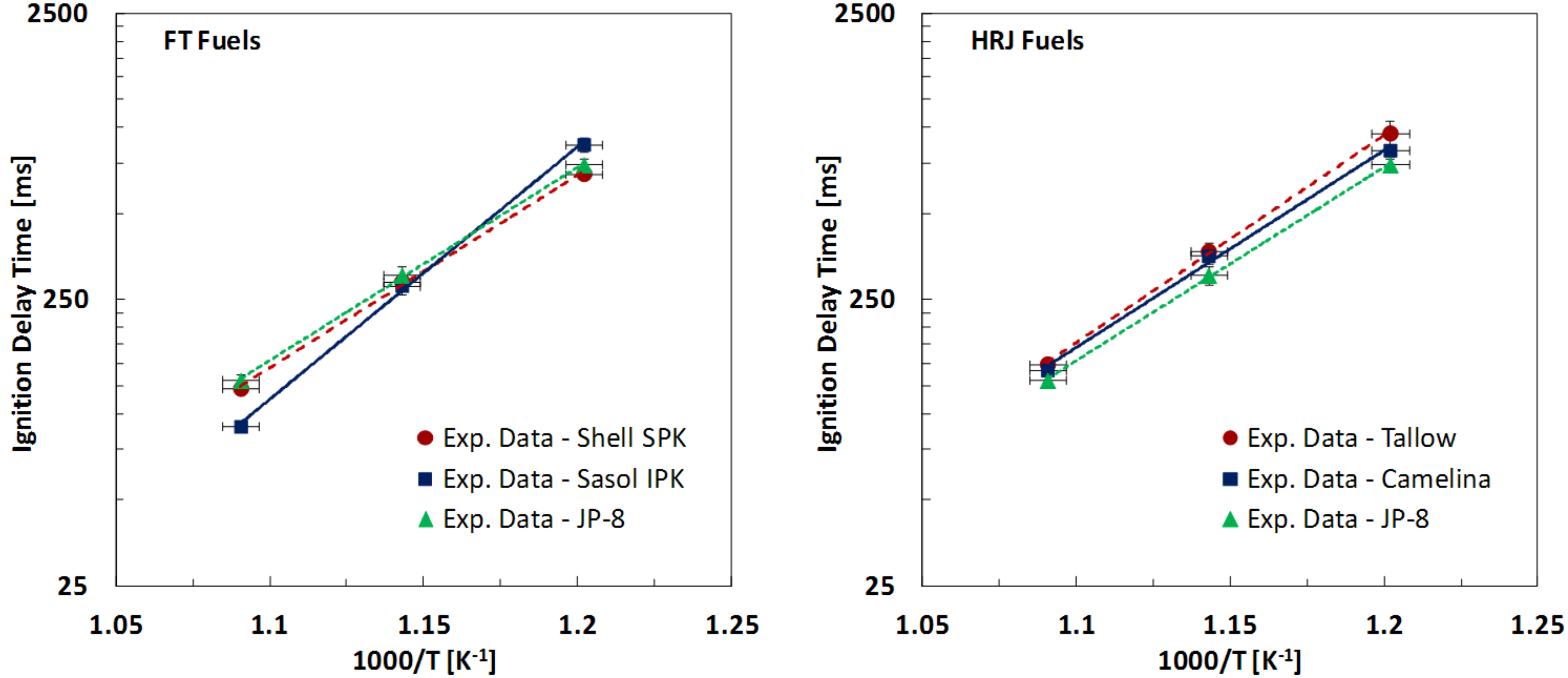
Hydrocarbon Oxidation Pathways



Experimental Conditions and Setup

- Pressure
  - 1 atm
- Temperature
  - 832 K, 875 K, & 917 K
- Equivalence Ratio
  - 0.5, 1.0, & 1.5
- Fuel:
  - JP-8, IPK, SPK, Camelina & Tallow
- Oxidizer Composition:
  - O_2: 17 mol% & 20 mol%
  - NO_x: 0 ppmv – 755 ppmv

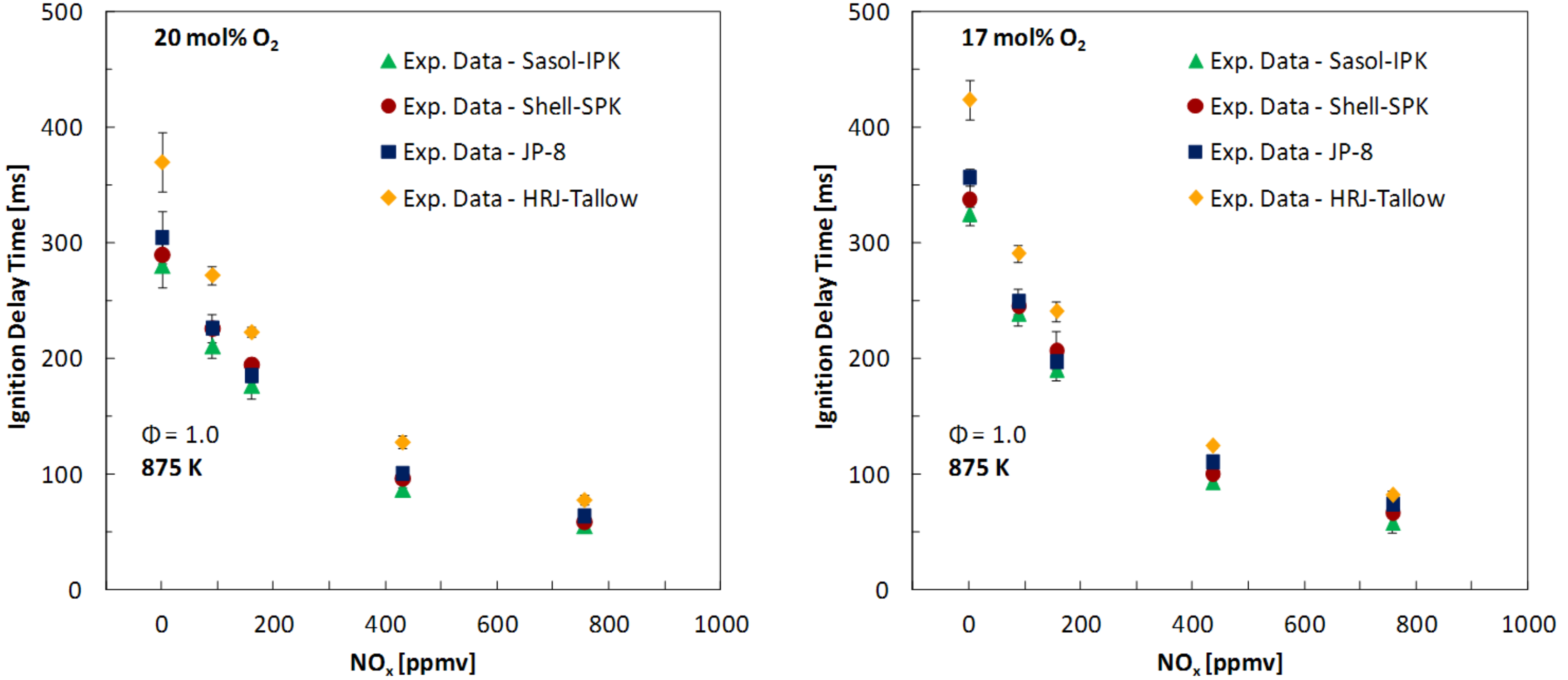
Ignition Delay Time w/out Vitiation



Experimental Activation Energies (832 – 917 K)

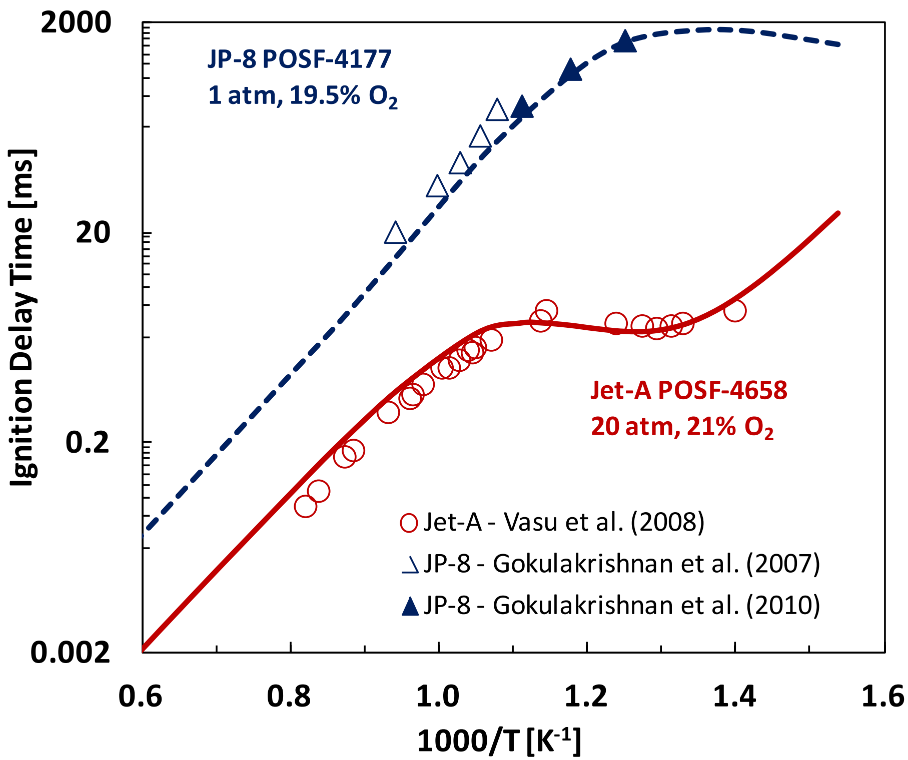
Fuel	E [kcal/mol]	DCN
JP-8	30.90	47.3
Sasol IPK	40.40	31.3
Shell SPK	30.78	58.4
Camelina	31.49	58.9
Tallow	33.11	58.1

Alternative Fuel Ignition w/ NO_x



- Variation in IDT between the fuels reduces with increased NO_x
- Sasol IPK has shorter IDT despite having the lowest DCN
- HRJ Tallow has longer IDT while DCN is higher than JP-8 and Sasol IPK
- The marginal effect on IDT diminishes with an asymptotic behavior as NO_x concentration approaches 800 ppm

Surrogate Model Development



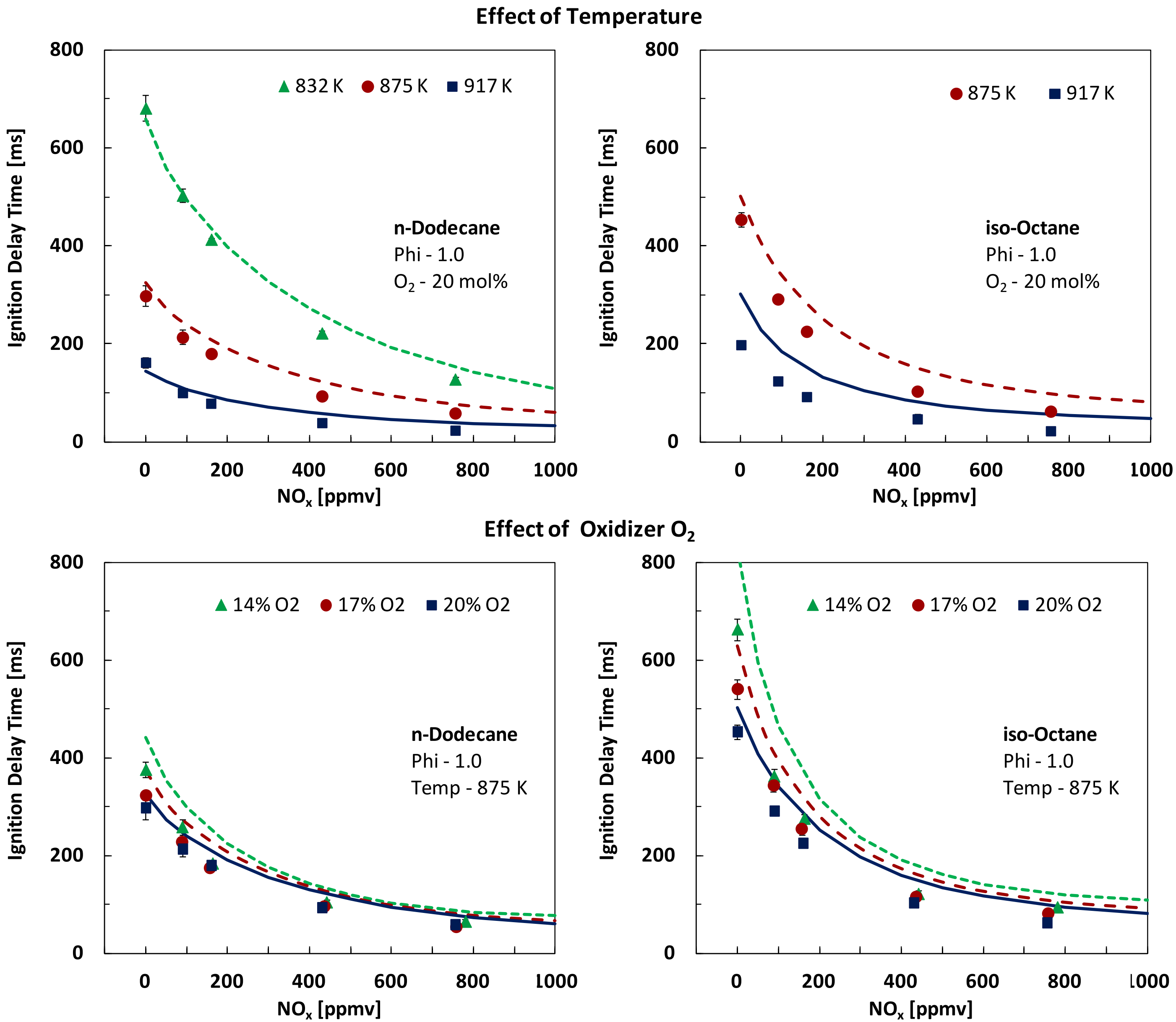
- CSE jet fuel surrogate kinetic model is a four-component surrogate kinetic model validated for each individual component.
- n-Paraffins:
  - n-decane & n-dodecane
- iso-Paraffins:
  - iso-octane
- Aromatics:
  - n-propyl-benzene
- For Jet-A and JP-8 mixtures the surrogate model predicts ignition delay time reasonably well but requires development for alternative fuels and vitiated combustion

Surrogate Model Composition

- Surrogate mixture compositions are determined by matching the following target characteristics (Dooley et al., 2010) :
  - hydrogen-to-carbon ratio (H/C)
  - derived cetane number (DCN)
  - threshold sooting index (TSI)
  - mean molecular weight (MW)
- Surrogate mixture compositions (mol %) for the fuels examined in this study are provided below:

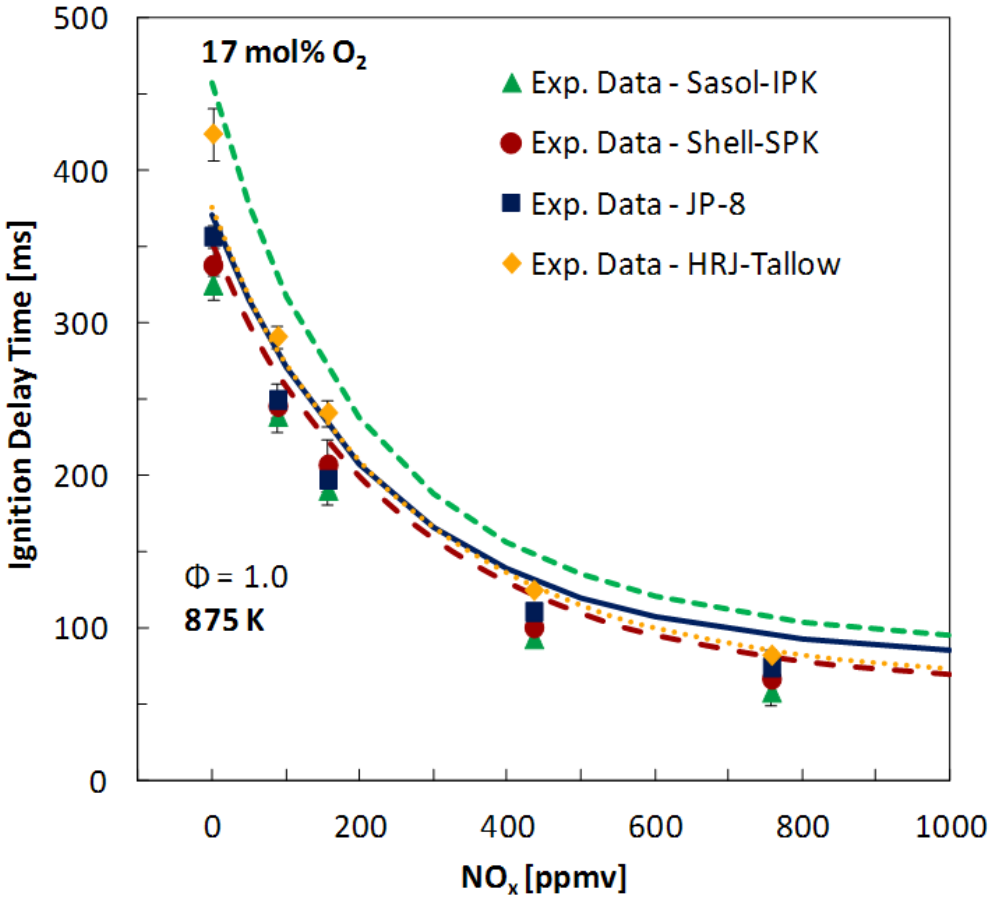
Surrogate	JP-8	Sasol IPK	Shell SPK	HRJ Camel.	HRJ Tallow
n-decane	0.0	0.0	74.6	0.0	0.0
n-dodecane	38.2	16.0	4.5	61.1	59.5
iso-octane	37.2	64.7	12.2	29.2	31.5
propyl-benzene	24.6	19.3	8.7	9.6	9.0

Surrogate Component Experiments

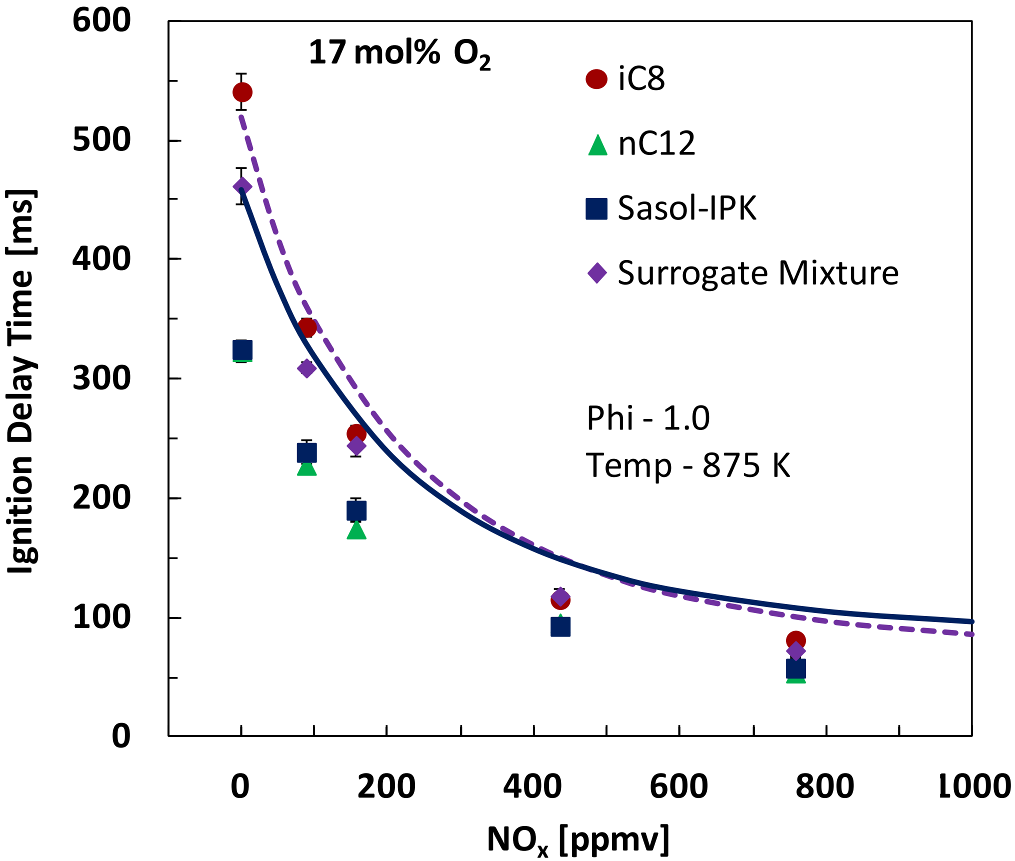


Surrogate Model Comparison

- Overall the model predicts effect of NO_x on IDT for JP-8, SPK and HRJ Tallow reasonably well.
- The model does not predict IDT well for the Sasol IPK fuel.
- Sasol IPK: ~95% iso-paraffins with the lowest DCN
- Current model uses highly-branched iso-octane to model iso-paraffinic fuel components



Sasol IPK Surrogate Mixtures



- 2-component surrogate for IPK, comprised of 82 mol % iso-octane and 18 mol % n-dodecane (DCN = 31) , was tested in the flow reactor
- Model predicts IDT of the iC_8 /nC_{12} mixture significantly better than the it does for the IPK fuel
- Work in progress to investigate weakly-branched iso-paraffinic fuels to improve the surrogate model

Modeling of Jet Fuel-NO_x Kinetics

- NO_x promotes oxidation in the low- and intermediate-temperature regimes through fuel independent and fuel dependent pathways
- Major fuel-independent reaction pathways of NO_x on jet fuel oxidation promotes OH radical production:
  - $HO_2 + NO = NO_2 + OH$
- Fuel dependent reactions involve NO_2 to form alkyl radicals and HONO/HNO_2 and eventually NO and OH:
  - $C_xH_y + NO_2 = C_xH_{y-1} + HONO/HNO_2$
  - $HNO_2 + M = HONO + M$
  - $HONO + M = NO + OH + M$
- Fuel dependent HC-NO_x interaction is relatively better understood for natural gas surrogate fuels (Gokulakrishnan et al. CNF 2014) than gasoline or jet fuels.

Lean, Premixed Prevaporized Combustion

- Ground-based power production is highly regulated for pollution emissions (NOx, CO, particulates)
  - Lean, Premixed combustion allows for control of flame temperature
  - Lower flame temperature reduces NOx production and minimizes soot production
- Typical Lean, Premixed Gas Turbines burn natural gas
- Many locations do not have access to low-cost natural gas
  - Need pipeline infrastructure to move natural gas from wells to users
  - Liquified natural gas (LNG) requires significant processing , adding expense
  - Liquid fuels typically have higher energy density and are easier to transport
- Techniques for 'clean' combustion of liquid fuels are needed

LPP Combustion Concept

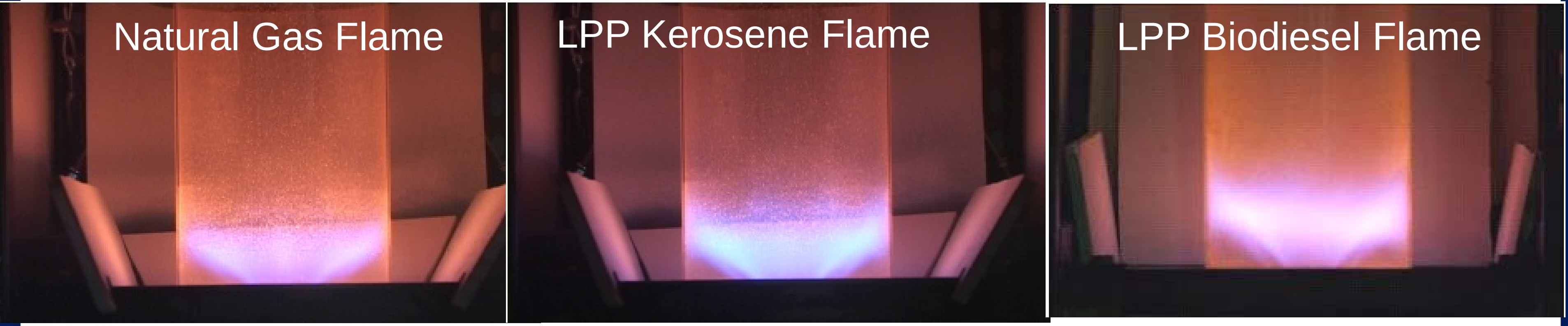
LPP = Lean, Premixed & Prevaporized

- LPP Skid converts liquid fuel into a substitute natural gas (LPP Gas) by vaporizing the liquid fuel into a reduced-oxygen background gas (diluent).
- LPP Gas properties adjusted with choice/quantity of diluent to match natural gas characteristics (heating value, Modified Wobbe Index, etc.)
- LPP Gas is burned with low emissions in place of natural gas in combustion device.
- Burning renewable liquid fuels (biodiesel, ethanol, etc.) creates a low-emissions, renewable energy power plant with no net CO_2 emissions.

Combustor Technology Review

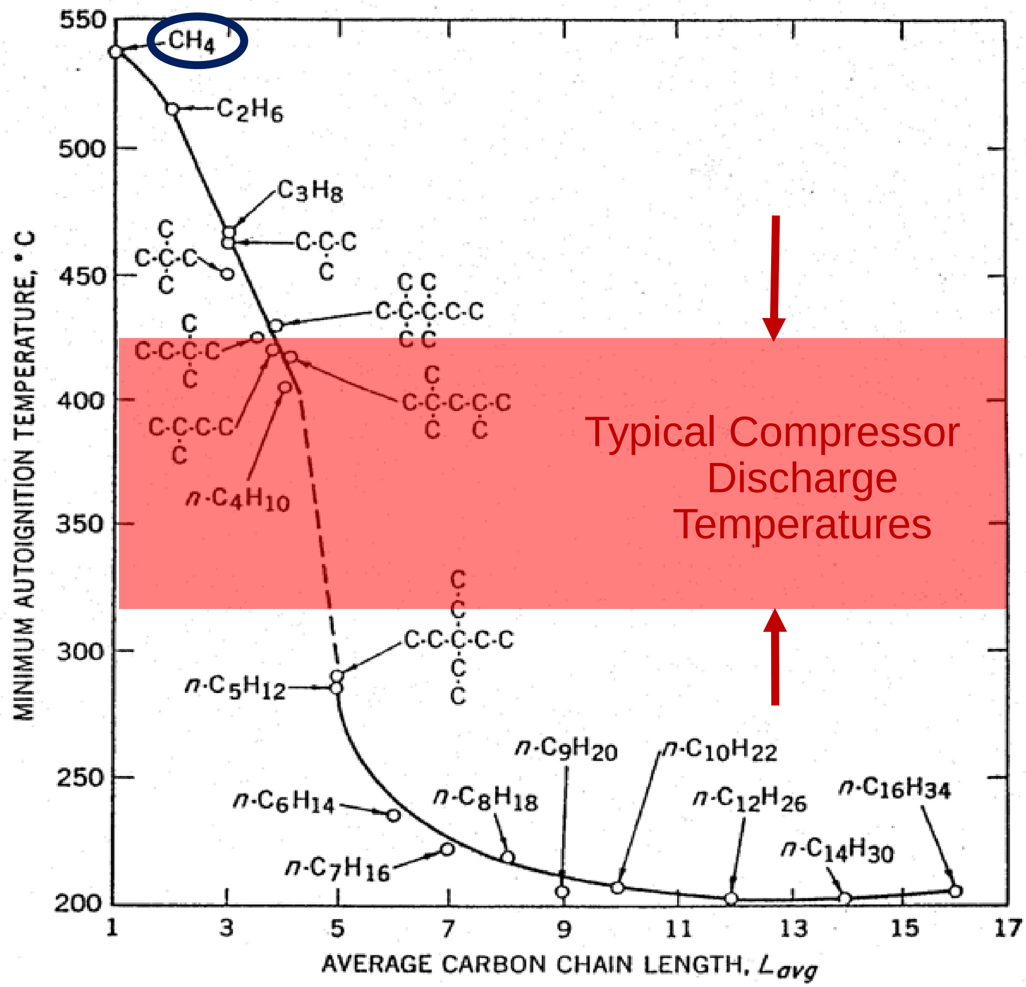
Traditional Combustion of Liquid Fuels in a Spray (Diffusion) Flame Creates High Levels of NOx, CO and Particulate Matter, even with Significant Water Injection to Reduce Emissions.

Gaseous Fuel Combustion (with Natural Gas or LPP Gas) in a Lean, Premixed Burner Creates a Low-Emissions Combustion



Fuel Autoignition Characteristics

Autoignition becomes a problem for higher hydrocarbons, at higher inlet temperatures, where it is not a problem for natural gas



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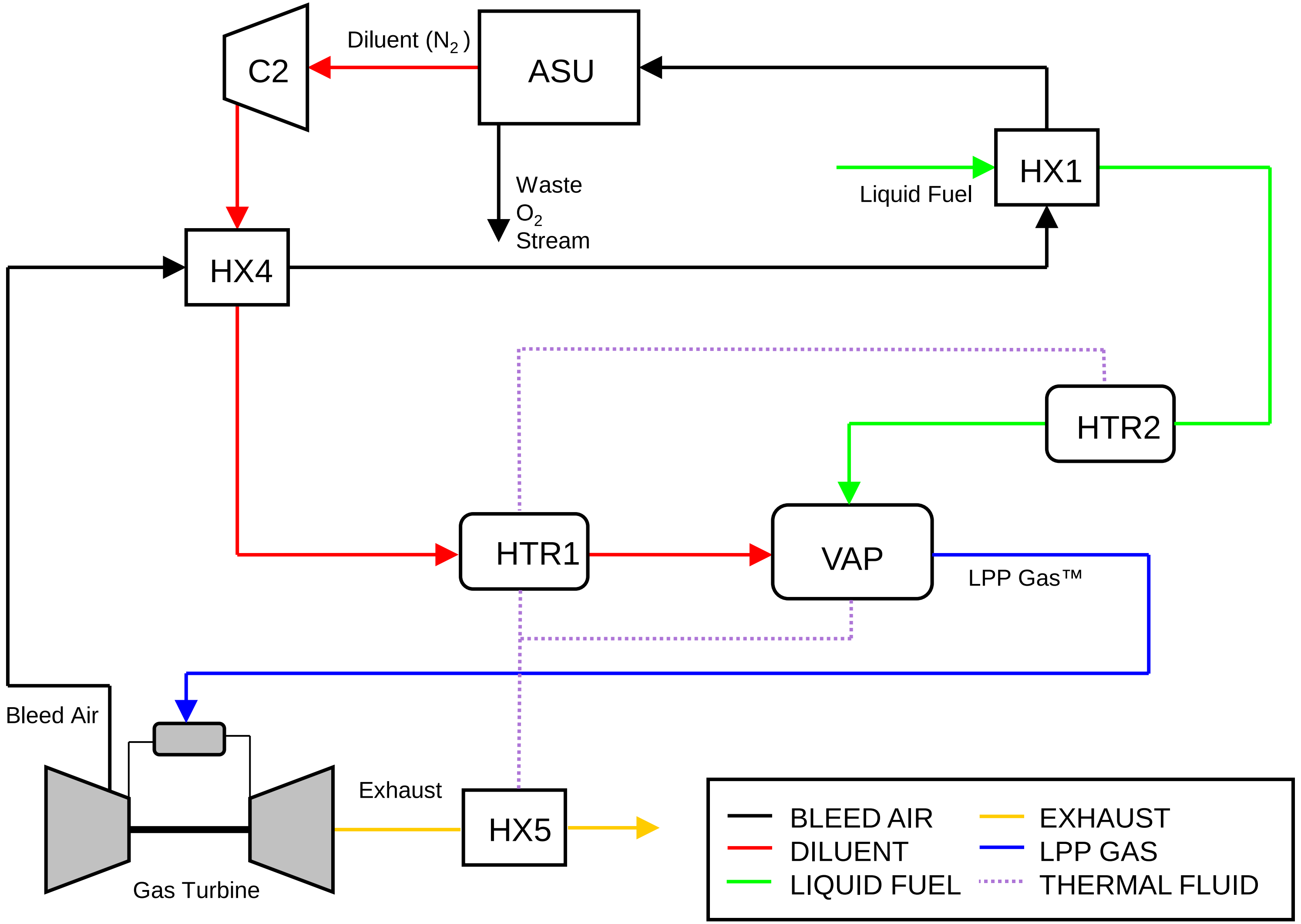
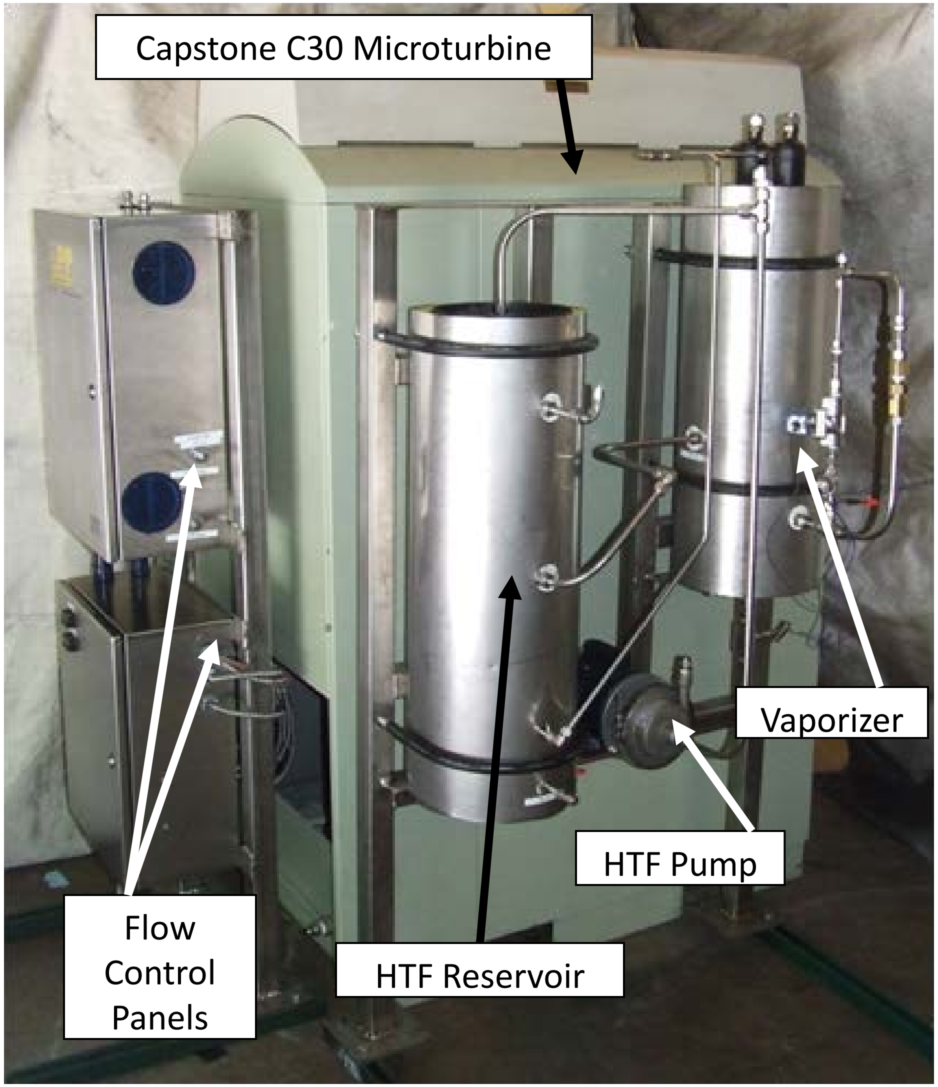
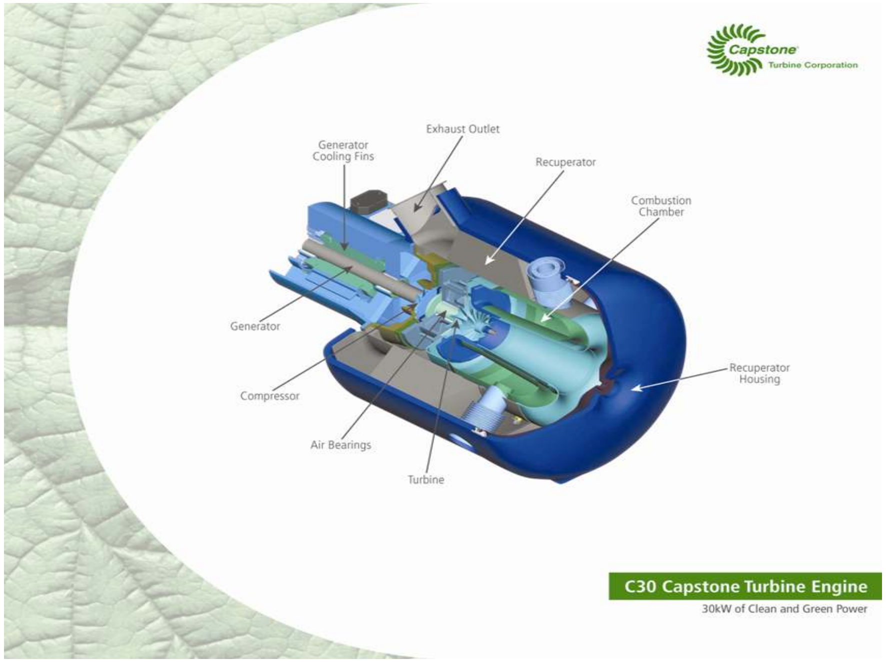
Gas Turbine/LPP Process Flow Diagram

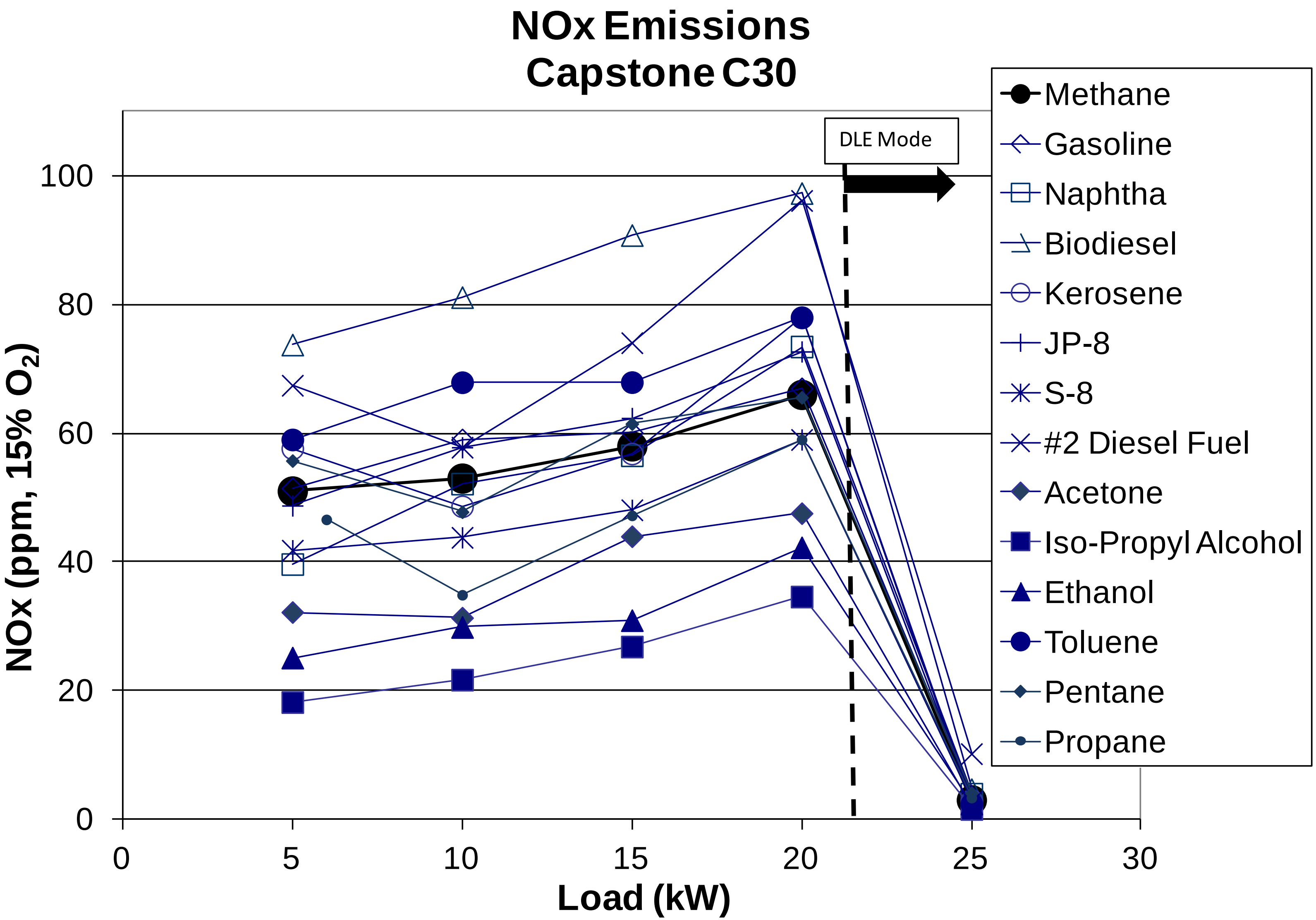


Demonstration Unit

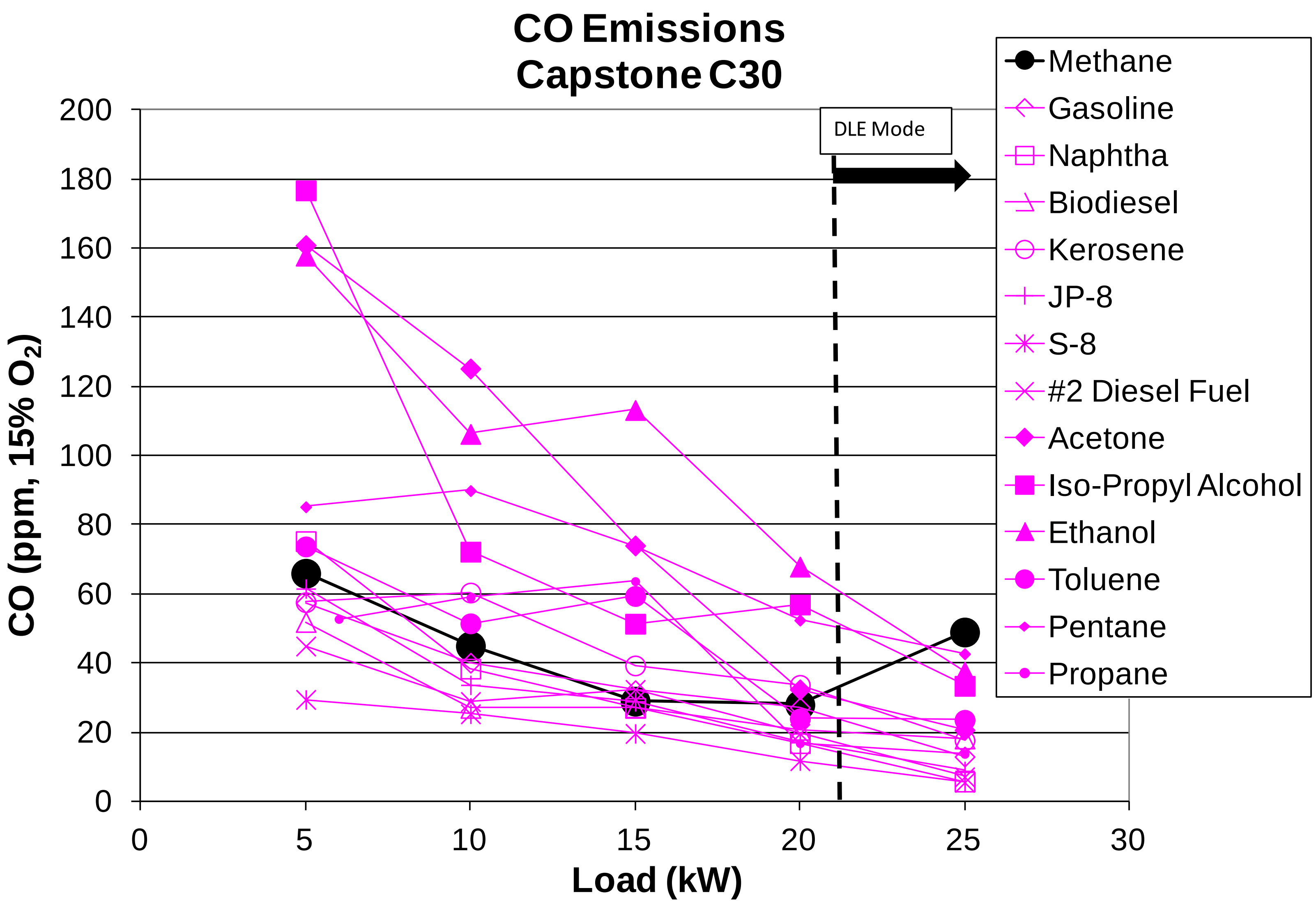




Premixed Combustion of Liquid Fuels



Premixed Combustion of Liquid Fuels



Conclusions

- Alternative fuels are viable ‘drop-in’ replacements for jet engines
- Differences in chemical composition can alter the combustion behavior of these fuels under both standard and vitiated conditions
- Current 4-component surrogate model predicts IDT for JP-8 and certain alternative fuels at the experimental conditions of this study with reasonable accuracy
- Vitiated combustion aspects of the model, specifically NO_x chemistry, are found to predict the enhancement of ignition, accounting for the change of reaction pathways in the low- and intermediate-temperature regimes
- Lean, Premixed, Prevaporized combustion is a viable option for burning alternative liquid fuels in gas turbines
  - Emissions are similar to those found for natural gas combustion
  - Wide-range of liquid fuels have been tested

Future Work

- Future research will focus on improvement of the surrogate model at both standard air and vitiated conditions including:
  - Inclusion of additional surrogate component(s) to represent larger, less-branched iso-paraffins
  - Investigation of additional target criteria to improve surrogate formulation

Acknowledgements

- U.S. Air Force Research Laboratory
- Dr. Barry Kiel, Air Force Research Laboratory
- Bethany Huelskamp at ISSI
- Dr. Tim Edwards, Air Force Research Laboratory

Thank You

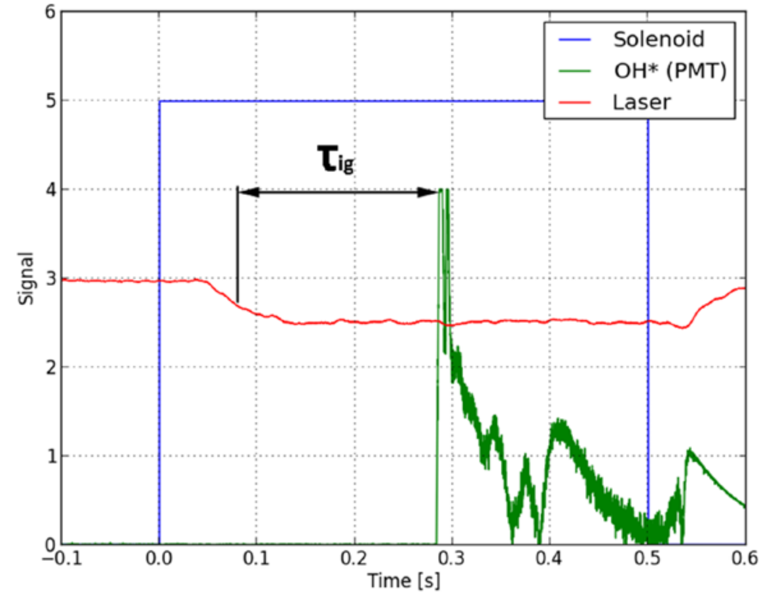
- Questions?

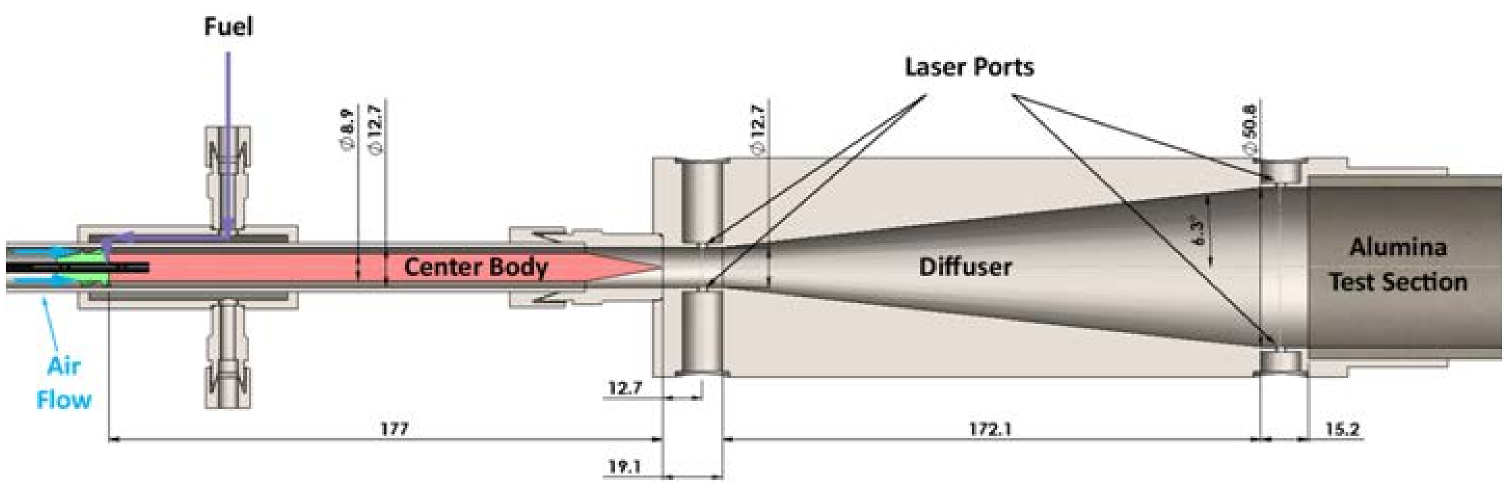
- Contact:
  - mklassen@csefire.com

Extra Slides

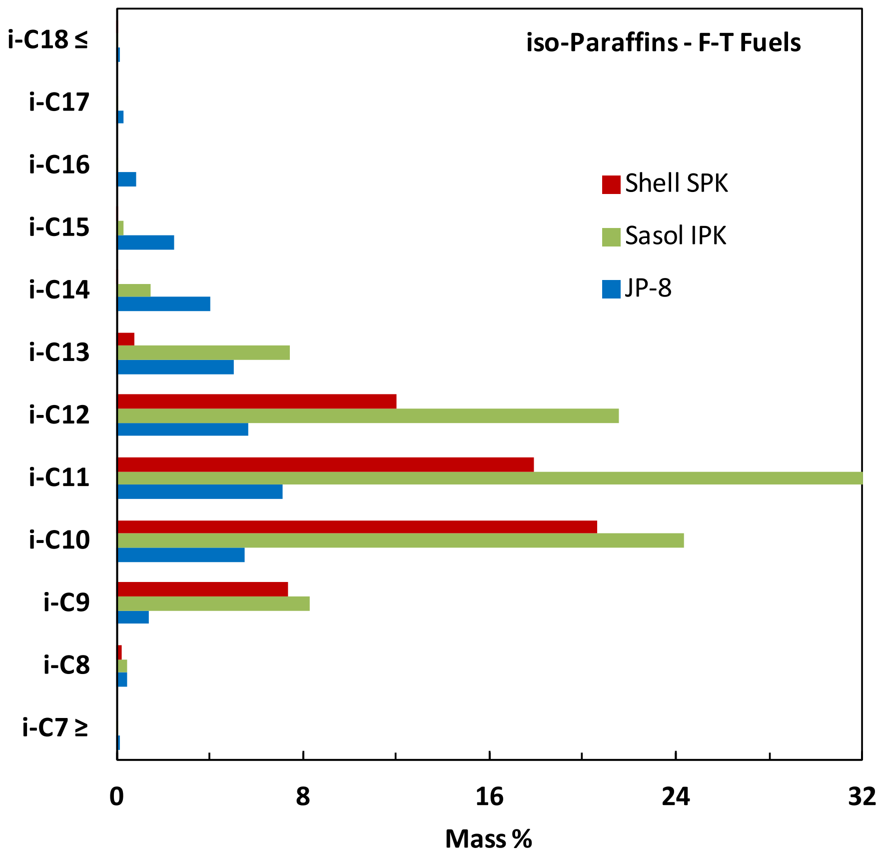
Ignition Delay Time Measurement

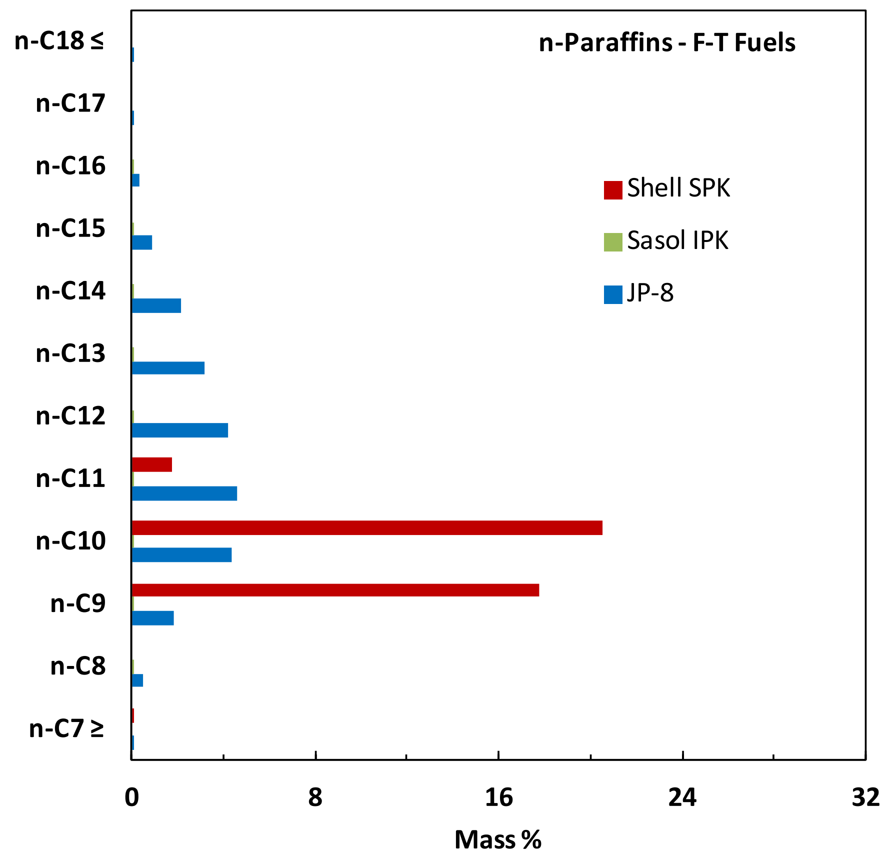
- Absorption of infrared HeNe beam (3.39 μm) by H-C bonds in the fuel/oxidizer mixture used to determine time delay between solenoid activation and fuel injection into the reactor
- OH* excitation measured by PMT equipped with 310 (± 5) nm band pass filter to determine ignition event
- IDT (τ_{ig}) measured as the time difference between initial PMT excitation and 50% reduction in the HeNe laser signal at the diffuser entrance





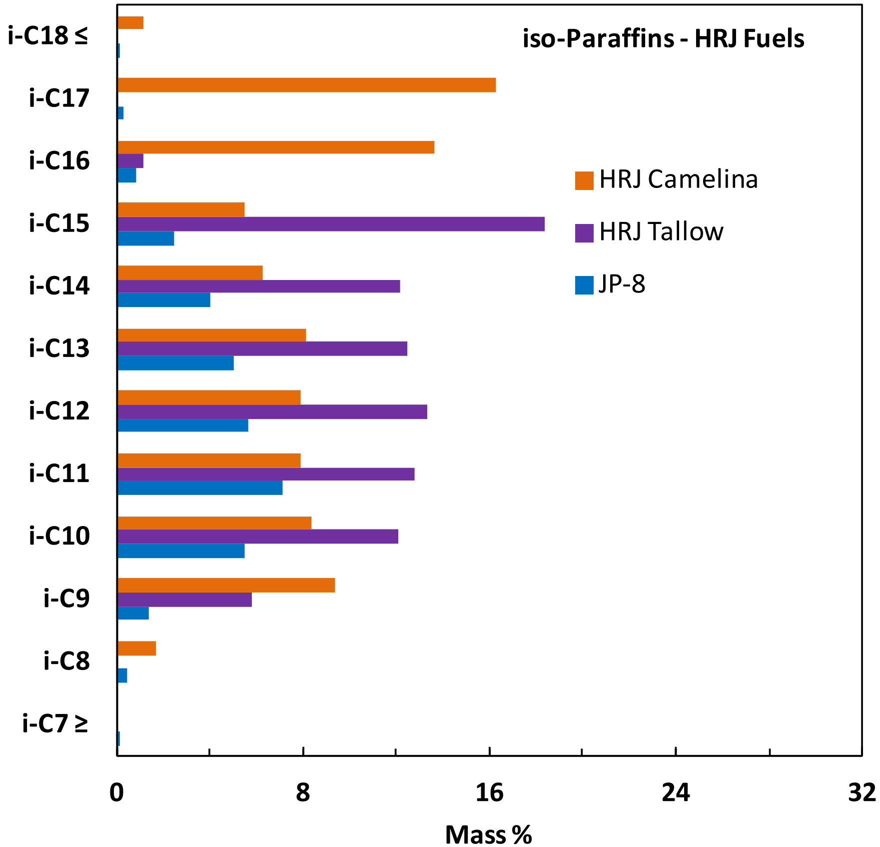
JP-8 & Fischer-Tropsch Fuel Comparisons

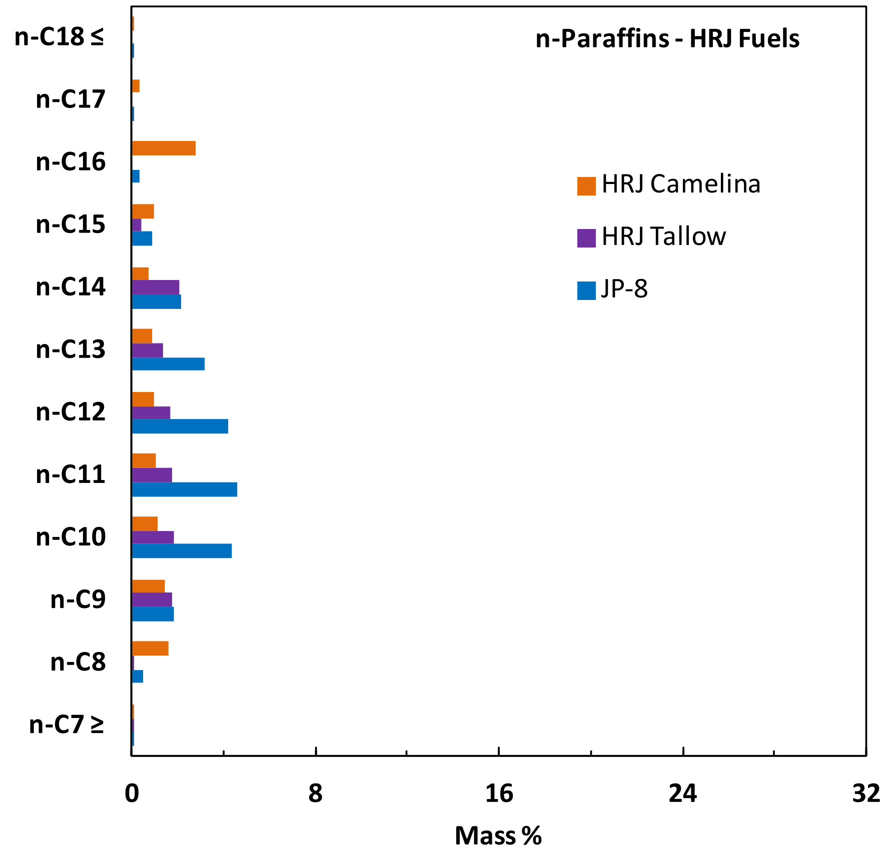




Data provided by Tim Edwards (AFRL) 2014

JP-8 & Hydrotreated Fuel Comparisons





Data provided by Tim Edwards (AFRL) 2014

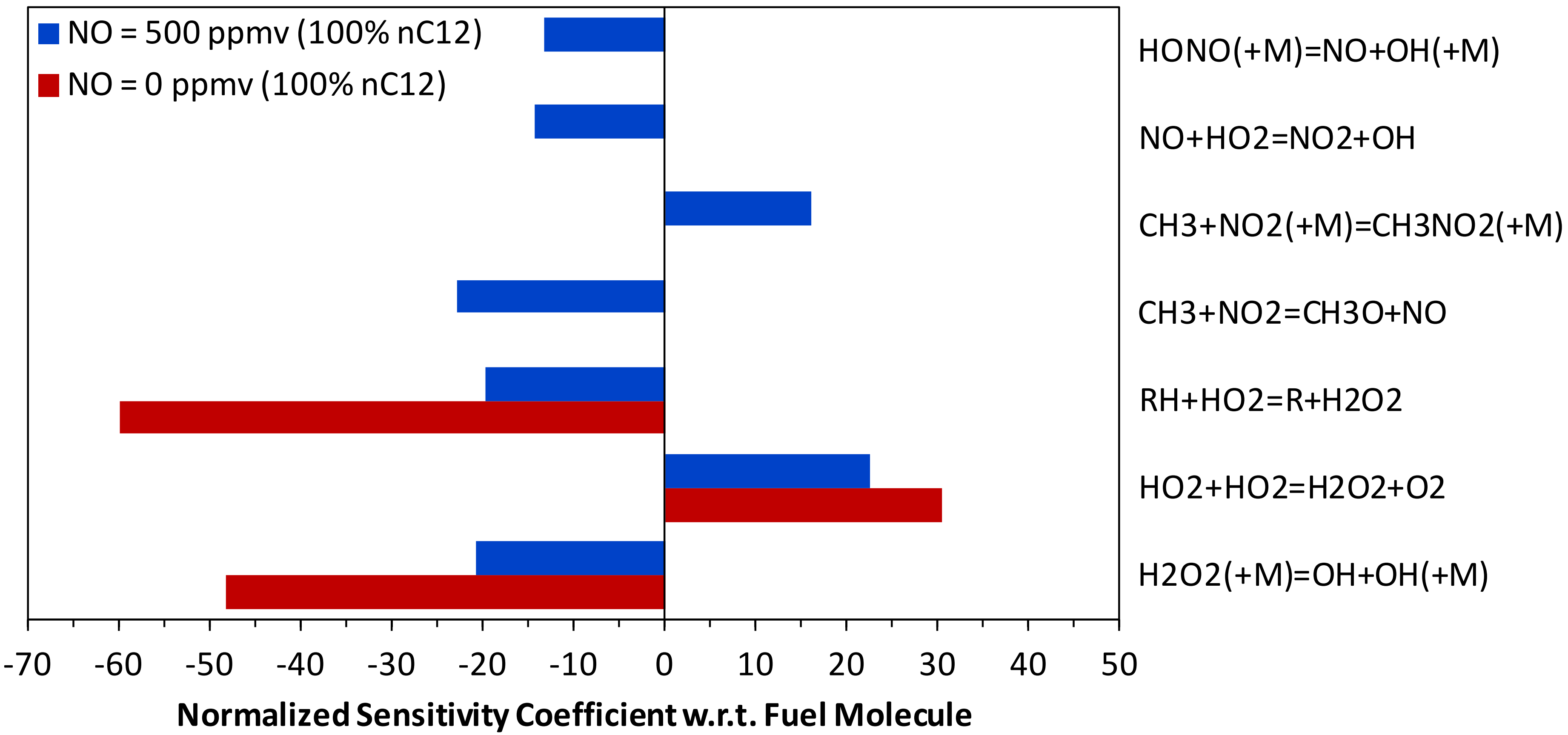
Jet Fuel Comparisons

- Five separate jet fuels were examined in this study:
  - Petroleum based: JP-8 6169
  - Fischer-Tropsch Fuels: Sasol IPK 7629 & Shell SPK 5729
  - Hydrotreated Renewable Jet Fuels: Camelina 7720 & Tallow 6308

Jet Fuel Type	Air Force POSF #	Density[a] [kg/m^3]	DCN[b]	TSI[b]	H/C Ratio[b]	MW[b] [g/mol]	Molecular Formula[b]
JP-8	6169	785	47.3	19.28	2.02	153.9	$C_{11.0}H_{22.1}$
F-T Sasol IPK	7629	739	31.3	17.28	2.20	149.2	$C_{10.5}H_{23.0}$
F-T Shell SPK	5729	730	58.4	9.11	2.24	136.7	$C_{9.6}H_{21.4}$
HRJ Camelina	7720	752	58.9	11.99	2.20	165.0	$C_{11.6}H_{25.5}$
HRJ Tallow	6308	748	58.1	11.58	2.18	161.0	$C_{11.3}H_{24.7}$

a – Edwards (2014); b – Won et al. (2013)

Reaction Sensitivity for NO_x Addition



Jet Fuel Chemical Class Composition