Generation of Comprehensive Surrogate Kinetic Models and Validation Databases for Simulating Large Molecular Weight Hydrocarbon Fuels

Principal Investigator: *Frederick L. Dryer*

Other Co-Investigators and Institutions:

Thomas A. Litzinger	*Penn State University (PSU)*
Robert J. Santoro	*Penn State University (PSU)*
Kenneth Brezinsky	*University of Illinois at Chicago (UIC)*
Chih-Jen Sung	*Case Western Reserve University (CWRU)*
Yiguang Ju	*Princeton University (PU)*

Visiting Researchers:

Henry J. Curran (NUI Galway)	*Princeton University (PU)*

Technical Management: *Dr. Julian Tishkoff, AFOSR*

2007 MURI Topic #12:Science-Based Design of Fuel-flexible Chemical Propulsion/Energy Conversion Systems

MULTI AGENCY COORDINATION COMMITTEE FOR COMBUSTION RESEARCH (MACCCR)
FUELS RESEARCH REVIEW
Los Angeles, CA
15-17 September 2009

MURI Purpose

Generate jet fuel surrogate component modeling concepts, cross-validated critical experimental data, detailed and reduced kinetic models, analytical tools and experimental methods to more accurately predict the complex gas phase combustion behavior of real fuels using mixtures of a small (minimal) number of chemical components.

- *Emulate gas phase, kinetic/transport coupled combustion properties for any specific real jet fuel*
- *Provide evolving tools/models as program progresses*
- *Provide foundation for additional refinements in future*
  - *Further refinement of target prediction accuracy*
  - *Additional kinetic property target inclusions*
  - *Consideration of fuel physical property targets*

Research Goals

- Validate novel principles to select surrogate components.
- Select and refine combustion target parameters to be matched.
- Validate methods and rules for formulating surrogate mixtures to replicate real fuel gas phase combustion properties.
- Characterize real fuel kinetic properties in same fundamental venues as those for surrogates and surrogate mixtures.
- Cross-validate comprehensive experimental database for selected components and component mixtures.
- Develop/validate detailed kinetic models for individual components, and their mixtures, including laminar transport.
- Compare real fuel data with surrogate model predictions.
- Advance tools for producing small dimensional models and improving CFD application integration.

Impact on DoD Capabilities

- Enhanced efficacy in evaluating fuel property variations on existing propulsion system performance and emissions.
- Improved paper design and development for advancing existing and developing new propulsion/combustion concepts.
- Assistance in integrating new non-petroleum-derived alternative fuel resources into the aero-propulsion sector.
- Provide fundamental assistance for developing “Rules and Tools” for expediting certification of alternative fuel candidates.

Team Presentations

MURI Overview: Real Aircraft Fuel Modeling Concepts, Surrogate Component Selection, and Observations
Frederick L. Dryer
Princeton University

A Study on TSI as a Property Target for Sooting of Jet Fuel Surrogates
R. J. Santoro, T. A. Litzinger
Pennsylvania State University

Combustion Data for Jet-A, its Constituent Components, and Surrogate Mixtures
Chih-Jen Sung
Case Western Reserve University

Kinetic Effects of n-alkane and Aromatic Mixtures on the Extinction Limits of Diffusion Flames

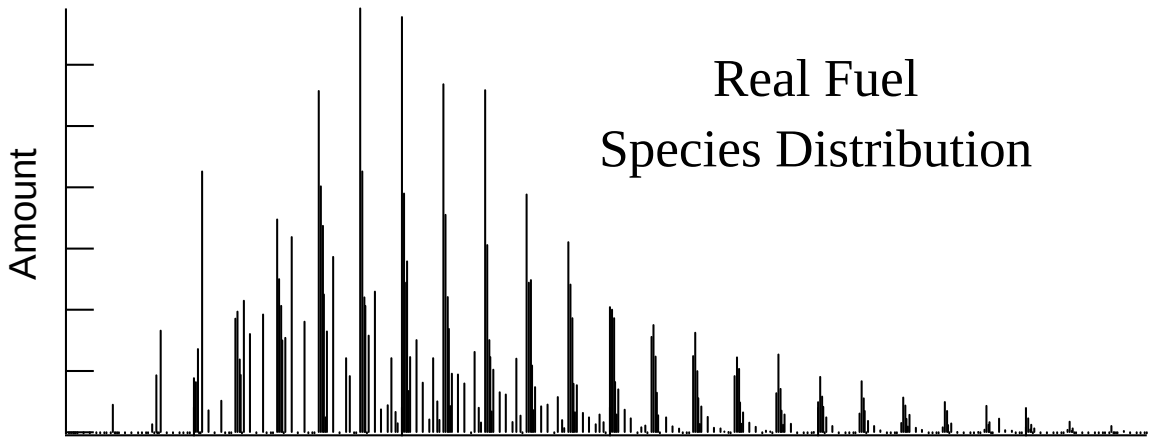
A New Dynamic Multi-time Scale Algorithm and Path Flux Analysis Method for Mechanism Reduction
Yiguang Ju
Princeton University

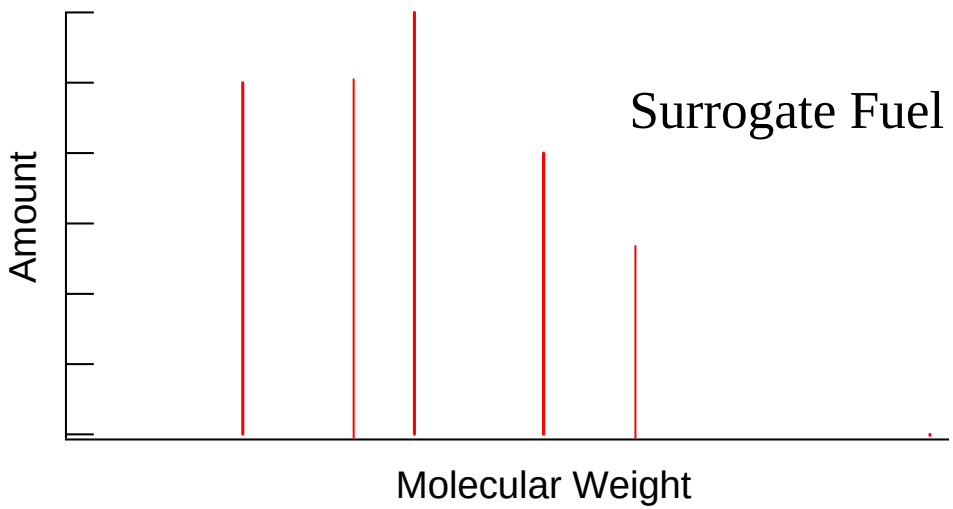
Oxidation of Potential Surrogate Fuel Components of JP-8
Kenneth Brezinsky
University of Illinois, Chicago

Detailed Chemical Kinetic Mechanisms for Combustion
Henry C. Curran
NUI Galway Ireland (Princeton University)

Flow Reactor Studies and Modeling Results
Frederick L. Dryer
Princeton University

Surrogate Mixtures





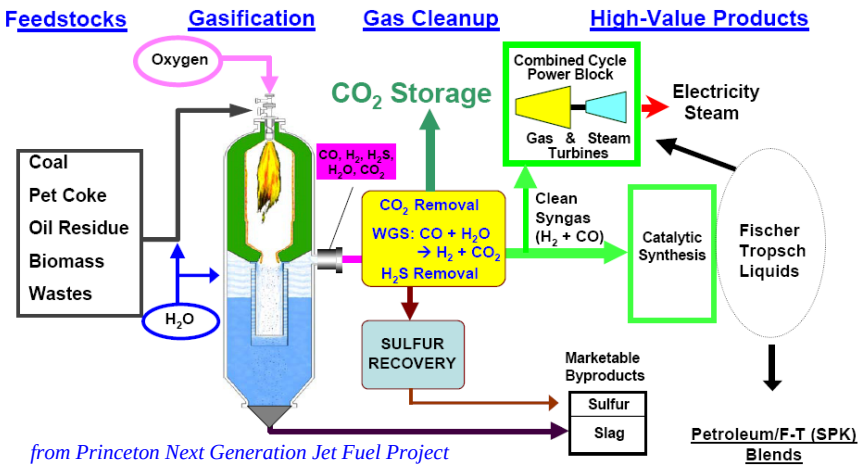
- *Real gas turbine fuels have 1000+ molecular species and presently vary significantly in composition*
- *Petroleum and petroleum/alternative fuel blend composition variability likely to increase*
- *Desire the ability to model fuel variations!*

Can we use a few component species to mimic the combustion properties of real fuels?

- *How to select component fuels for a surrogate model.*
- *What are the component fuel blending rules.*
- *Validated kinetic models for surrogate fuel mixtures.*
- *How to facilitate CFD applications.*

Future Petroleum and Petroleum/non-Petroleum Aircraft Fuels

Thermochemical (Gasification)-Based Fuels



from Princeton Next Generation Jet Fuel Project

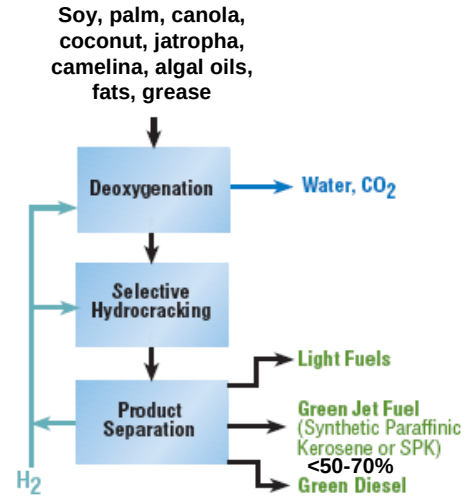
< 50% F-T/petroleum blends now reaching certification for aircraft use

Fully Deoxygenated "Green Fuels"

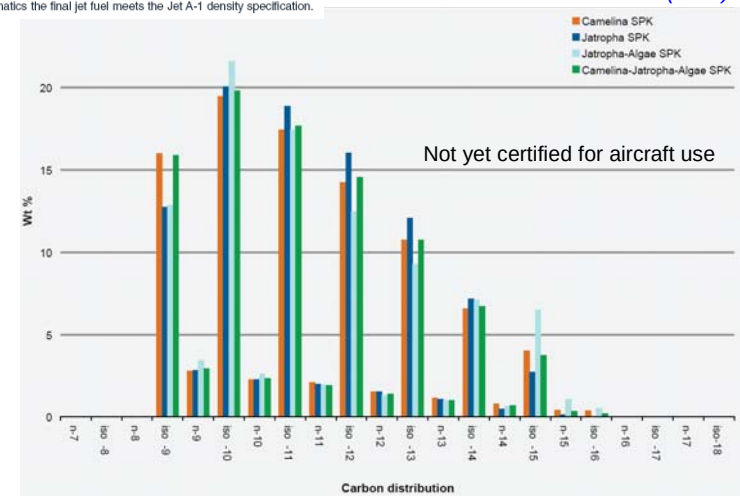
Analysis of Renewable Jet Samples

	Jet A-1	Jatropha	Camelina
Property	Spec	SPK	SPK
Flash point, °C	38 min	46	42
Freeze point, °C	-47	-57	-63.5
Net heat of combustion, MJ/kg)	42.8 min	44.3	44.1
JFTOT (2.5h at control temp, °C)	260 min	300	300
Filter pressure drop, mmHg	25 max	0	0
Tube deposits	<3	<1	<1
Distillation, 10%	185 max	168.5	163
50%	report	186.0	183.5
End boiling point	340 max	248	242
Density, kg/m³	775 - 840	749*	753*
Sulfur, ppm	-	<0.01	<0.01
Trace metals (each), ppm	-	<0.05	<0.05

* by definition SPK fuels have a lower density. However once blended with aromatics the final jet fuel meets the Jet A-1 density specification.



from UOP 4972-2 0409 (2008)



Neat Bio-SPK data for Carbon Structure

from Kindler and Rahmes, The Boeing Co. (2009)

- Future Petroleum based fuels and blends with alternative resources will continue to have variable fuel compositions.
- All chemical structures of these fuels will continue to fall within the classes of those presently considered in the MURI research.
- Approach taken should be applicable for emulating all of these real fuel compositions.

Surrogate Component Selection and Mixture Formulation

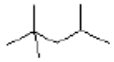
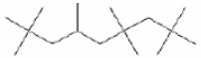
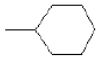
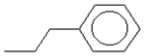
- At least one component from each molecular class found in real fuels.
  - Use components that in appropriate combination permit matching real fuel H/C ratio, sooting, and autoignition behavior over ranges found for real petroleum-derived and alternative fuels.
- Component Mixing Rules *(in addition to matching **H/C** ratio of the real fuel):*
  - *Sooting* - Evaluate **TSI** as combustion property target for relating surrogate mixture sooting behavior to real fuel sooting behavior.
    - Develop self consistent TSI reference database for surrogate components.
    - Validate appropriate functional relationships for predicting mixture TSI.
    - Compare mixture TSI with real fuel TSI to verify methodology.
    - Compare sooting predictions and measurements in a high pressure turbulent combustor.
  - Autoignition behavior – investigate Derived Cetane Number (**DCN**) for similar use as TSI to empirically adjust mixture to real fuel properties.
- Compare real fuel behavior and surrogate mixture behavior in wide variety of fundamental test venues.
    - Use well-characterized jet fuel samples (AFRL) to evaluate surrogate selections and mixing rules.
    - Perform validation experiments against each real fuels in specialized instrumentation (e.g. flow reactors, RCM, shock tubes, flames….) over appropriate pressure, equivalence ratio, and temperature range.

Guiding Kinetic/Transport Concepts

- Overall net active radical pool defined by production/consumption rates
- H/C ratio affects radical and hydrogen production rate, intermediate fragments, diffusion rates, and reaction zone structure.
- Radical pool of alkanes, cyclo-alkanes typically suppressed by aromatics. Pure component reactive radical pools are ordered as:
  - Alkanes>cyclo alkanes> long alkyl chain single ring aromatics> small alkyl chain single ring aromatics.
- Hydrocarbon mixtures exhibit two stage ignition; first stage, ntc and hot ignition behavior are coupled through kinetic properties and first stage heat release – Two stage behavior may be important in *both* diesel *and* gas turbine applications.
- Hydrocarbon mixture sooting strongly related to both fuel hydrogen content (premixed) and aromatic content/structure (TSI, mixing limited).
- Hydrocarbon mixture transport effects related to reactant molecular weights as well as their intermediate fragments

Surrogate Component Candidates

- Keep 8-9 < Carbon number < 14-16, ave.~12
- Use alkanes, cycloalkanes in combination with single ring aromatics to define base net radical level, two-stage ignition character, H/C ratio, and sooting
- Use at least two single ring aromatics of same molecular weight but different alkyl side chain structure to adjust two stage autoignition behavior while adjusting total aromatic content (aromaticity is constrained by sooting and H/C ratio)
- Small amounts of 1-methyl naphthalene to adjust sooting of mixture (if necessary)

Component	Molecular Formula	Structure	NTC
n-Heptane	C_7H_{18}		Yes
n-Decane	$C_{10}H_{22}$		Yes
n-Dodecane	$C_{12}H_{26}$		Yes
Iso-Octane (2,2,4 Trimethylpentane)	C_8H_{18}		Sml
Iso-Cetane (Heptamethylnonane)	$C_{16}H_{34}$		No
Methylcyclohexane	C_7H_{14}		Yes
Toluene	C_7H_8		No
n-Propyl Benzene	C_9H_{12}		?
1,3,5 Tri Methyl Benzene	C_9H_{12}		?
1-methyl naphthalene	$C_{11}H_{10}$		No

Several models available, more refinements, substantial validation.
Several models available, more validations emerging.
Fewer validation data, models under construction for n-PB, 124- TMB, 135-TMB, MCH, iso-alkanes with weak to medium branching

Experimental Research

- **Princeton University (PU)**
  - Variable Pressure Flow Reactor (VPFR) Experiments 2-12 atm, 550-950 K, dilute mixture conditions (Dryer)
  - Premixed Flame (1-30 atm) and Ignition Experiments (1-8 atm), initial T range, (450 K-1400 K), diluent differences (Ju)
  - Non-Premixed Flame Extinction &Ignition Experiments, coordinated with CWRU (Ju)
  - Mixture Formulation Concepts Based on Combustion Chemistry-Related Property Targets (H/C ratio, TSI, Autoignition behavior)
    - Ignition Quality Testing (IQT) for DCN, Dryer
- **Case Western Reserve University (CWRU)** → **UCONN** (8/09)
  - Rapid Compression Machine Experiments: 10-50 atm, 600-1100 K, low dilution
  - Premixed Flame Experiments (coordinated with PU)
  - Non-Premixed Flame Experiments: 1-6 atm (coordinated with PU)
- **Pennsylvania State University (PSU)**
  - Autoignition Experiments, (HPFR) 5-30 atm, 600-950 K, low dilution mixtures
  - Sooting Characteristics (MGTC), < 800K inlet to 20 atm
  - Threshold Soot Index Reference Database and Component Mixture Rule Verification
- **University of Illinois, Chicago (UIC)**
  - Single Pulse Shock Tube Experiments: ignition delays and stable species evolution, 10-40 atm, 800-2500 K

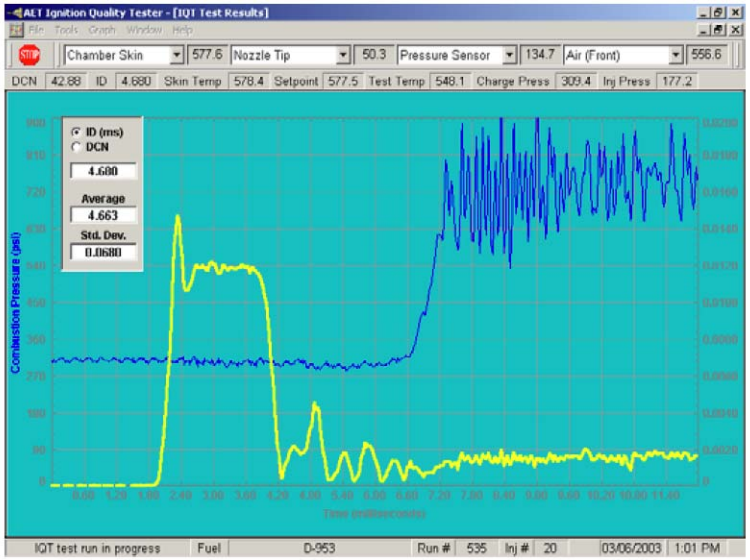
IQT™Method - Derived Cetane Number (DCN)

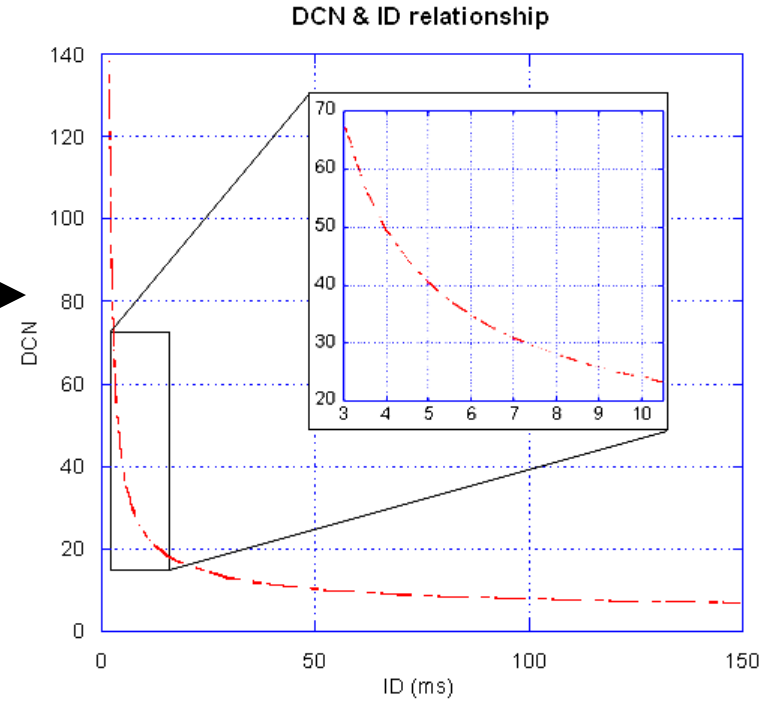
- ASTM D 6890 test procedure– fully accepted (internationally) for diesel fuel property determination.
- More reproducible than CFR engine characterization of CN (ASTM D 613).
- More universally comparable to CN than calculated Cetane Index Correlation (ASTM D 973).
- Reproducible from lab to lab and day to day, <1 CN: PU (new instr; PSU (older instr).

Blends (volumetric)	PU	PSU
50/50 Dec/n-PropBz	38.1	38.3
50/50 Dec/135TMB	32.2	31.9

- Better operation and reproducibility for blends with 34<DCN<61 (ASTM D6890)
- Standard operation more representative of gas turbine than piston engine operating conditions.
  - Constant volume combustion process. (~0.213 liters)
  - Heated chamber (~829 K)
  - Elevated Pressure (~22 atm)
  - Combustion air is “zero” air, (but non-standard use could tailor with contaminants)
    - < 5 ppm HC & H_2O
  - Fixed volume of fuel is injected
    - Equivalent to 0.0786 g/test of *n*-heptane (dilute, non-wall impingement small droplet size)
- Requires less than 100 ml of sample for accurate measurement.
- Can be applied to real fuels and surrogate mixtures as a correlation tool as well as for scanning effects of molecular structure on autoignition characteristics.
- Versatile operation at other pressures and temperatures are means of emphasizing low/intermediate and high temperature phenomena on autoignition.

Derived Cetane Number (DCN) Test Method





- Single Characterization:
  - Total fuel sample ~50 ml
  - 15 “warm-up” & 32 recorded injection/ignition events per test ~ 15 minutes
  - Ignition delay is derived from ASTM correlation of absolute ignition delay v. CN, 34<DCN<61

Procedure for Surrogate Blend Tests:

- Choose base n-alkane (n-decane, dodecane).
- Define statistical experiments for blending components.
- Obtain DCN data for all blend options for 34>DCN>61.
- Develop regression correlation for results.
- Check regression predictions vs. new data.

SwRI DCN Measurements on Real Fuels

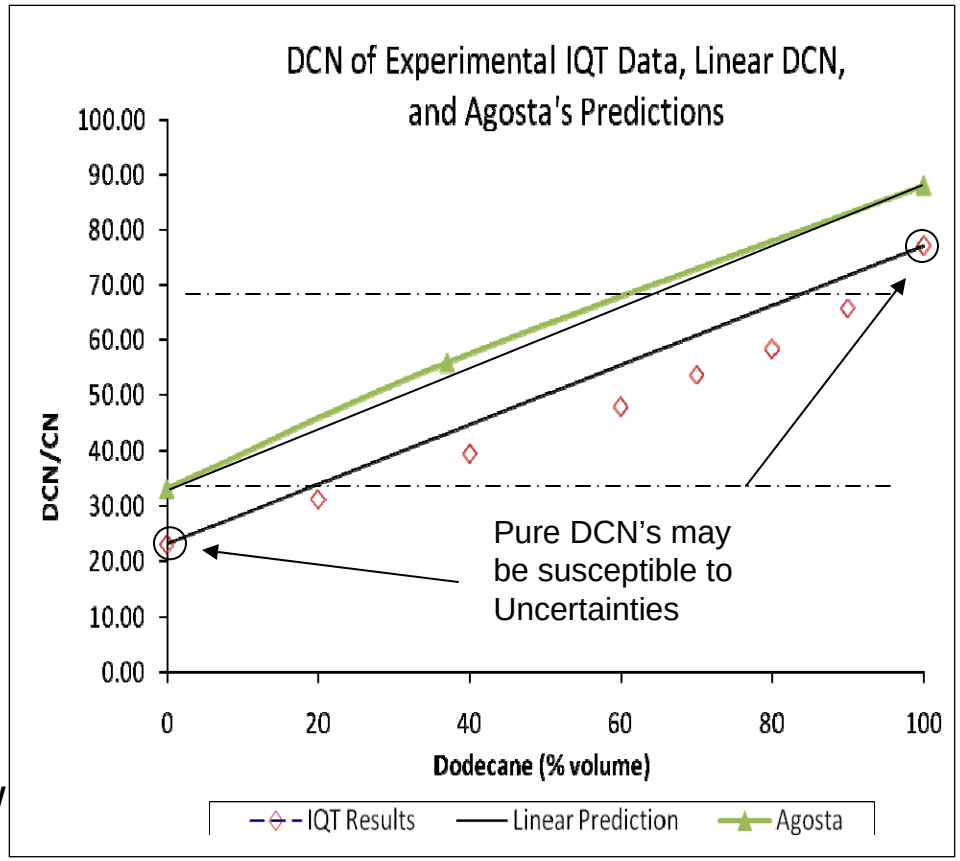
Sample Description (Wright Patterson AFB)	IQT DCN	ASTM D613	ASTM D976
AFB-POSF-3602-Jet A	38.35		
AFB-POSF-3638-Jet A	44.74		
AFB-POSF-3684-JP-8	43.14		
AFB-POSF-3773-JP-8	47.79		
AFB-POSF-4177-JP-8	40.15		
AFB-POSF-4658-Jet"A"Blend	45.27		
AFB-POSF-4765 coal-based Jet A	32.95		
AFB-POSF-4795/JP-10	18.64		
AFB-POS5140-TS-1 Jet fuel	40.81		
POSF 4751 JP-8	44.43	45.2	
POSF 5018 S-8 Syntroleum GTL F-T	59.67	58.4	68
50/50 blend 4751/5018	51.60	52.9	
POSF 5172 Shell SPK GTL F-T	59.08	57.4	57
50/50 blend 4751/5172	50.75	51.1	
Sasol IPK (POSF 5642)	31.28		51

Courtesy of AFRL, Tim Edwards

Example of IQT DCN Screening Capability

MCH Blending in n-Dodecane Targets

- DCN's of n-dodecane/component blends typically non-linear near pure component for several experimental reasons.
- Very short/short long ignition delays (experimental value).
- DCN/Tau correlation uncertainties.
- Determine DCN's in regions where blending values are in real fuel DCN range.
- DCN for many n-dodecane blends are linear in 35<DCN< 70 range – iso-oct/n-dod is an exception.
- Synergetic blending found in Drexel flow reactor correlation.
- Antagonistic blending found in IQT.
- Screening requires only very small. amounts of test component and a few hours.

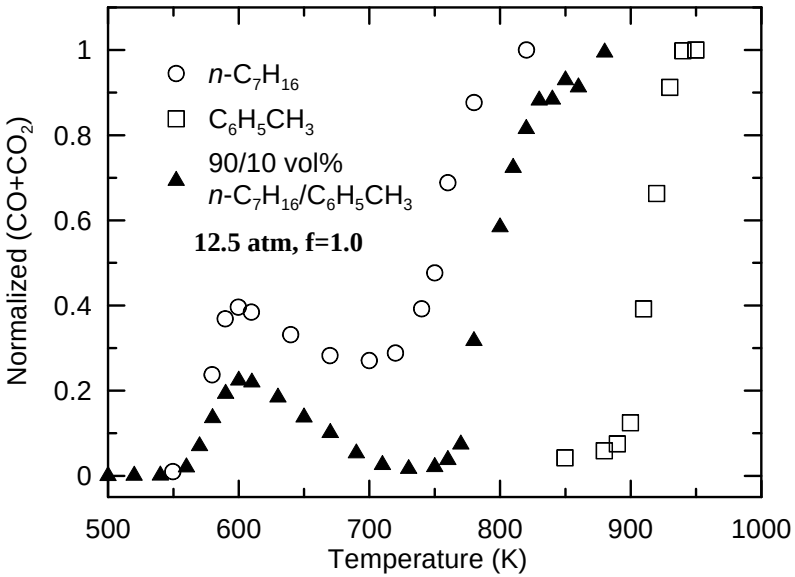


Blending MCH In Drexel Flow reactor: y = 39.732x - 1359.5 and CO max production of 860 ppm using reported ASTM D-613 pure component CN's.

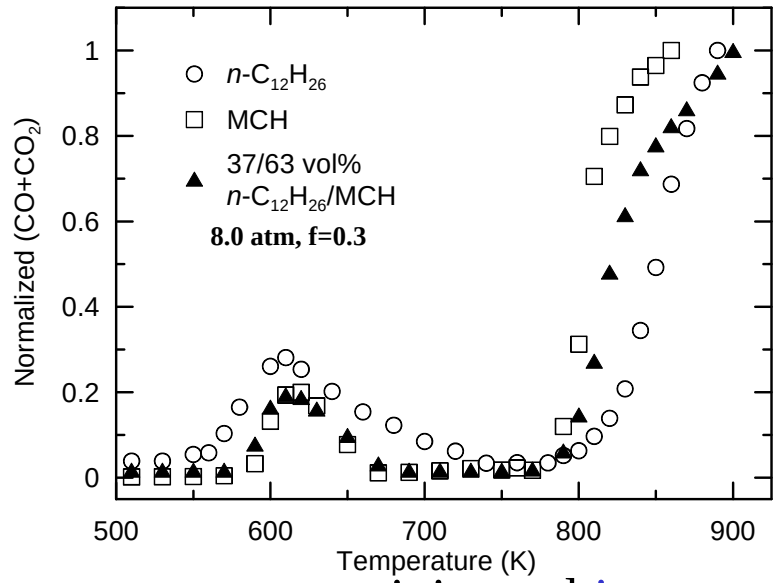
Agosta (2002) "Development of a Chemical Surrogate for JP-8 Aviation Fuel Using a Pressurized Flow Reactor", Drexel University, May.

Blending Effects on Autoignition Behavior

n-heptane/toluene blending



n-dodecane/ methylcyclohexane blending



- Addition of toluene to n-heptane inhibits low temperature reactivity and *increases* the hot ignition temperature.
- Addition of MCH to n-dodecane inhibits low temperature reactivity and *decreases* the hot ignition temperature.
- Overall autoignition properties of blends are affected by influences on both low temperature/NTC ("pre-ignition") activity and as well as hot ignition behavior.
- DCN blending correlations for surrogate components need experimental verification.

DCN Regression Results: Dec, i-Oct, Tol Mixtures

Preliminary Results further analysis proceeding

$$DCN = \sum_i (Coeff_i * Term_i)$$

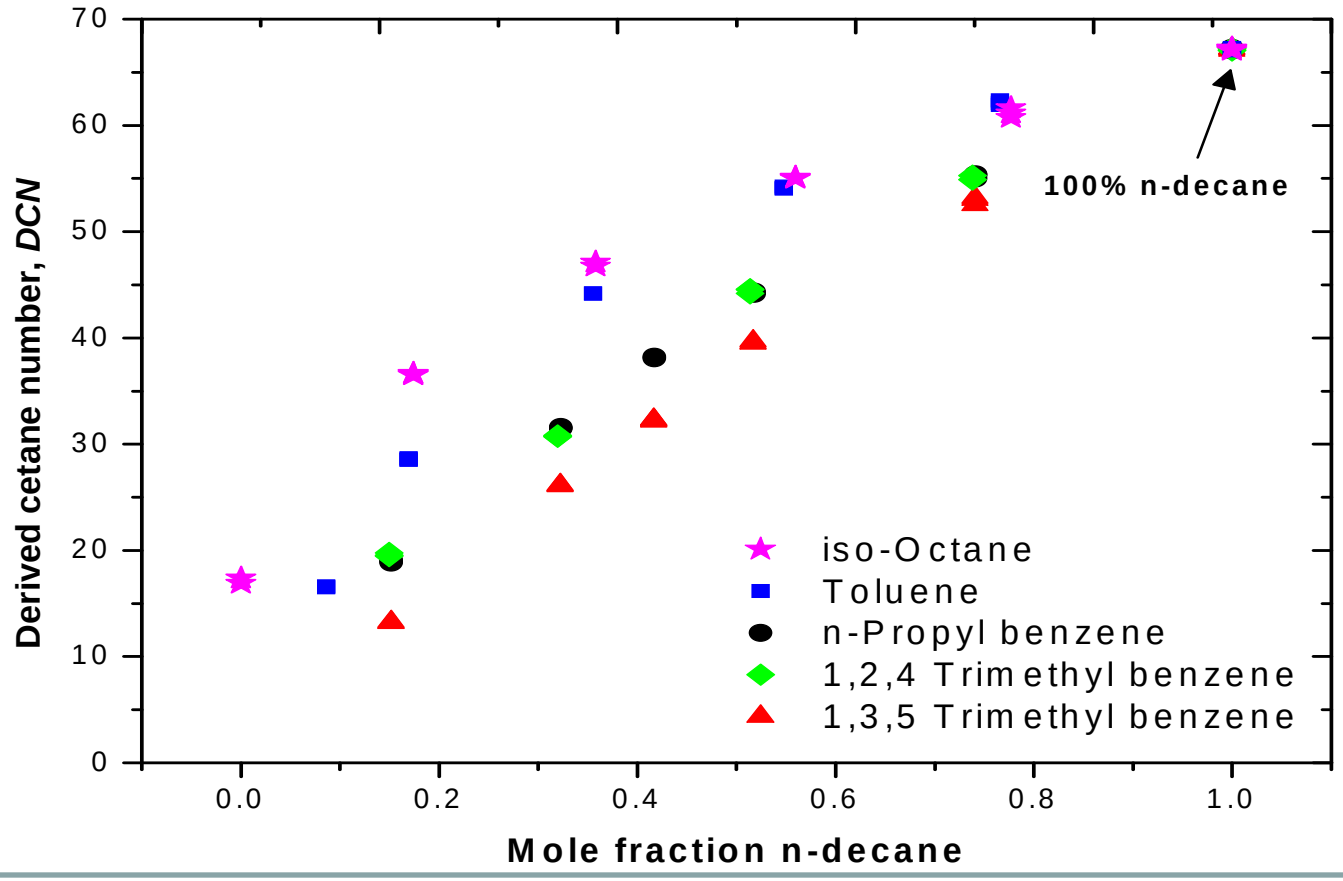
- Volume Correlation more linear than mass or molar cases
- Correlation for range of 35<CN<55
- Examples of reproducibility here to be added
- Typical reproducibility better than 0.5

N-Dec/i-Oct/Tol	Pred	Meas
36/44/21	39.5	39.6
46/27/27	43.2	43.2

$Term_i$ (Volume Fractions)	$Coeff_i$
Dec	7
i-Oct	2
Tol	2
Dec*i-Oct	9
Dec*Tol	4
Dec*i-Oct*(Dec-Oct)	5
Dec*Tol*(Dec-Tol)	5
Dec*Tol *(Dec-Tol) ^{2}	9

Preliminary results: Contact PI for further information

Typical Results: n-Decane Mixture Data



Derived cetane numbers for n-decane/aromatic mixtures from Ignition Quality Tester, at ~865K and 20atm.

Results: Model for n-Decane and n-Dodecane Blending with i-Oct, nPB, and 135TMB

(Preliminary, in Construction)

n-Decane Quaternary Mixtures

$Term_i$ (Volume Fraction)	$Coef_i$
n-Dec	*Preliminary results: Contact PI for further information*
i-Oct	
135TMB	
nPB	
Dec vol*nPB	
Decvol*135TMB*(-)	
Dec vol*Decvol*i-Oct*135TMB	
i-Oct*i-Oct*nPB*135TMB	

S = 0.837840 R-Sq = 99.03%

Dec/i-Oct/nPB/135TMB (vol%)	Pred	Meas
58/15/13/14	43.1	44.8

n-Dodecane Quaternary Mixtures

$Term_i$ (Mole Fraction)	$Coef_i$
n-Dod	*Preliminary results: Contact PI for further information*
i-Oct	
nPB	
135TMB	
n-Dod*i-Oct	
n-Dod*nPB	
n-Dod*135TMB	
n-Dod*i-Oct*(n-Dod – i-Oct)	
n-Dod*nPB*(n-Dod – nPB)	
i-Oct*nPB*(i-Oct – nPB)	
i-Oct*nPB*nPB*135TMB	
i-Oct*nPB*135TMB*135TMB	
n-Dod*i-Oct*(n-Dod – i-Oct)^2	
n-Dod*135TMB*(n-Dod – 135TMB)^2	

S = 0.382053 R-Sq = 99.95%

n-Dod/i-Oct/nPB/135TMB (vol%)	Pred	Meas
30/10/0/60	32.4	31.6
33/13/31/24	38.0	40.9
26/17/15/42	31.3	33.7

Additional data can further refine the accuracy of these correlations

Reproducing Global Average Jet-A Property Targets

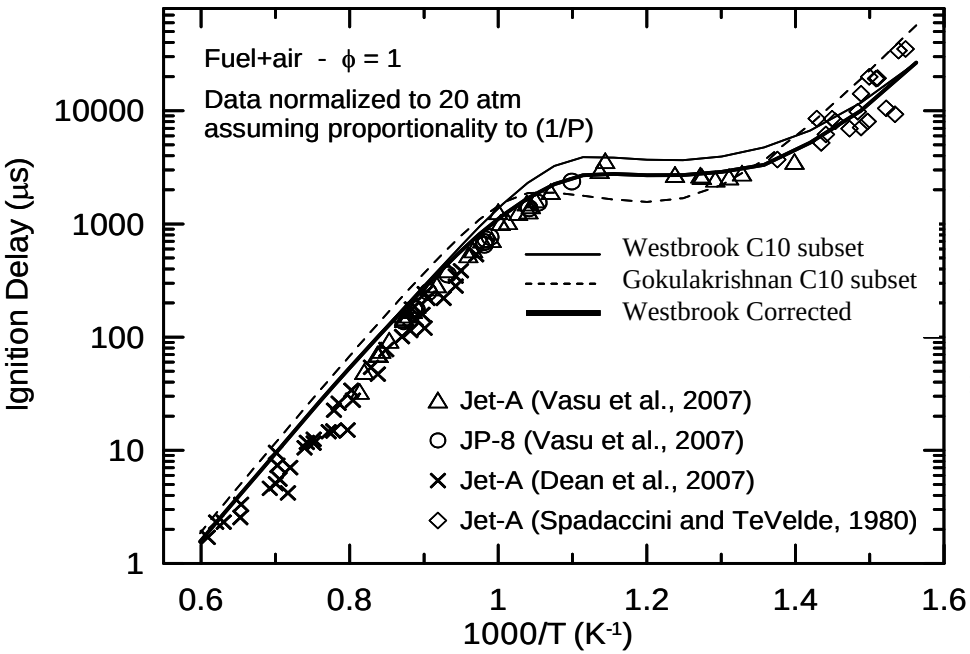
	Liquid volume fractions			
Component	**A**	**B**	**C**	**D**
n-decane	48.73%		52.47%	
n-dodecane		41.73%		42.45%
iso-octane	27.76%	35.43%	18.33%	29.10%
toluene	23.51%	22.84%		
n-propylbenzene			2.20%	14.57%
1,3,5-trimethylbenzene			27.00%	13.88%
H/C	1.909	1.909	1.909	1.909
CN linear blending (DCN)	43.9 (45.0)	43.9 (NA)	43.9 (38.6)	43.9 (45.0)
TSI (TSI from PSU Database)	18.55 (17.5)	19.19 (17.6)	21.47 (25.0)	21.47 (24.4)
Aromatics (vol %); avg.=17.86%	23.51%	22.84%	29.20%	28.45%

- Targets can be reproduced with a variety of class distributions, without reproducing that of a the real fuel.
- Sooting propensity does not correlate with aromatic fraction alone
- Consistent reference data sets for component TSI, CN and blending characteristics are under refinement

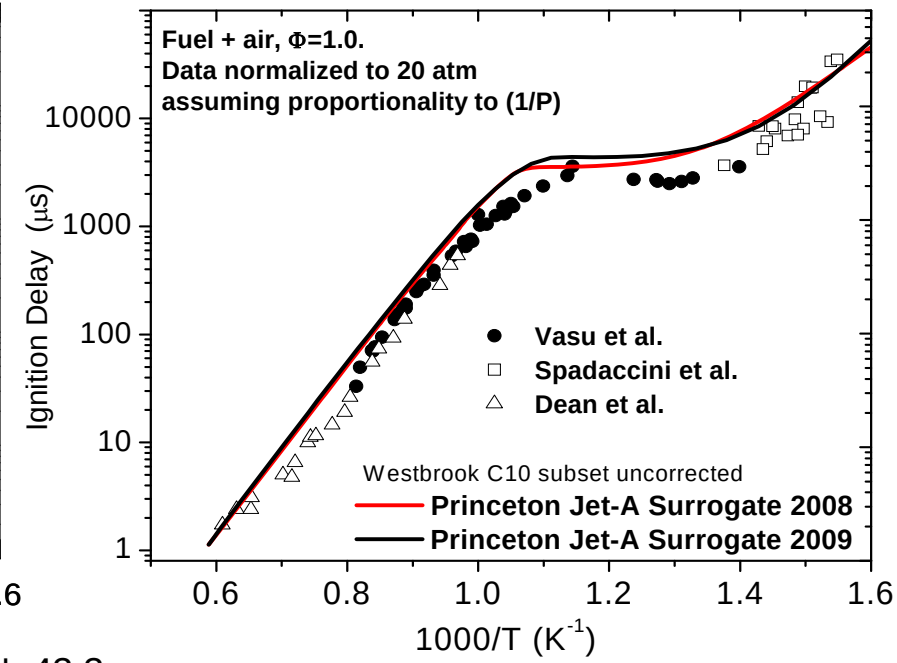
Linear blending data in Xu et al., JANNAF 42nd Meeting, Hanscom AF Base, Newton, MA. May 12-16, 2008

Updated Ignition Delay Prediction for Jet A

H/C 1.924, DCN 47.5 – 2008 Surrogate Mixture (vol %):
49.5% n-decade, 28.2% iso-octane, 22.3% toluene



H/C 1.925, DCN 43.4 – 2009 Surrogate Mixture (vol %):
43.04% n-decade, 38.38% iso-octane, 18.57% toluene



- Jet A Target Data: 13.9 wt% hydrogen (H/C=1.924); CN=43.3
- Base kinetic model: n-heptane/iso-octane/toluene developed for gasoline surrogate by Chaos et al. (*Joint Combustion Meeting, San Diego, CA, 2007. Paper E-26*)
- Augmented with high temperature n-decane oxidation based upon prior rules for n-alkane modeling of Chaos et al. (*Int.J. Chem. Kin. 39, 2007, 399*)
- Low temperature n-decane subsets taken from Gokulakrishnan et al. (*J. Eng. Gas. Turb. Power 129, 2007, 655*) and Westbrook et al. (*Combust. Flame, 2009)*:

2008-2009 MURI Accomplishment Highlights

Surrogate Mixture formulation

- Continuing to evolve specific surrogate component list for forming mixtures.
- Further evaluated H/C ratio, threshold sooting index (TSI), and derived cetane number (DCN) as reasonable targets for determining surrogate mixtures to match combustion behavior of real fuels.
- Continuing to evolve database of TSI's from component smoke point measurements.
  - Further testing of abilities to reproduce real fuel sooting properties under high pressure turbulent combustion conditions.
- Investigating DCN as a means of formulating surrogate mixture autoignition properties:
  - DCN measurements of surrogate component mixtures can be used to determine autoignition behavior and functional blending rules for determining DCN of mixtures
  - DCN can be derived for and compared with real fuel DCN's using simple, efficient methods
  - Ignition Quality Testing (IQT) methods can be used to qualitatively evaluate autoignition blending properties of surrogate candidate species (e.g., iso-alkanes) and alternative fuel formulations with minimal volumes of sample required
  - Numerical model predictions of ignition delay for simple component mixtures with matching H/C, DCN with those of real jet fuels show are continuing to evaluate the concept.

Experimental Validation Data-base Contributions

- Flow reactor experiments confirm that none of the selected aromatic components, toluene, n-propyl- (n-PB) and trimethyl- (TMB) benzenes, exhibit low temperature (cool flame) chemistry. New data produced on reactivity characteristics of n-decane at high pressure. Data show that n-dod/nPB/135-TMB preferred over using 124-TMB blends.
- High pressure, single pulse shock tube data obtained for m-xylene, n-PB, 1,3,5-TMB, and a 1,3,5-TMB/n-PB (1.5:1) mixture.
- Elevated pressure, rapid compression machine (RCM) data at low/intermediate temperatures acquired for jet-A, JP-8, and S-8 fuels, n-decane, methylcyclohexane, iso-octane, toluene, and iso-octane/toluene blends.
- Atmospheric pressure laminar flame speeds of two jet fuels with preheat determined.
- New data on extinction limits of and soot volume fractions in toluene/n-decane counterflow diffusion flames obtained.

Modeling

- Numerical model predictions of ignition delay for simple component mixtures by matching mixture H/C and DCN to a real jet fuel show promise for mixture formulation concepts.
- Model development on full range decane, dodecane, MCH, and alkylated single ring aromatics underway.
- C0-C4 detailed sub-model refinements underway; Refined toluene model developed. 1,3 xylene model advancements made. n-propyl benzene model development initiated.
- Dynamic multi-scale method for detailed kinetic model reduction was developed.

2008-2009 Archival Publications

G. Mittal and C. J. Sung, “Homogeneous Charge Compression Ignition of Binary Fuel Blends,” *Combust Flame* 155, 431-439 (2008).

G. Mittal, M. Chaos, C. J. Sung, and F. L. Dryer, “Dimethyl Ether Autoignition in a Rapid Compression Machine: Experiments and Chemical Kinetic Modeling,” *Fuel Processing Technology* 89 (12), 1244-1254 (2008).

K. Kamal, G. Mittal, and C. J. Sung, “Autoignition of *n*-Decane under Elevated Pressure and Low-to-Intermediate Temperature Conditions,” *Combust Flame* 156, 1278-1288 (2009).

Y. Ju, X. Gou, W. Sun, and Z. Chen, “An On-Grid Dynamic Multi-Timescale Method with Path Flux Analysis for Multi-Physics Detailed Modeling of Combustion (invited review paper)”, *Journal of the Combustion Society of Japan*, Vol.51, 2009, in press.

S. H. Won, W. Sun, Y. Ju, “Kinetic Effects of Toluene Blending on the Extinction Limit of n-Decane Diffusion Flames,” *Combust. Flame* in review (2009), also presented at *6th U.S. National Combustion Meeting*, Ann Arbor, Michigan (2009).

G. Mittal and C. J. Sung, “Autoignition of Methylcyclohexane at Elevated Pressures,” *Combust Flame,* In Press.

K. Kamal and C. J. Sung, “An Experimental Study of the Autoignition Characteristics of Conventional Jet Fuel/Oxidizer Mixtures: Jet-A and JP-8,” *Combust Flame,* (2009). Accepted with revisions

K. Kamal and C. J. Sung, “A Comparative Experimental Study of the Autoignition Characteristics of Alternative and Conventional Jet Fuel/Oxidizer Mixtures,” *Combust Flame* (2009). Submitted.

A. Mensch, R.J. Santoro, T.A. Litzinger and S.-Y. Lee “Sooting Characteristics of Surrogates for Jet Fuels”, *Combust. Flame*, (2009). Accepted with revisions.

X. Gou, W. Sun, Z. Chen and Y. Ju, “A Dynamic Multi-Timescale Method for Combustion Modeling with Detailed and Reduced Chemical Kinetic Mechanisms”, *Combust Flame* (2009). Submitted.

W. Sun, Z. Chen, X. Gou, and Y. Ju, “A Path Flux Analysis Method for the Reduction of Detailed Chemical Kinetic Mechanisms”, *Combust Flame* (2009). Submitted.

Presentations and Preprints

H. Xu, Z. Yang, M. Chaos, and F.L. Dryer, “Surrogate Jet Fuel Mixture Formulation and Development of Experimental Databases,” JANNAF 42nd Combustion Joint Sub-Committee Meeting, Modeling and Data For Combustion Simulation, Boston Marriott Newton, Hanscom AF Base, Newton, MA. May 12-16, 2008.

T.Malewicki, S.Gudiyella, K. Brezinsky, “Oxidation of potential surrogate fuel components of JP-8”, Work in Progress Poster (W5P108) presented at *32nd International Symposium on Combustion*, Aug 3-8, 2008.

G. Mittal and C. J. Sung, “Methylcyclohexane Oxidation in a Rapid Compression Machine,” Work in Progress Poster (W5P071) presented at 32nd International Symposium on Combustion, Montreal CA, Aug 3-8, 2008.

S. H. Won, W. Sun, and Y. Ju, “Effect of Toluene Blending on n-Decane Diffusion Flame Extinction Limit,” Work in Progress Poster (W4P202) presented at *32nd International Symposium on Combustion*, Montreal CA, Aug 3-8, 2008.

Z. Yang, H. Xu, M. Chaos, and F.L. Dryer, “Surrogate Fuel Component Selections and Mixture Properties for Emulating Fuel Combustion Chemistry of Real Petroleum-Derived and Non-Oxygenated Alternative Fuels,” Work in Progress Poster (W4P138) presented at *32nd International Symposium on Combustion*, Montreal CA, Aug 3-8, 2008.

A. Mensch, S.-Y. Lee , R. J. Santoro, and T. A. Litzinger, “Sooting Characteristics Of Surrogates For Jet Fuels,” Work in Progress Poster (W5P137) presented at *32nd International Symposium on Combustion, Montreal CA, Aug 3-8, 2008.* G.

G. Mittal and C. J. Sung, “Methylcyclohexane Oxidation in a Rapid Compression Machine,” Work in Progress Poster (W5P071) presented at 32nd International Symposium on Combustion, Montreal CA, Aug 3-8, 2008.

S. H. Won, W. Sun, and Y. Ju, “Effect of Toluene Blending on n-Decane Diffusion Flame Extinction Limit,” Work in Progress Poster (W4P202) presented at 32nd International Symposium on Combustion, Montreal CA, Aug 3-8, 2008.

K. Kumar and C. J. Sung, “An Experimental Study of the Autoignition Characteristics of Jet-A/Oxidizer Mixtures in a Rapid Compression Machine,” *Spring Technical Meeting of the Western States Section of the Combustion Institute*, University of Southern California, CA, 2008.

G. Mittal and C. J. Sung, “An Experimental Study of Autoignition of Methylcyclohexane,” *Technical Meeting of the Central States Section of the Combustion Institute*, Tuscaloosa, AL, 2008.

K. Kumar and C. J. Sung, “Autoignition of Conventional and Alternative Jet Fuels,” *Second International Symposium on Jet Propulsion and Power Engineering*, Guilin, China, 2008.

S. H. Won, W. Sun, Y. Ju, “Kinetic Effects of Toluene Blending on n-Decane Diffusion Flame Extinction Limit,” *47th AIAA Aerospace Sciences Meeting*, Orlando, Florida (2009), AIAA-2009-0993.

X. Gou, Z. Chen, W. Sun, Y. Ju, “Multi-scale Method for Detailed Chemistry in Simulation of Reacting Flows,” *47th AIAA Aerospace Sciences Meeting*, Orlando, Florida (2009), AIAA-2009-1369.

W. Sun, Z. Chen, X. Gou, Y. Ju, “A Path Flux Analysis Method for the Reduction of Chemical Kinetic Mechanisms,” *6th U.S. National Combustion Meeting*, Ann Arbor, Michigan (2009).

K. Kamal, C. J. Sung, and X. Hui, “Laminar Flame Speeds and Extinction Limits of Conventional and Alternative Jet Fuels,” *Forty-Seventh Aerospace Sciences Meeting*, AIAA Paper No. 2009-991 (2009).

K. Kamal and C. J. Sung, “Autoignition of Jet Fuels under High Pressure and Low-to-intermediate Temperatures,” *Forty-Seventh Aerospace Sciences Meeting*, AIAA Paper No. 2009-1527 (2009).

A. Mensch, R. J. Santoro, T. A. Litzinger and S.-Y. Lee, “Sooting Characteristics of Surrogates for Jet Fuels”, AIAA-2009-1525, 47th AIAA Aerospace Sciences Meeting, Orlando, Florida, Jan. 5-8, 2009

K. Kamal and C. J. Sung, “Autoignition of Fully Blended Jet Fuels and Neat Hydrocarbons: Effect of Cetane Number,” *Sixth Joint Meeting of the U.S. Sections of the Combustion Institute*, Ann Arbor, MI, 2009.

K. Kamal, X. Hui, and C. J. Sung, “Fundamental Combustion Properties of Jet Fuels,” *Sixth Joint Meeting of the U.S. Sections of the Combustion Institute*, Ann Arbor, MI, 2009.

K. Kamal and C. J. Sung, “Flame Propagation and Extinction Characteristics of Neat Hydrocarbon Surrogate Fuel Components,” *Sixth Joint Meeting of the U.S. Sections of the Combustion Institute*, Ann Arbor, MI, 2009.

Acknowledgements

- Princeton staff contributions:
  - M. Chaos, S. Dooley, W. Metcalfe, J. Heyne
  - Collaborations on IQT/DCN:
  - A. Boehman and J. Henye (PSU) –Initial measurements (supported under AFOSR Contract FA9550-07-1-0451; Program manager: Julian Tishkoff).
  - Continued interactions with G. Webster (AET. Ltd.) on IQT testing.
- J. (Tim) Edwards (AFRL) – Jet fuel samples & DCN data
- C.K. Westbrook and W.J. Pitz of LLNL – Collaboratively sharing recent C_8-C_{16} alkane and toluene oxidation models.
- Helpful discussions with:
  - Advisory Board Members – J. (Tim) Edwards, AFRL;J. Farrell, Exxon-Mobil; C. Fotache, UTRC; H. Mongia, GE Aviation (retired); W. Pitz, LLNL; W. Tsang, NIST.

Thank You

MURI Five Year Deliverable

- Provide a 5 liter sample of any specific gas turbine hydrocarbon fuel, and experimentally characterize a small number of key properties for the fuel using relatively simple procedures.
- These simple procedures will determine a specific mixture of selected surrogate components for which accompanying detailed and reduced models that emulate its global combustion features, including autoignition, laminar burning rate, extinction, and sooting behavior will be provided.

We are developing concepts, base surrogate component slates, and models that can be expanded upon to encompass additional property and combustion targets in the future….

Questions