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:

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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
Princeton, New Jersey
20-22 September, 2010

MURI Research Goals

- Validate novel principles to select surrogate components.
- Select and refine combustion target parameters to be emulated.
- 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.
- Compare real fuel data with formulated surrogate mixture data.
- Further develop cross-validated, comprehensive experimental database for components and component mixtures.
- Develop/validate detailed kinetic models for individual components, and their mixtures, including laminar transport.
- 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” efforts for expediting certification and integrating alternative fuels with petroleum derived fuels.
  - T. Edwards, C. Moses, and F. Dryer (2010). Evaluation of Combustion Performance of Alternative Aviation Fuels, 46th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit 25-28 July 2010, Nashville, TN AIAA-2010-7155 *(Panel Discussion).*

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MURI Accomplishments in 2009-2010

Major progress on *experimentally evaluating* jet fuel surrogate mixture formulation concepts developed in the originating proposal.

- Collaborative, cross-validated critical experimental data comparisons of a real jet fuel sample (POSF 4658) and surrogate mixture behavior at PU, PSU, UCONN, RPI (Oehlschlaeger): ignition delay (RS, RCM), VPFR reactivity, diffusive strained extinction.
  - First generation surrogate (n-C_{10}/iso-C_8/tol) on line, Combust Flame, July 2010 (PU, PSU, UCONN, *RPI*)
  - Second generation surrogate (n-C_{12}, iso-C_8/nPB/1,3,5TmB study progress (all members + *RPI*).
- More concept testing; additional components (e.g. MCH), added gas phase kinetic targets (e.g. strained extinction). (all members , *RPI, others*).
- Advancing sooting comparisons under high pressure dump combustor conditions (PSU).
- Property data (H/C, DCN, TSI, MW_{ave}) for other jet fuel samples in progress (PU, PSU)
  - Associated 1st /2nd generation component surrogate compositions to be made available.
- Initiated efforts on emulating liquid phase physical properties (PU).
  - *Continue to emphasize mixtures of a small (minimal) number of chemical components constrained by gas phase kinetic considerations.*

Additional surrogate component experimental validation data

- *High pressure single pulse shock tube (UIC): n-C10, n-C12,nPB,* 1st /2nd generation *surrogates.*
- *RCM data (UCONN): n-C_{10}, n-C_{12}, i-C_8, MCH, Tol, nPB, 1,2,4 TmB, 1,3,5 TmB,* 1st /2nd generation *surrogates.*
- *Laminar flame speeds,1atm (UCONN): n-C_7, n-C_{10}, n-C_{12}, MCH, Tol, nPB, 1,2,4 TmB, 1,3,5 TmB.*
- *Premixed strained extinction (UCONN): n-C_7, nC_{10}, n-C_{12}, MCH, Tol, nPB, 1,2,4 TmB, 1,3,5 TmB.*
- *Diffusive strained extinction (PU): n-C_{12}, i-C_8, n-PB, 1,2,4 TmB, 1,3,5 TmB, kinetic effect analysis.*
- *VPFR reactivity and species time history (PU): n-C_{10}, n-C_{12}, n-PB, 1,3,5 TmB.*

Fundamental supporting research

- *Model reduction (UCONN, PU)*
- *TSI (PSU) and DCN(PU) fundamentals.*
- *Radical Index and extinction limit correlations.*
- *Flame speed comparisons - counter flow v spherical flame (PU).*
- *Multi-time scale and path analysis integration with adaptive griding (PU).*
- *Kinetic modeling: 1st generation surrogate modeling predictions; toluene model development (PU), nPB (UIC, PU), 1-olelfin and small molecule (C_2,C_3) sub-model components: (Curran/LLNL).*

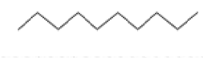
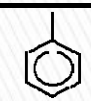
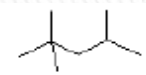
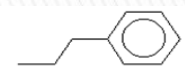
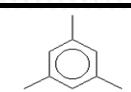
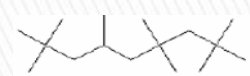
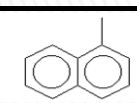
Jet Fuel Kinetic Modeling

- Postulated jet fuel surrogate mixtures have typically been developed by representing each generic molecular class within a real fuel by one or more individual components.
- Formulations haven't considered the real word variability of properties even for petroleum derived fuels. *The need to encompass fuel variability effects has been a primary driver for the MURI endeavors.*
  - Synthetic fuels potentially add new dimensions to composition variability.
- Historically, there have been many surrogate studies, but no generally accepted, widely validated methodology for surrogate fuel mixture formulation. *In 2007-2008, the MURI proposed an alternative approach.*[1]
- Key to the MURI effort: comprehensive testing of the fidelity for *apriori* surrogate compositions to emulate gas phase combustion properties of a specific real fuel in a wide range of fundamental experimental venues.
- The MURI emphasis is on utilizing small numbers of surrogate components to emulate gas phase kinetic characteristics.
  - **Kinetic model reduction strongly depends on model construction (i.e. the # of individual components)!**
  - **Kinetic complexity (*not* physical property emulation) strongly constrains the optimal component choices!**

1. Xu et al. (2008) JANNAF 42nd Comb. Jnt Sub-Cmte Mtg., 5/12-16

Surrogate Component Philosophy

- *Radical pool of alkanes is typically suppressed by aromatics. Component reactive radical pools are ordered as: alkanes>cyclo alkanes>iso alkanes > long alkyl chain mono aromatics> short alkyl chain mono aromatics.*
- Keep 8-9 < Carbon number < 14-16, so as to emulate real fuel molecular average weight.
- Use alkanes, mono-cycloalkanes in combination with single ring alkylated aromatics to define base net radical level, two-stage ignition character, H/C ratio, and sooting.
- Use at least two single ring alkyl-aromatics of same molecular weight but different alkyl side chain structure to permit adjustment of two-stage autoignition behavior, sooting and H/C ratio of surrogate mixtures.
- *Avoid multi-ring naphthenes and aromatics, if possible (kinetic model development even more complicated).*

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

Several models available, continuing refinements, substantial validation.
Fewer validation data and models available, especially for mixtures.
Components for which some modeling/validation data are available; may be considered in the future.

Hydrocarbon Type Classification of Jet Fuels

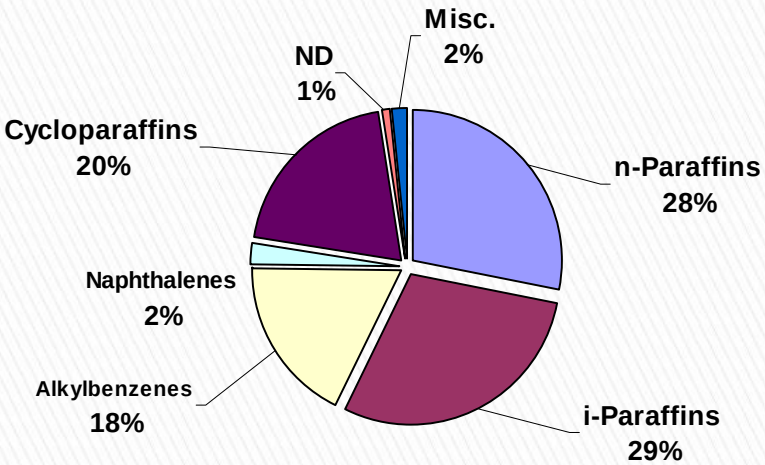
An Exemplar Method:

ASTM D2425 - 04(2009) Standard Test Method for Hydrocarbon Types in Middle Distillates by Mass Spectrometry

• Eleven hydrocarbon types can be identified: paraffins, noncondensed cycloparaffins, condensed dicycloparaffins, condensed tricycloparaffins, alkylbenzenes, indans or tetralins, or both, CnH2n-10 (indenes, etc.), naphthalenes, C_nH_{2n}-14 (acenaphthenes, etc.), C_nH_{2n}-16 (acenaphthylenes, etc.), and tricyclic aromatics.

Organic Class	World survey average, vol %	Composite Jet A blend (POSF-4658)	POSF 4751 JP-8	
Paraffins (normal + iso)	58.8	55.2	59.6	
monocycloparaffins	10.9	17.2	14.5	
dicycloparaffins	9.3	7.8	5.9	
tricycloparaffins	1.1	0.6	<1	
alkyl benzenes	13.4	12.7	12.0	
indans+tetralins	4.9	4.9	6.3	
naphthalene	<0.2	<0.2	<0.2	
substituted naphthalenes	1.6	1.3	<0.2	

Hydrocarbon Class Distribution in Jet-A (wt.%)



- ***Other methods exist, but all are complex and may yield different class compositions.***
  - ***Are ASTM characterizations sufficiently accurate for fundamental research purposes in constructing surrogate mixtures?***
- ***The MURI effort is not basing surrogate formulation on these data.***

MURI Strategy for Modeling a Specific Jet Fuel

Identify critical fuel property targets that manifest in important practical combustion behavior of each real fuel:

- Adiabatic flame temperature
- Local air fuel stoichiometry
- Enthalpy of combustion
- Flame velocity
- Overall active radical production
- Premixed sooting

} Ratio of Hydrogen to Carbon (H/C)

- Non-premixed sooting → Threshold Sooting Index (TSI), By standardizing smoke point measurement
- Fuel diffusive transport properties → Average Molecular Weight (MW_{ave})
- Autoignition/global kinetics → Derived Cetane Number (DCN), Correlative for macro ignition measure

H/C, TSI, DCN, MW_{ave} can each be determined for the real fuel sample, as well as for the surrogate mixture, using the same, simple experimental procedures.

=> no quantitative species classification measurements used to formulate the surrogate mixture.

Surrogate Mixture Construction Method

Characterize the specific real fuel.

- Determine empirical formula for C_nH_m using CHN analysis (ASTM D5291).
  - Derive average molecular weight and H/C ratio.
- Determine DCN of fuel using Ignition Quality Testing (ASTM D6890).
- Determine TSI from smoke point measurement (ASTM D1322) and average molecular weight.

Characterize chosen surrogate components and their mixtures

- Develop experimental self-consistent library of TSI values for surrogate components and mixtures.
- Develop experimental self-consistent DCN database for surrogate component mixtures composed of a base n-alkane to which other components that are added yield 30 <DCN<65 (ASTM D6890).

Emulate the H/C, DCN, TSI, and average molecular weight of specific fuel by choice of surrogate components and mixture fractions.

Compare gas phase experimental observations using the specific fuel with those for the apriori formulated surrogate mixture:

- Reflected shock tube ignition delay (in collaboration with RPI).
- Rapid Compression Machine (RCM) ignition properties (UCONN).
- Variable Pressure Flow Reactor (VPFR) reactivity (PU).
- Diffusive strained extinction (PU).

Compared in Dooley et al. doi:10.1016/j.combustflame.2010.07.001

- Premixed laminar burning rate (UCONN, PU).
- Premixed strained extinction (UCONN, PU).
- Species evolution as extent of reaction (VPFR, PU; Single pulse shock tube, UIC); Others?

In progress

“Cetane” Autoignition Indicators

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

Cetane Index (CI)

Cetane Number (CN)

Derived Cetane Number (DCN)

Courtesy of AFRL, Tim Edwards

- **IQT DCN (ASTM 6890) known to differ from CN (ASTM 613) values.**
- **“CI” (yielded by data correlation) is not always a reliable indicator of DCN, CN.**
- **Compilations frequently report all three indiscriminately as “cetane number”.**

Exemplar Cases Using POSF 4658 Jet A

POSF 4658 Jet A Sample Comparison

- POSF 4658 is considered to be very similar to the "Global average" in terms of Jet-A fuel properties. (Considerable data involving this sample are already in the literature.).
- All properties of the fuel (as determined experimentally by the MURI project:
  - Empirical Formula of $C_{10.17}H_{19.91}$ determined by C/H direct experimental measurement.

    => "Molecular" weight = 142.01 g/mol and H/C = 1.957.
  - Derived Cetane Number of 47.1±0.3 from Ignition Quality Testing (PU).
  - Threshold Sooting Index of 21.4 from smoke point measurement (PSU).

First Generation Surrogate formulation (n-decane, iso-octane, and toluene mixture) to emulate the real fuel property targets

- Well-developed, validated detailed model descriptions of all of the selected surrogate components yield an ability to compare/interpret predictions against the surrogate mixture experimental results.
- Not major components of the real fuel.
- TSI, MW_{ave} similar to POSF 4658 can not be generated with 1st generation mixtures => compare results with only non-sooting experimental observations.

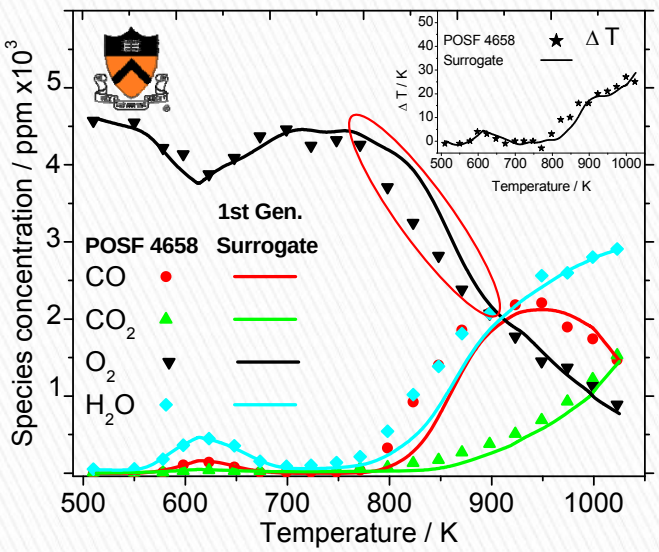
Result

- Promising emulation of real fuel ignition delays (shown in earlier presentation of *Oehlschlaeger*)
  - Dooley et al. doi:10.1016/j.combustflame.2010.07.001 (on line, July 23)*.

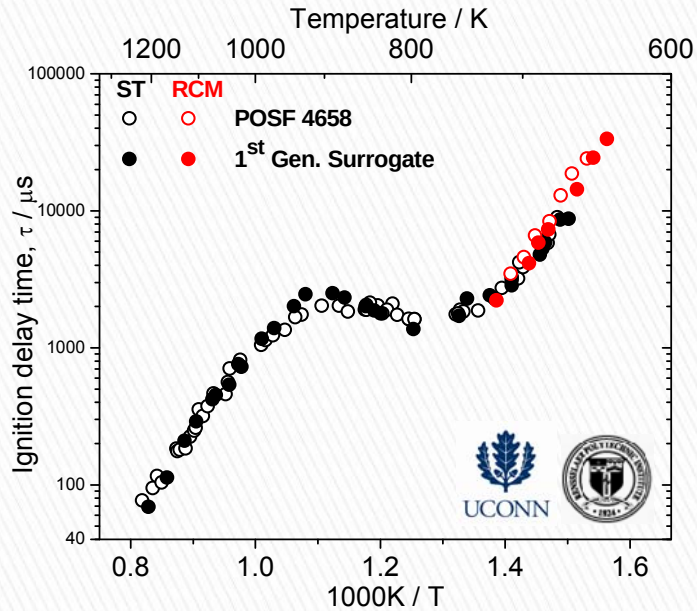
*presented at the 33rd International Symposium on Combustion

1st Generation POSF 4658 Surrogate

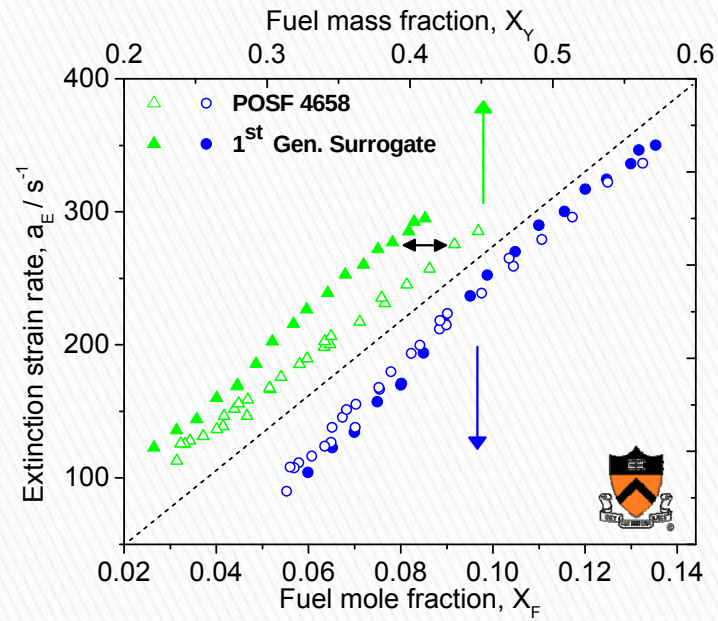
Mole Fraction			DCN	H/C	MW / g mol^{-1}	TSI
Jet-A POSF 4658			47.1	1.957	142.01	21.4
***n*-decane**	***iso*-octane**	**Toluene**				
0.4267	0.3302	0.2431	47.1	2.01	120.7	14.1



Flow reactor oxidation data for conditions of 12.5 atm, 0.3% carbon, φ= 1.0 and *t* =1.8s, for POSF 4658 and 1st generation POSF 4658 surrogate. Inset;DT.



Ignition delay times, φ= 1.0 in air at ~20 atm for POSF 4658 and 1st generation POSF 4658 surrogate.



Strain rates of extinction for counter flow diffusion flames at 1 atm, for POSF 4658 and 1st generation POSF 4658 surrogate.

Results are strikingly similar to real fuel results over a wide range of experimental venues, but the mixture cannot emulate sooting properties.

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Second Generation Surrogate

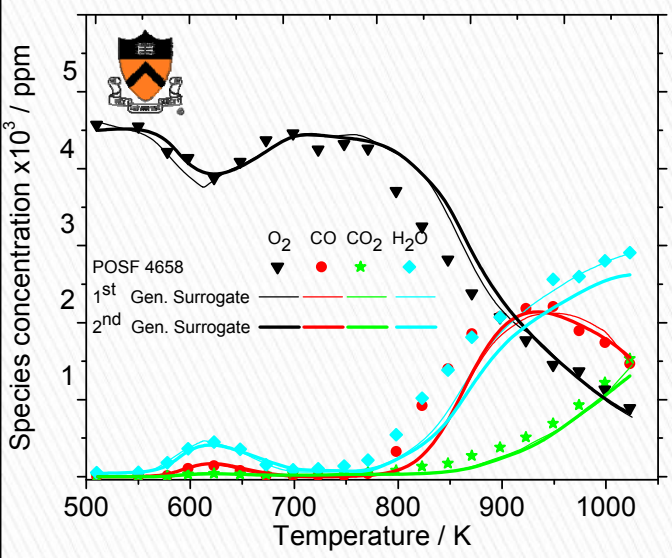
Using higher molecular weight "base" n-alkane permits emulation of all property targets for full range of observed properties for other jet fuel samples.

	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	43.9	43.9	43.9	43.9
(Typical JP-8 values in blue) **TSI**	18.55	19.19	21.47	21.47
Aromatics (vol %); avg.=17.86%	23.51%	22.84%	29.20%	28.45%

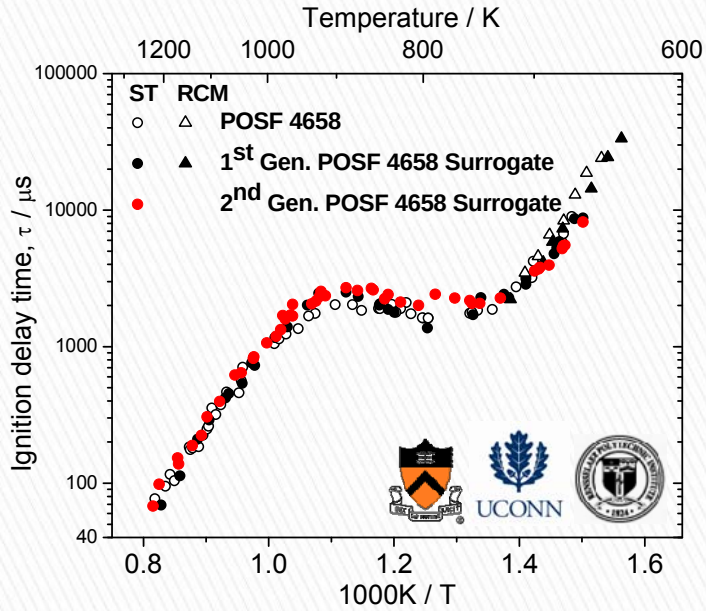
- Second generation DCN map generated for n-C10/iso-C8/nPB/1,3,5 TmB.
- Property targets can be reproduced with a variety of class distributions, no "unique" surrogate blend.
- Are other component chemical classes required, for example weakly branched- or cyclo-alkanes?
- Cyclo alkane component addition is discussed in a later presentation (Dooley).

2nd Generation POSF 4658 Surrogate

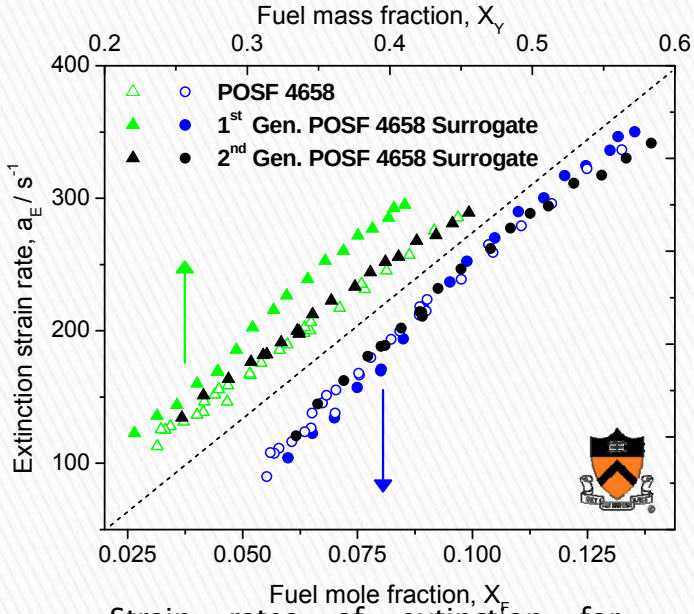
Mole Fraction					DCN	H/C	MW / g mol^{-1}	TSI
Jet-A POSF 4658					47.1	1.957	142.01	21.4
1st Generation surrogate	*n*-decane	*iso*-octane	Toluene		47.1	2.01	120.7	14.1
	0.427	0.33	0.243					
2nd Generation surrogate	*n*-dodecane	*iso*-octane	Mesitylene	n-propyl benzene	48.5	1.95	138.7	20.4
	0.40	029	0.07	0.23				



Flow reactor oxidation data for conditions of 12.5 atm, 0.3% carbon, φ= 1.0 and *t* =1.8s, for POSF 4658, 1st generation POSF 4658 and 2nd generation POSF 4658 surrogate.



Ignition delay times, ϕ= 1.0 in air at ~20 atm for POSF 4658, 1st generation POSF 4658 surrogate and 2nd generation POSF 4658.



Strain rates of extinction for counter flow diffusion flames at 1 atm, for POSF 4658, 1st generation POSF 4658 surrogate and 2nd generation POSF 4658.

1st and 2nd generation surrogates produce nearly identical results!

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Team Presentations

MURI Overview
Frederick L. Dryer
Princeton University

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

Detailed Studies on the Oxidation of Surrogate Fuel Components and Surrogates of JP-8
Kenneth Brezinsky
University of Illinois, Chicago

Sub-mechanism Advancements for Surrogate Fuel Modeling
Henry J. Curran
NUI Galway Ireland (Princeton 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

Fundamental Combustion Data for Jet-A, Constituent Components, and Surrogate Mixtures
Chih-Jen Sung
University of Connecticut

Surrogate Mixture Concepts and Associated Kinetic Studies
Stephen Dooley
Princeton University

Publications

Archival publications (2009-2010)

- M. P. Burke, F.L. Dryer, Y. Ju (2010). ”Assessment of Kinetic Modeling for Lean H2/CH4/O2/Diluent Flames at High Pressures”, *Proc. Combust. Inst.* 33. In Press.
- Z. Chen, M. P Burke, Y. Ju, (2010). “Effects of Extrapolation Method And Flame Radii Range on the Determination of Laminar Flame Speed and Markstein Length Using Propagating Spherical Flames”, *Proc. Combust. Inst.* 33. In Press.
- S. Dooley, S.H. Won, M. Chaos, J. Heyne, Y. Ju, F.L. Dryer, K. Kumar, C.J. Sung, H. Wang, M. Oehlschlaeger, R. Santoro, T. Litzinger (2010). “A Jet Fuel Surrogate Formulated By Real Fuel Properties,” *Combust Flame (on-line).* doi:10.1016/j.combustflame.2010.07.001 *Presented at the 33rd Symposium on Combustion, Beijing China, August 2010.*
- K. Kumar and C.J. Sung (2010). “Flame Propagation and Extinction Characteristics of Neat Surrogate Fuel Components,” *Energy and Fuels* 24, 3840-3849.
- Y. Ju, W. Sun, M. P. Burke, X. Gou, Z. Chen (2010). “Multi-Timescale Modeling of Ignition and Flame Regimes of n-heptane-Air Mixtures Near Spark Assisted Homogeneous Charge Compression Ignition Conditions”, *Proc. Combust. Inst.* 33. In Press.
- X. Gou, W. Sun, Z. Chen, Y. Ju (2010). “A Dynamic Multi-Timescale Method for Combustion Modeling with Detailed and Reduced Chemical Kinetic Mechanisms”, *Combust Flame* 157, 1111–1121.
- K. Kamal and C.J. Sung (2010), “A Comparative Experimental Study of the Autoignition Characteristics of Alternative and Conventional Jet Fuel/Oxidizer Mixtures,” *Fuel* 89, 2853-2863.
- K. Kumar C.J. Sung (2010). “An Experimental Study of the Autoignition Characteristics of Conventional Jet Fuel/Oxidizer Mixtures: Jet-A and JP-8,” *Combust Flame* 157, 676-685.
- A. Mensch, R. J. Santoro, T. A. Litzinger, and S.-Y. Lee (2010). “Sooting Characteristics of Surrogates for Jet Fuels”, *Combust Flame* 157 1097–1105.
- G. Mittal and C. J. Sung (2009). “Autoignition of Methylcyclohexane at Elevated Pressures,” *Combustion and Flame*, 156, 1852-1855.
- K. Kamal, G. Mittal, and C.J. Sung (2009), “Autoignition of *n*-Decane under Elevated Pressure and Low-to-Intermediate Temperature Conditions,” *Combustion and Flame* 156, 1278-1288.
- W. Sun, Z. Chen, X. Gou, Y. Ju (2010). “A Path Flux Analysis Method for the Reduction of Detailed Chemical Kinetic Mechanisms”, *Combust Flame*, 157, 1298–1307.
- S. H. Won, W. Sun, Y. Ju (2010). “Kinetic Effects of Toluene Blending on the Extinction Limit of n-Decane Diffusion Flames,” *Combust Flame* 157, 411–420.
- S. H. Won, S. Dooley, F. L. Dryer, Y. Ju (2010). “Kinetic Effect of Molecular Structure on Extinction Limit of Aromatic Diffusion Flames”, *Proc. Combust. Inst.* 33. In press.

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Dr. Julian Tishkoff; Program Manager; Dr. Timothy Edwards AFRL, technical discussions, fuel samples.

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Conclusions and Future Drivers

- The important issue in selecting surrogate components is the identification of the controlling common intermediate chemical functionalities formed in the combustion of the real fuel.
  - This does not necessarily require inclusion of all of the initial fuel molecular structures to obtain an adequate real fuel emulation.
- We have shown experimentally that the MURI methodology constrains gas phase combustion chemistry properties for likely any mixture of surrogate components used to emulate a real gas turbine fuel.
- Even the most developed and studied kinetic models (n-decane, iso-octane, toluene) need further refinement to predict the transition from low temperature kinetic behavior (hot ignition regime) into beta-scission governed oxidation and the pressure effects on combustion behavior.
- Further validation and kinetic model development for n-C_{12}/iso-C_8/1,3,5 TmB/n-PB underway; more validation data desirable.
  - *N-alkane chemistry is controlling but aromatic chemistry is limiting.*

Model reduction begins with limiting the surrogate selections.

=> Engineering Questions *(Industry input needed)*:

- What level of emulation of real fuel properties must surrogates meet?
- Gas phase kinetic property targets?
- Kinetic model predictive accuracy?
- Liquid fuel thermophysical properties?

Continuing MURI Efforts

- Demonstrate added cases of surrogate mixture comparisons with other gas turbine fuel samples over wide range of fundamental venues
- Test/proof approach for translating MURI mixture formulation concept to applied research investigations.
- Provide further validation data for n-dodecane, n-decane, iso-octane, and alkyl aromatics in kinetic transition to high temperature (beta scission/chemical branching behavior).
- Improve alkane and aromatic oxidation kinetic models for surrogate mixtures.
- Further evaluate/validate MCH kinetic modeling and inclusion of MCH as a surrogate component.
- Produce validation data and evaluate weakly branched alkane surrogate component needs.
- Produce MURI mixture kinetic model and appropriate reductions for validations and applications.
- Strong emphasis on advancing model developments for n-dodecane, n-propyl benzene, and 1,3,5 trimethyl benzene.
- Further evaluate MURI surrogate mixtures to emulate real fuel sooting behavior in fundamental and applied venues.