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

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

Three year program plus two year option

Initiation Date: July 1, 2007

MULTI AGENCY COORDINATION COMMITTEE FOR COMBUSTION RESEARCH (MACCCR)
FUELS RESEARCH REVIEW
National Institute of Standards and Technology (NIST), Gaithersburg MD
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Today's Team Presentations

MURI Overview: Real Aircraft Fuel Modeling Concepts, Surrogate Component Selection, and Observations

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A Study on TSI as a Property Target for Sooting of Jet Fuel Surrogates

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Oxidation of Potential Surrogate Fuel Components of JP-8

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Fundamental Combustion Data for Surrogate Components, Blends, and Jet Fuels

Chih-Jen Sung
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Case Western Reserve University
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Effects of Aromatic Fuel Blending on Extinction Limits and Soot Formation of n-Decane Diffusion Flames

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MURI Purpose

Generate a base jet fuel surrogate component model, cross-validated critical experimental data, detailed and reduced kinetic mechanisms, analytical tools and experimental methods to more accurately predict the complex gas phase combustion behavior of real fuels using 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*

Anticipated Outcome

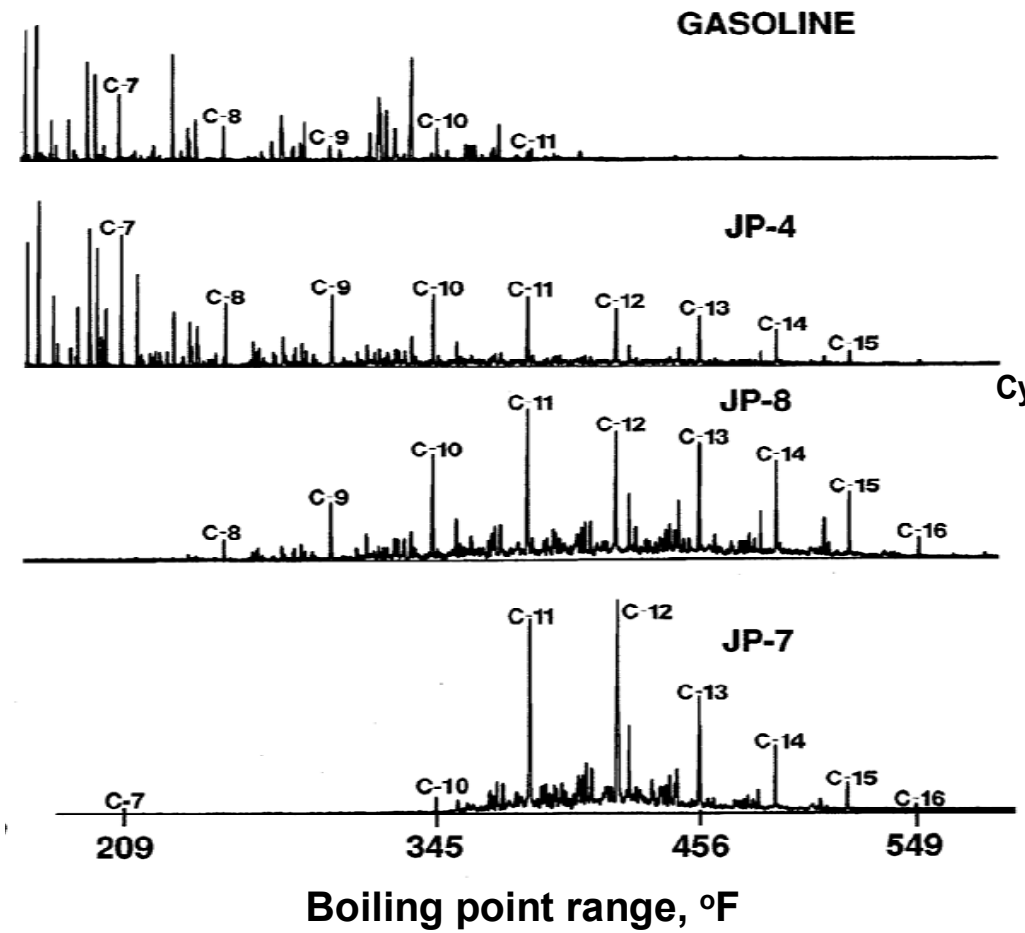
- Validated principles to select surrogate components
- Cross-validated comprehensive experimental database for the selected components and component mixtures
- Detailed kinetic models for individual components, and their mixtures, coupled with laminar transport
- Selection and refinement of combustion target parameters
- Validated rules and methods for formulating surrogate mixtures to replicate real fuel gas phase combustion properties
- Characterizations of real fuel kinetic properties in same fundamental venues as those used to characterize surrogates and surrogate mixtures
- Tools to produce small dimensional models for CFD applications

Impact on DoD Capabilities

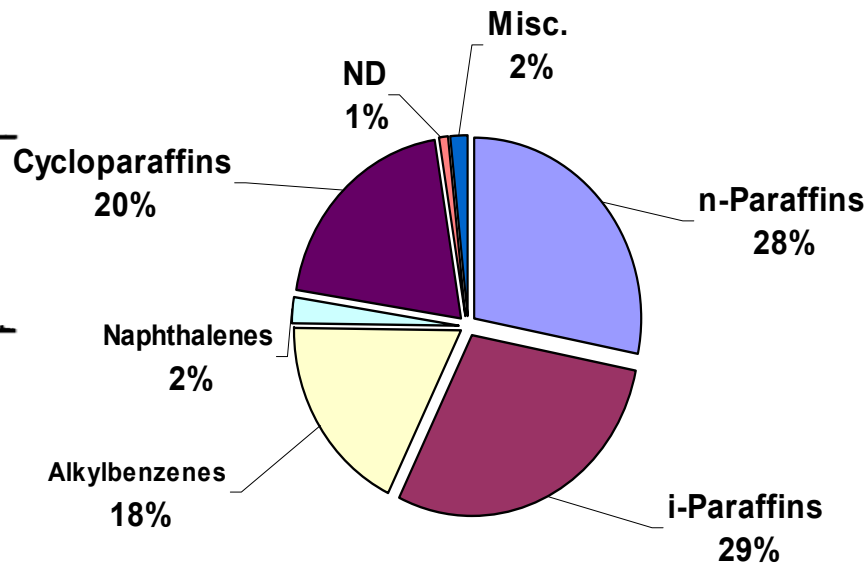
- Enhanced efficacy in evaluating fuel property variations on existing propulsion system performance and emissions
- Improved paper design and development for advancing existing and developing new propulsion/combustion concepts
- Assistance in integrating new non-petroleum-derived alternative fuel resources into the aero-propulsion sector

See http://www.princeton.edu/~combust/MURI/ for further background and program specifics

Real Fuel Chemical Characteristics



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



Distillation properties and class compositions vary with region and time

Colket et al. AIAA Paper 2007-770

Petroleum-derived Jet Fuel Variability(+)

Select ASTM Test Properties	JP-8			JA-1		
	Min	Max	Avg.	Min	Max	Avg.
Hydrogen Content (mass %)	13.40	14.78	13.81	NR	NR	NR
H/C Ratio	1.844	2.067	1.909	NR	NR	NR
Cetane Index (CI)	31.8	56.8	43.9	NR	NR	NR
Smoke Point (SP, mm)	19.0	31.0	22.7	24.0	27.0	26.2
Aromatics (liq. vol %)	0.10	24.60	17.86	15.20	19.40	17.58
(TSI)**	15.72	25.66	21.47	19.71	22.17	20.31
Density (g/ml, 15°C)	0.7800	0.8325	0.8038	0.7865	0.7986	0.7904

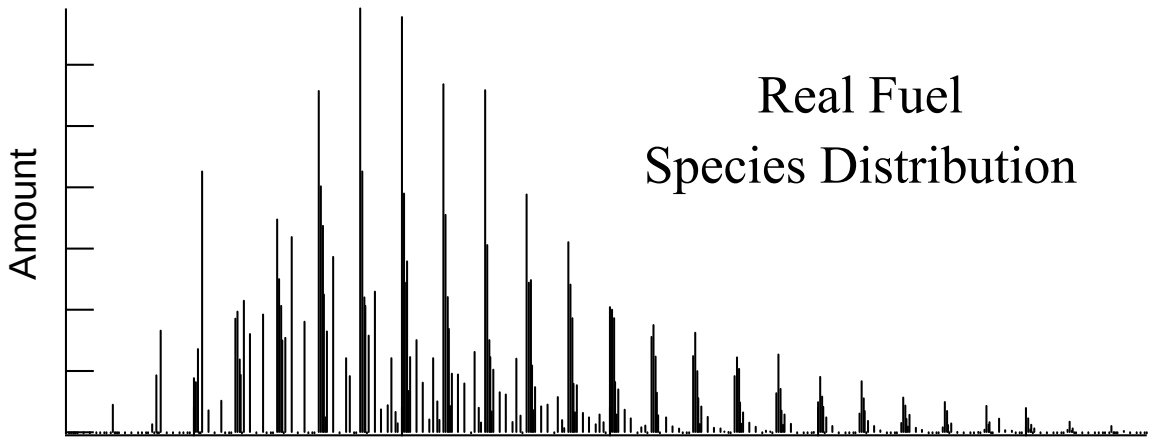
NR - Not Reported

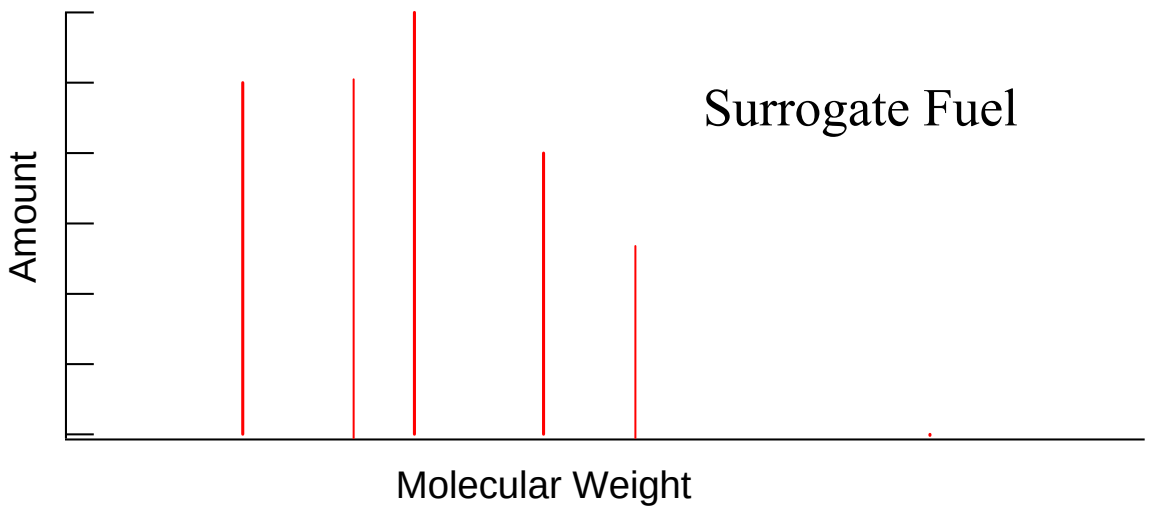
Data from http://www.desc.dia.mil/DCM/Files/2006PQISreport.pdf

(+) - No oxygenated species present. F-T alternative fuel liquids are typically sulfur free, mostly alkanes, and increase hydrogen content, and lower aromaticity when blended with conventional petroleum derived fuels

(**) -Threshold Sooting Index (TSI) values estimated assuming $C_{11}H_{21}$ for JP-8 and $C_{12}H_{23}$ for Jet-A:
TSI = 3.18 (*MW*/SP) where *MW* is the molecular weight (*Yang et al. (2007) Combust Flame 149, 191*)

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!*

- *Which components are needed to emulate real fuel variability?*
- *How many are needed?*
- *Component blending rules to match any real fuel?*

Surrogate Component Selection and Mixture Formulation

Typical approach in the literature:

- Types of components to include:
  - At least one component from each molecular class found in real fuels
- Surrogate mixture composition to model real fuel behavior:
  - Match surrogate molecular class composition to that of the real fuel
  - Compare real fuel behavior and surrogate mixture behavior in wide variety of fundamental test venues
    - Use well-characterized jet fuel samples to validate the result (AFRL)
    - Determine chemical class composition of the real fuel to be emulated
    - Perform numerous validation experiments against each real fuel in specialized instrumentation (e.g. flow reactors, RCM, shock tubes, flames….) over appropriate pressure, equivalence ratio, and temperature ranges

This approach is excellent for proof of concept, but not amenable for producing specific surrogate mixtures to emulate specific real fuels

Desire mixture formulation concepts that permit matching surrogate and real fuel gas phase combustion-related properties without extensive additional testing

Surrogate Fuel Model Construction

I. Select minimum number of components that will permit emulating chosen real fuel combustion property targets (Princeton-Dryer)*

II. Expand experimental validation database for individual components, component mixtures, and real fuels (All)

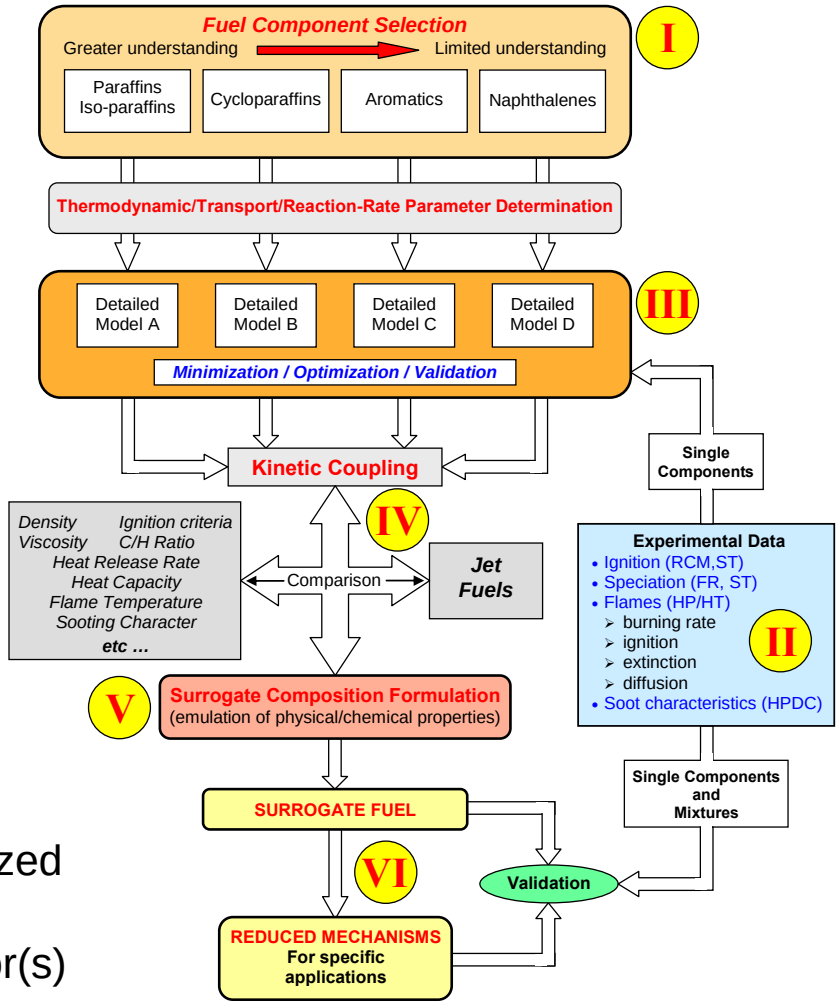
III. Develop minimized/optimized models for chosen targets and operating parameter ranges (Princeton-Dryer/Curran, UIUC-Brezinsky)

IV. Define appropriate targets that surrogate mixtures should emulate (Princeton-Dryer)

V. Cross-compare jet fuel and surrogate mixture target behavior (All)

VI. Develop/apply methods to produce smaller dimensional representations of minimized/optimized models (Ju)

*Principal contributor(s)



http://www.princeton.edu/~combust/MURI/

Guiding Kinetic/Transport Concepts

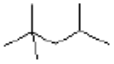
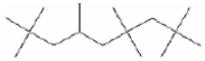
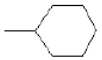
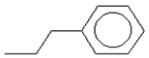
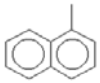
- Overall net active radical pool defined by production/consumption rates
- H/C ratio affects radical and hydrogen production rate, intermediate fragments, diffusion rates, and reaction zone structure
- Radical pool of alkanes, cyclo-alkanes typically suppressed by aromatics. Pure component reactive 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 fuel hydrogen content and aromatic content (and structure)
- Hydrocarbon mixture transport effects related to reactant molecular weights as well as their intermediate fragments

Current 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)

  Comprehensive C7/C8/Toluene model exists

  High Temperature models available now; further validation studies underway presently

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

Experiments

- Comprehensive experimental database for developing and validating kinetic models for individual components and their interactions
  - First and second stage autoignition behavior in both dilute and higher fuel concentration conditions
  - Heat release rate
  - Major species evolution histories
  - Laminar flame speed
  - Premixed and non-premixed extinction limits
  - Premixed and non-premixed ignition
  - Sooting under more applied fluid dynamic conditions
- Develop and verify concepts for reproducing combustion property targets of a specific real fuel with a surrogate mixture

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)
    - Autoignition: Ignition Quality Testing (IQT) and Derived Cetane No. (DCN), Dryer
- **Case Western Reserve University (CWRU)**
  - 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

H/C Ratio Constraint and Molecular Class Composition

- H/C affects flame temperature and local equivalence ratio, important in mixing-limited systems
- If H/C is *not matched*, then for the same overall equivalence ratio, air/fuel mass flow rates for predictions will not emulate those in the real device
  - Mixing/turbulence effects may be mismatched for specific device design and operating conditions
  - Local equivalence ratios will be incorrect in non-premixed reacting environments
- Reproducing class composition fractions of the real fuel is an imprecise method for reproducing H/C ratio
  - ASTM reported H/C ratios, hydrogen content, and aromatic fraction are based on correlations with properties that include distillation curve, etc., typically *not* direct measurements

Use components that in appropriate combination permit matching real fuel H/C ratio, sooting, and autoignition behavior over ranges found (expected) for present (and future) real petroleum-derived and alternative fuels

Sooting Properties and Real Fuel Data

- Smoke Point (SP) typically reported for real fuels (ASTM D1322)
  - Standardized flame height empirical method
- Threshold Sooting Index (TSI) – apparatus independent re-interpretation of smoke point measurements (Calcote and Manos)
  - TSI= a(MW/SP)+b, correlation parameters developed by several investigators (Gill and Olsen)
    - Extensive data available but derived based from several different sources
- TSI based approach predicts well jet fuel sooting in real combustors (Yang et al., 2007)
- TSI properties of hydrocarbons (Yan et al., 2005) and hydrocarbon oxygenates (Pepiot-Desjardins, 2008) can be predicted through structural group contributions – fundamentally supports ability to reproduce real fuel TSI's with appropriate component mixtures

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

Yan et al. (2005) Energy & Fuels 19, 2408; Pepiot-Desjardins et al. DOI:10.1016.combustflame.2008.03.017

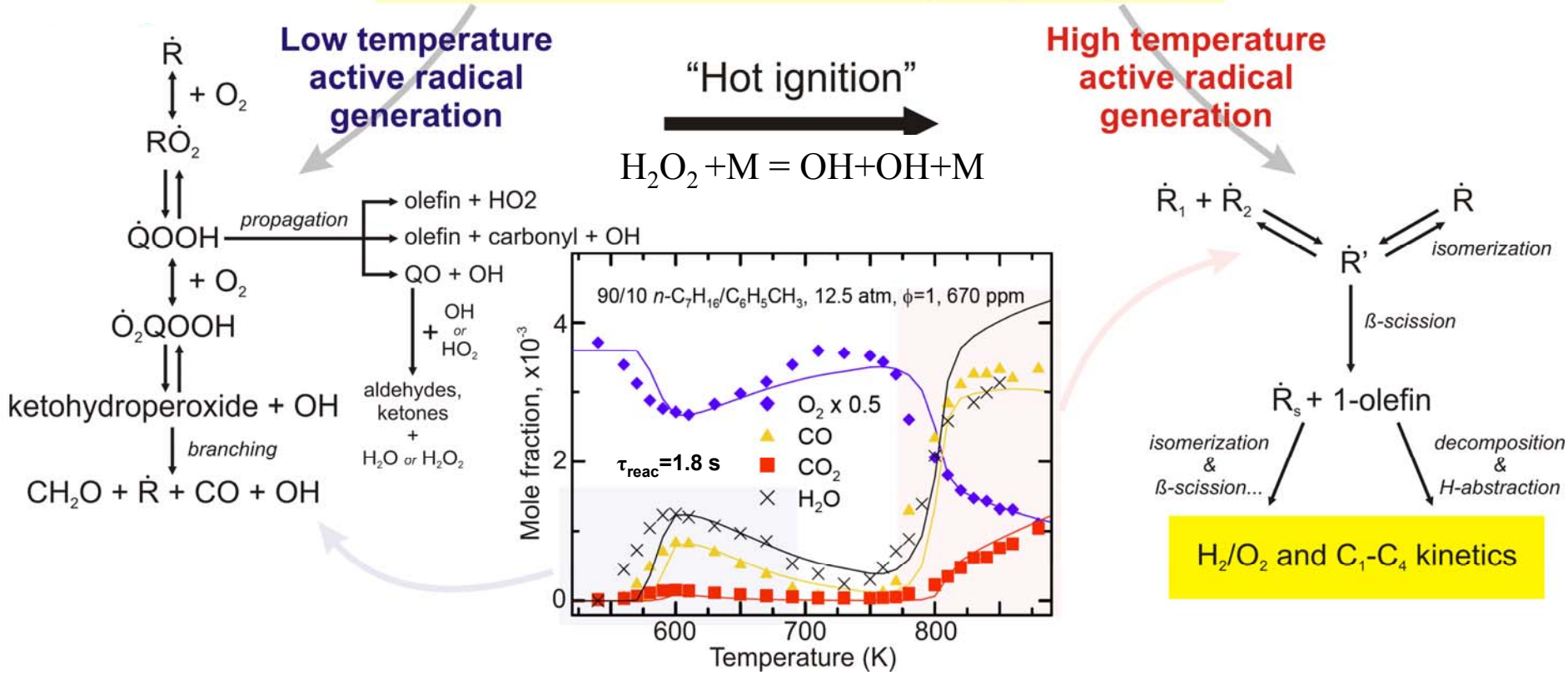
Autoignition of High Carbon Number Hydrocarbons

$RH + O_2 \rightleftharpoons \dot{R} + HO_2$ Low Temperature

$RH \rightleftharpoons \dot{R}_1 + \dot{R}_2$ High Temperature

Chemical initiation

$RH + X \rightleftharpoons \dot{R} + HX$ $X = OH, HO_2, CH_3, H, O$ Fuel destruction



Species Mole Fraction v Initial Reaction Temperature

Autoignition Properties of Aircraft Fuels

- Comparing surrogate mixture two stage autoignition behavior with real fuel in fundamental experiments (i.e. shock tube, RCM, and flow tube experiments) is ineffective for *formulating* appropriate mixture compositions
- Octane (ON) or Cetane (CN) numbers are used as autoignition property targets for conventional gasoline and diesel fuel applications
  - Ghosh et al. (2006) show Octane and Cetane numbers of real fuel mixtures correlate with hydrocarbon "lumps" measured using GC – indicative that chemical functional groupings control autoignition behavior.
  - Cetane Number blending for components may be non-linear
    - Example – Using "pre-ignition" flow reactor studies, Natelson et al (2008) suggest non-linear CN number blending of n-dodecane and MCH.

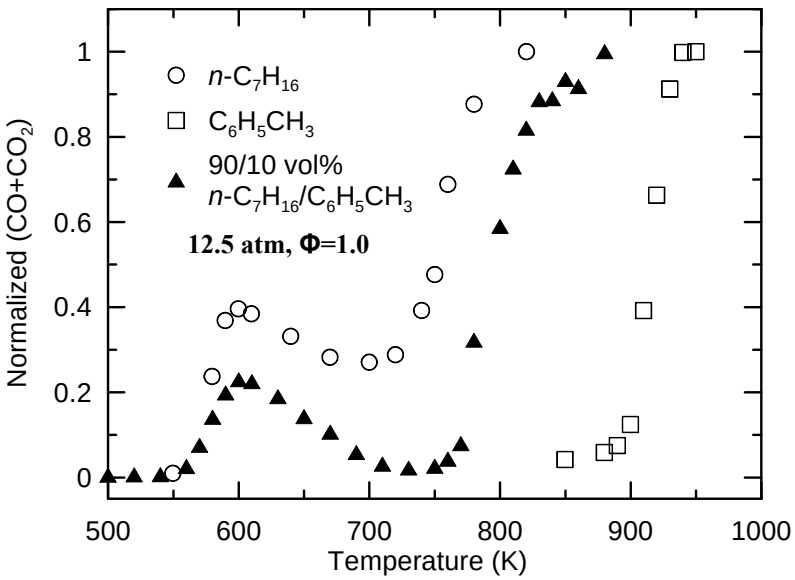
Consider CN as appropriate autoignition measure for gas turbine as well as diesel applications

- Need a self consistent database for components and mixture CN's as well as comparison with real fuel behavior for rigorous validation of the concept

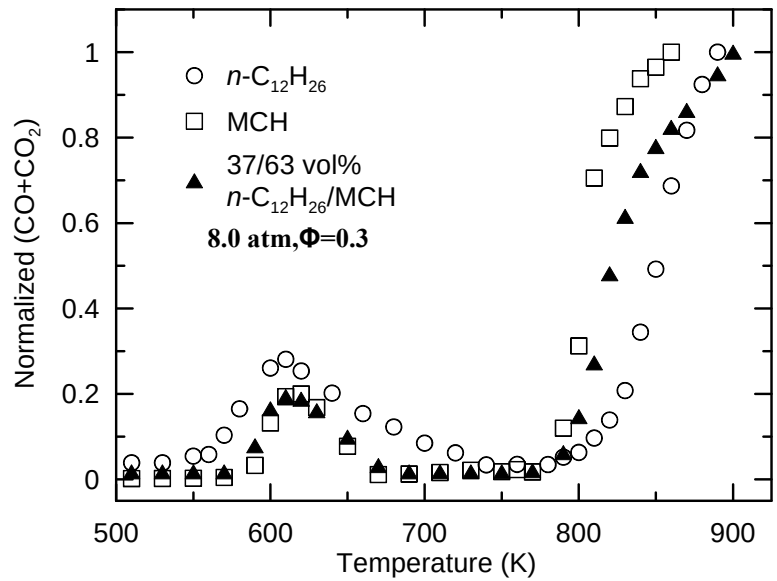
Ghosh et al. (2006) Ind. Eng Chem. 45 337 and 346; Natelson et al. (2008) Fuel 87, 2339

Blending Effects on Autoignition Behavior

n-heptane/toluene blending



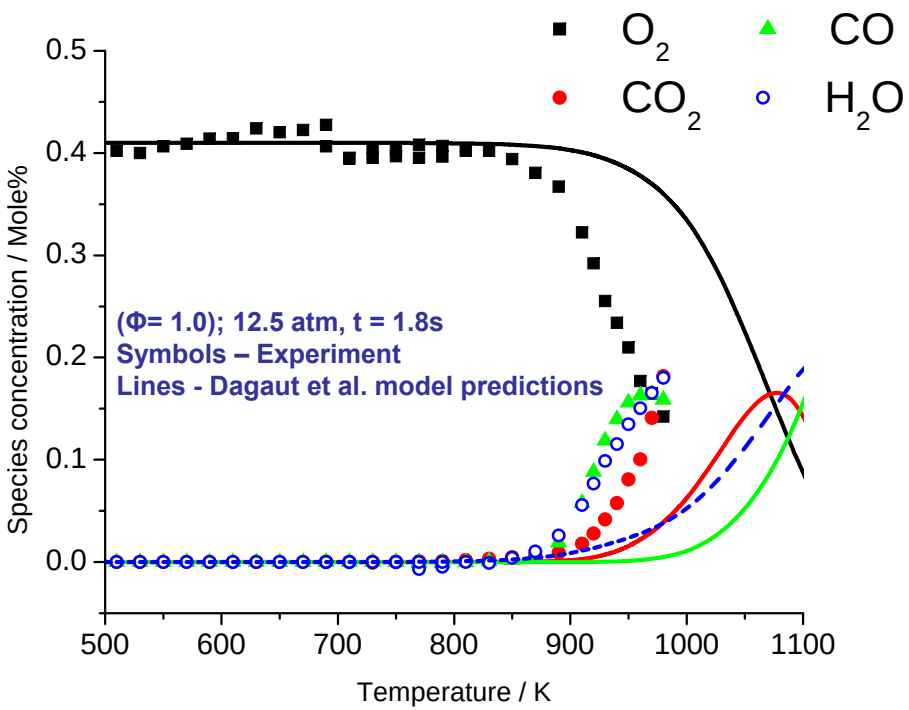
n-dodecane/ methylcyclohexane blending

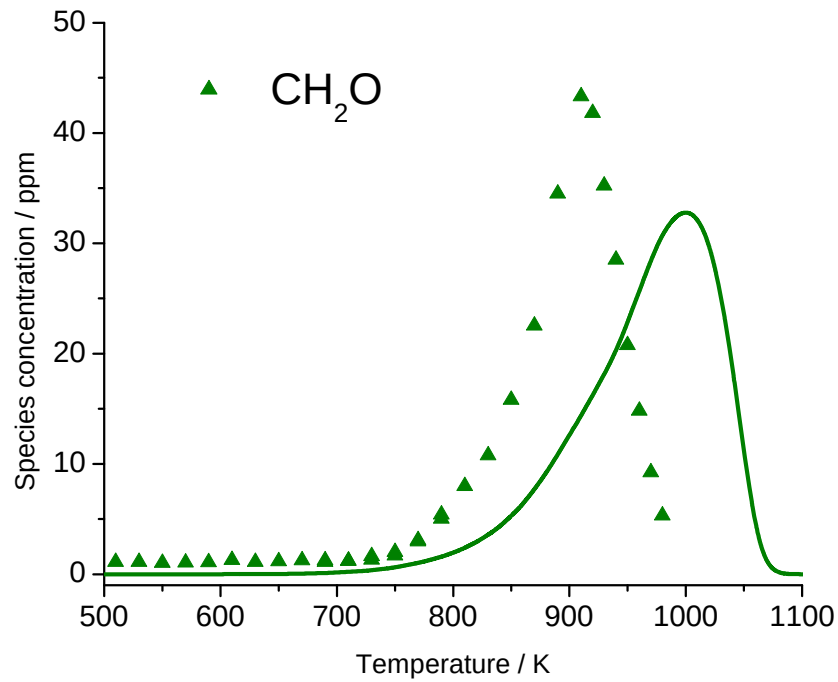


- Addition of toluene to n-heptane inhibits low temperature reactivity and *increases* the hot ignition temperature
- Addition of MCH to n-dodecane inhibits low temperature reactivity and *decreases* the hot ignition temperature
- Overall autoignition properties of blends are affected by influences on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

n-Propylbenzene Reactivity Properties

Preliminary Data



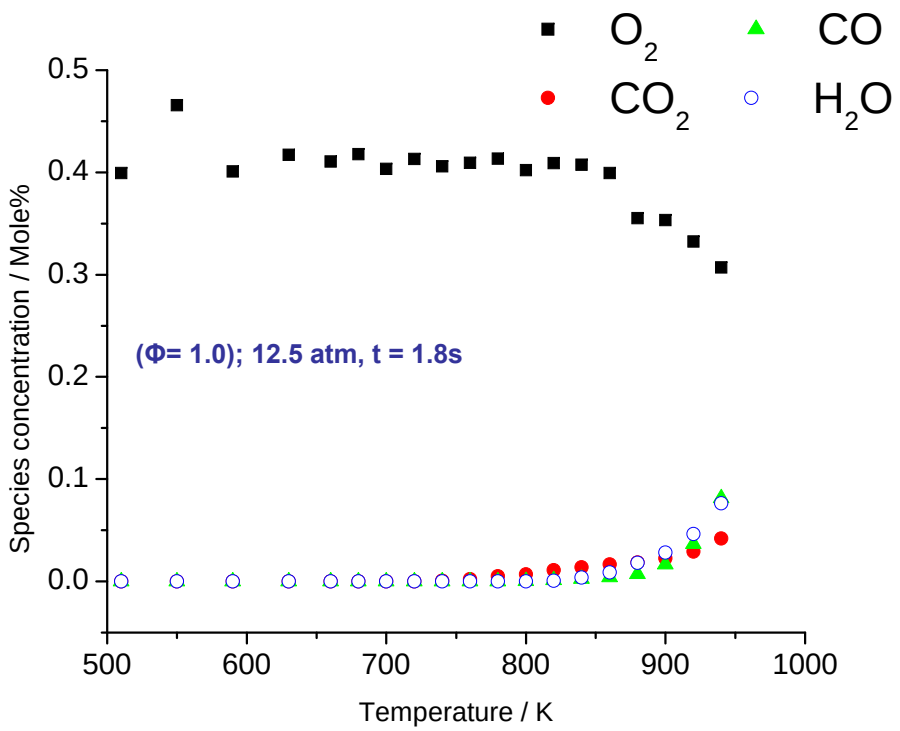


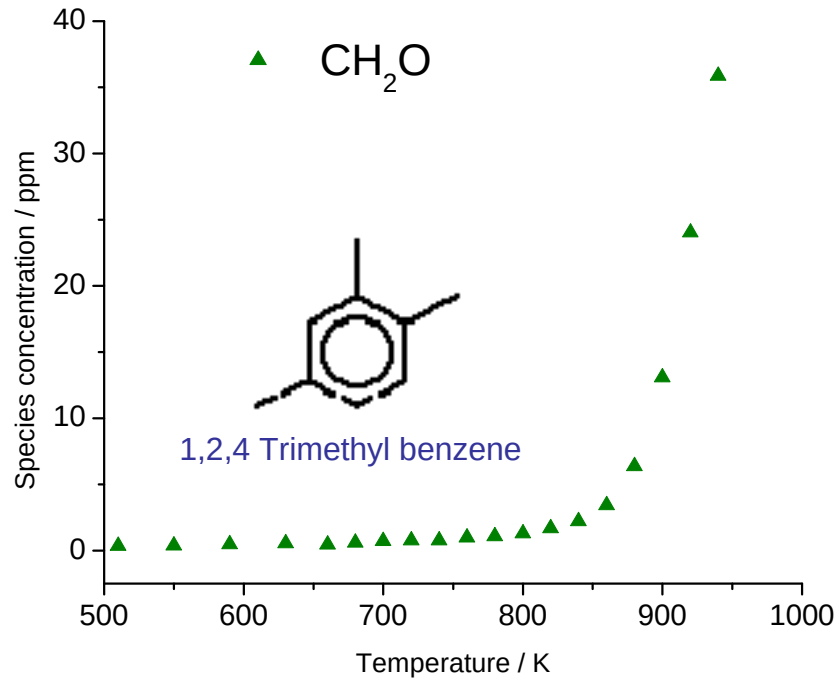
- No NTC, no low temperature reactivity observed
  - Similar result shown previously for pure toluene oxidation
- Comparison against only model in the literature shows further model development/validation are needed

Dagaut et al. (2002) Fuel, 81, 173

1,2,4-Trimethyl Benzene Reactivity Properties

Preliminary Data

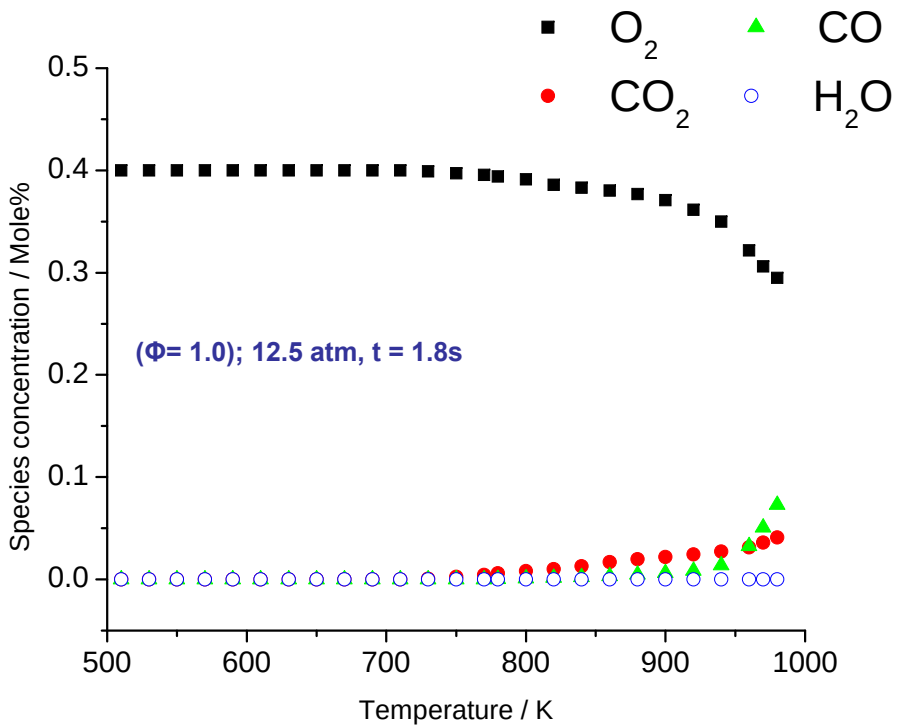


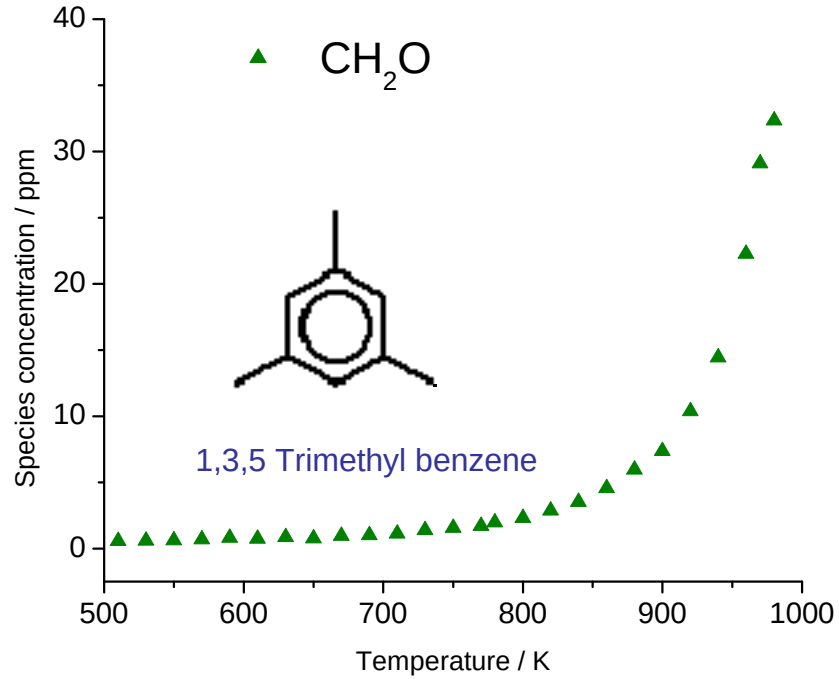


- No NTC, no low temperature reactivity observed
- Higher hot ignition temperature than n-propyl benzene
- No model available in the published literature

1,3,5-Trimethyl Benzene Reactivity Properties

Preliminary Data





- No NTC, no low temperature reactivity observed
- 1,3,5 isomer has similar hot ignition temperature to 1,2,4 TMB, but is less reactive thereafter
- No model available in the published literature

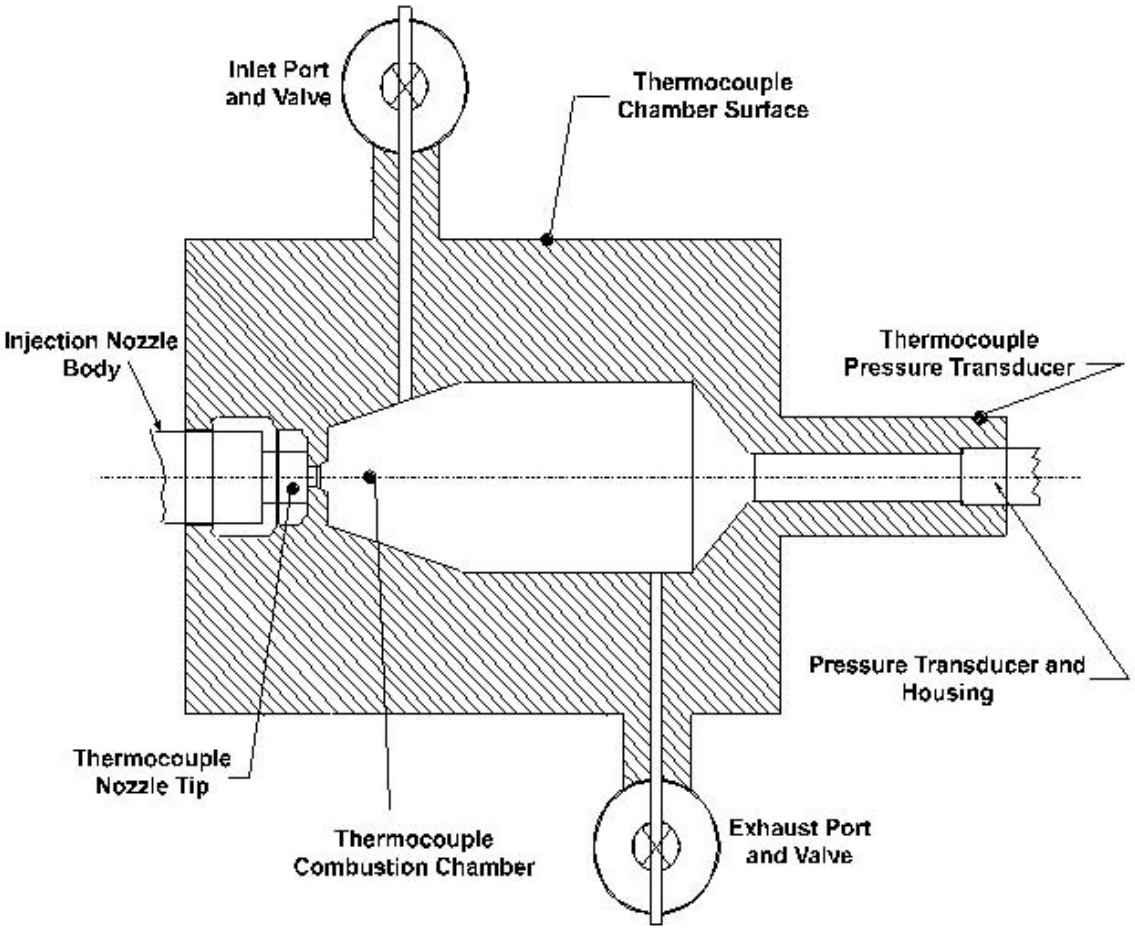
Advances in Cetane Determination Methods

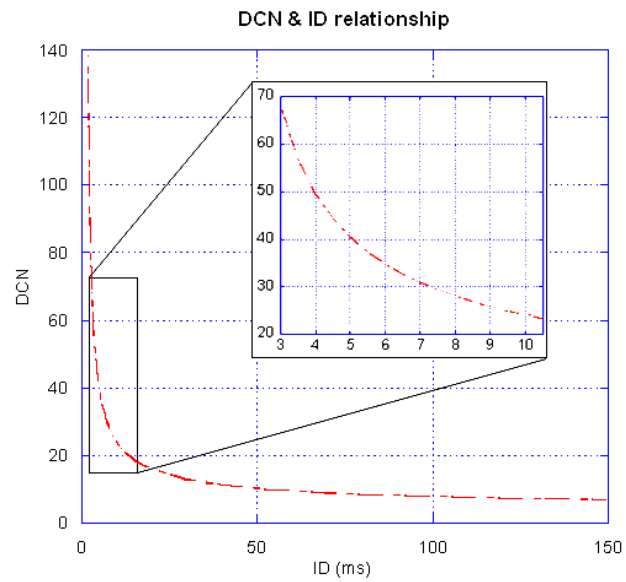
Is there a simple method for surrogate mixture and real fuel applications?

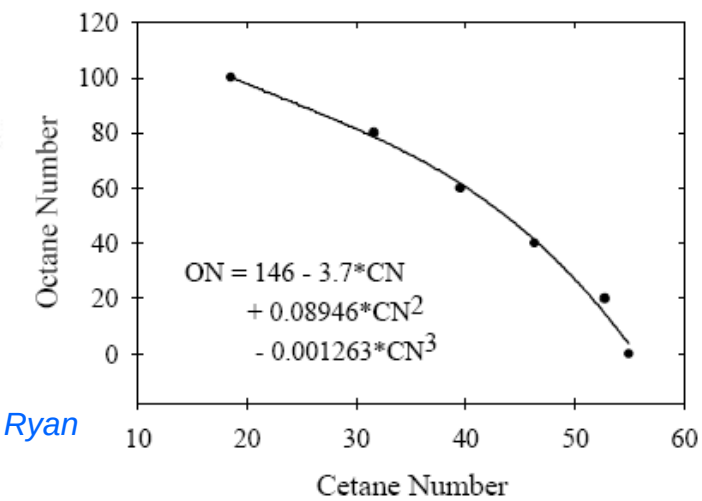
- ~~*Cetane Number (CN)* - Determined by **Engine Testing (ASTM D-613)**~~
  - ~~Requires industry standard test engine and instrumentation, operated under specific conditions~~
  - ~~Compression ratio is varied for the test sample and reference fuels of known cetane number to obtain a fixed ignition delay.~~
- ~~*Cetane Index (CI)* - **(ASTM D-976 or D-4737)** – presently reported for JP-8~~
  - ~~Frequently substituted for CN because D-613 is expensive and time-consuming.~~
  - ~~Derived from the fuel's density and distillation curve parameters.~~
  - ~~May also have larger uncertainties for fuels with disparate distillation curves~~
  - ~~Cannot be used in determining CN of surrogate components or mixtures~~
- *Derived Cetane Number (DCN)* **- IQT , i.e. Ignition Quality Testing*** (**ASTM D6890, IP 498, ASTM - 7170)**
  - Rapid, constant volume combustion method
  - Determines the pressure- and temperature-dependent autoignition characteristics
  - Can be used with surrogate components, mixtures, and real fuels (with/without additives)
  - Emerging as an internationally accepted testing method for fuel qualification. Easily applied to single components, mixtures, and real (both petroleum derived and alternative) fuels to determine CN and test CN emulations.
  - Operating methodology can also be re-configured to determine high pressure autoignition temperatures
  - Only low sample volumes are required per test (~50 ml)
  - *Twenty minute test vs. many hours of experiments with flow tubes or shock tubes to determine surrogate blending rules and matching of surrogate mixtures and real fuels*

**http://www.aet.ca/index.php?section=1*

Ignition Quality Testing (IQT) and DCN







From extensive work on IQT, DCN and autoignition temperature research of T. Ryan and co-workers, at Southwest Research Institute (SWRI), San Antonio, TX

DCN's for Reference Aircraft Fuel Samples

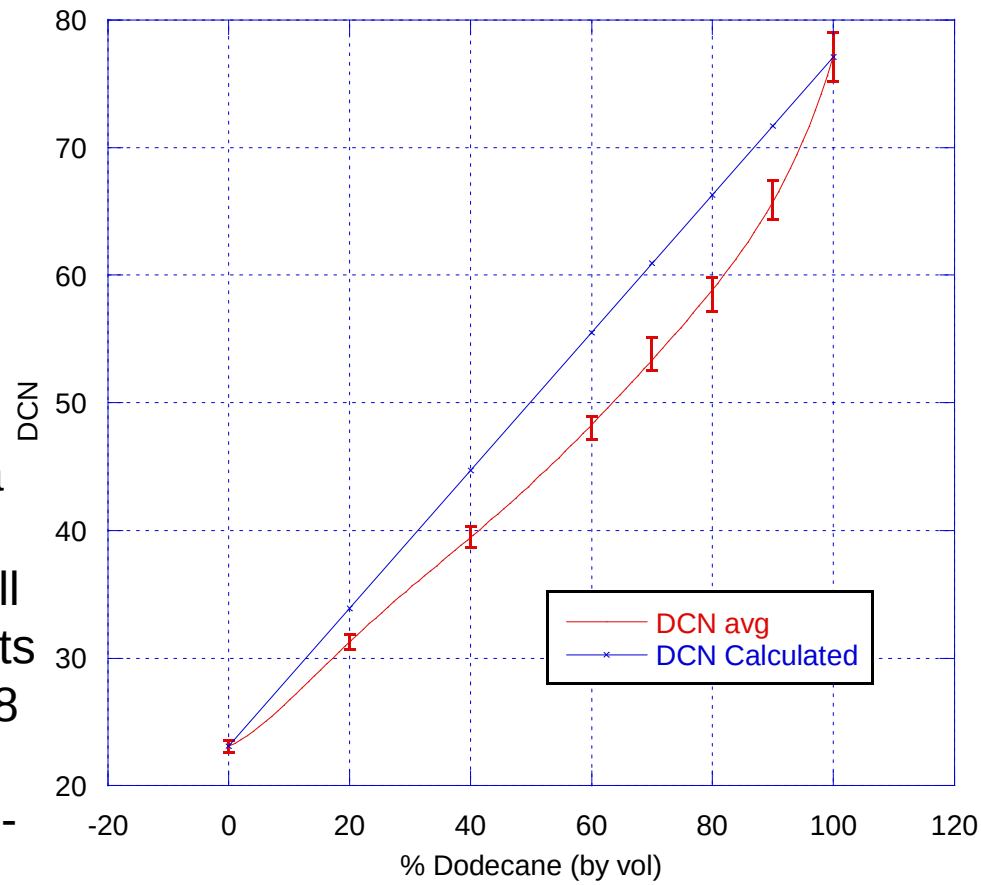
Sample Description	DCN
Wright Patterson AFB-POSF-3602-Jet-A	38.35
Wright Patterson AFB-POSF-3638-Jet-A	44.74
Wright Patterson AFB-POSF-3684-JP-8	43.14
Wright Patterson AFB-POSF-3773-JP-8	47.79
Wright Patterson AFB-POSF-4177-JP-8	40.15
Wright Patterson AFB-POSF-4658-Jet"A"Blend	45.27
Wright Patterson AFB-POSF-4765 - coal based naphthenic fuel	32.95
Wright Patterson AFB-POSF-4795/JP-10	18.64
Wright Patterson AFB-POSF 5140-TS-1 Jet fuel	40.81

- DCN's of real fuels with and without additives are easily determined
  - Provides a real fuel property target for surrogate fuel mixtures if DCN's and blending functions of surrogate components are known.

Courtesy of AFRL, Tim Edwards (2008); Data obtained using IQT at SWRI

DCN and Blending Function for n-dodecane/MCH Mixtures

- Functional relationship derived in less than two hours
- DCN blending is non-linear, especially outside 35<DCN<65 (typical real fuel range)
  - DCN outside of this range may be affected have larger measurement uncertainties
  - CN, CI, and DCN may also differ as a result of inaccuracy and/or reproducibility of each method, as well as relative sensitivities to contaminants
    - Example: DCN of n-dodecane is 78 but literature CN is ~88
- Similar blending interactions found for n-decane/ iso-octane, n-decane/1,3,5 trimethylbenzene, and n-decane/n-propylbenzene blends



Unpublished DCN data from J. Henye and A. Boehman at PSU, (2008)

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	43.9	43.9	43.9	43.9
TSI	18.55	19.19	21.47	21.47
Aromatics (vol %); avg.=17.86%	23.51%	22.84%	29.20%	28.45%

- Property targets can be reproduced with a variety of class distributions, without reproducing that of a particular Jet A
- Sooting propensity does not correlate with aromatic fraction alone
- Consistent reference data sets for component TSI, CN and blending characteristics are needed to rigorously test the concept

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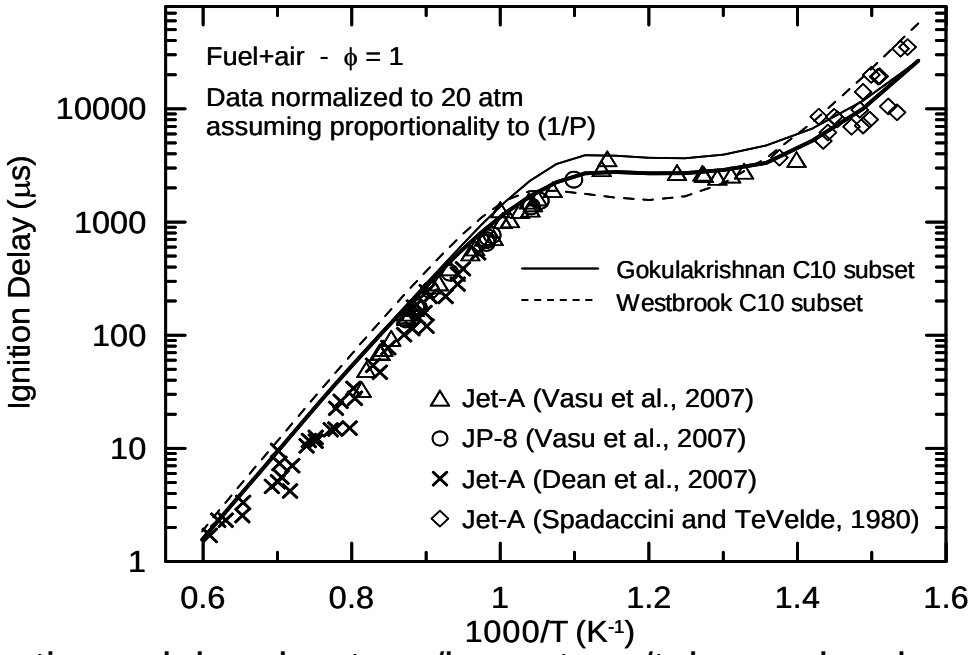
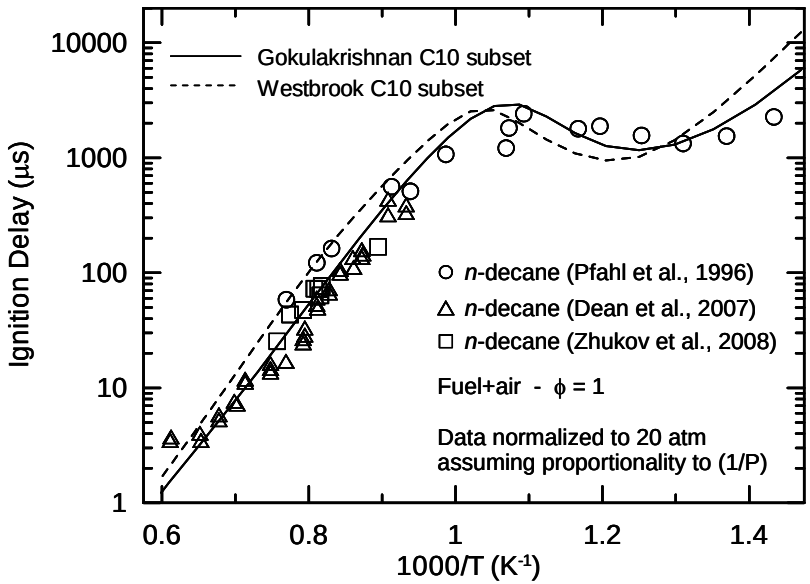
Ignition Delay Predictions for Jet Fuels

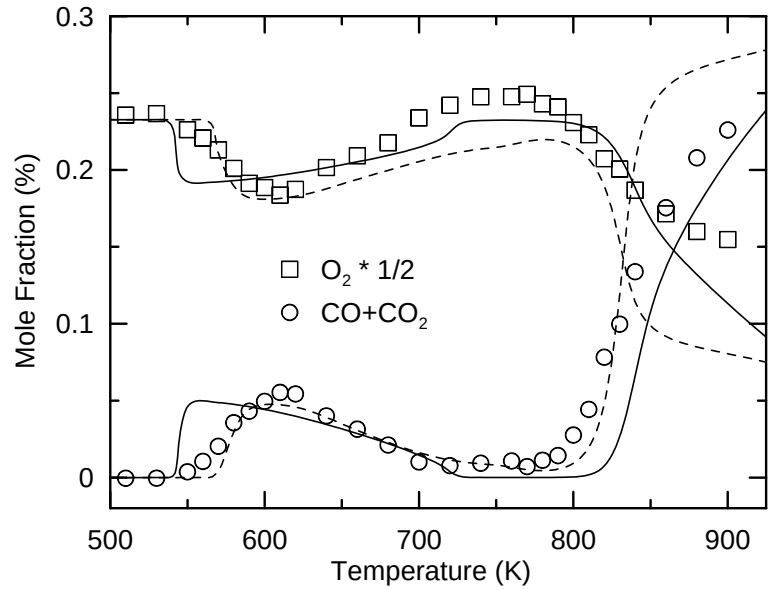


- Jet A Target Data: 13.9 wt% hydrogen (H/C=1.924); CN=43.3 TSI unknown
- Surrogate Mixture (vol %): 49.5% n-decane, 28.2% iso-octane, 22.3% toluene

- 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, 2008, submitted*)
- Constant U, V modeling assumptions, except for bold solid line which considers reflected shock pressure rise and polytropic compression prior to ignition (~10%/ms)

Model Predictions for n-Decane





- Surrogate model ability to reproduce jet fuel NTC characteristics depends on ability to reproduce data for pure alkanes
- Model predictions differ in simulations of data collected in different experimental venues
- In example above models predict turnover temperatures differently under shock tube and flow reactor conditions
- Stresses need for self-consistent dataset for pure, binary, ternary, etc. mixtures
- Availability of data collected over a wide range of parameters and in different facilities ensures proper model optimization so that a “comprehensive” model can be developed
- Data needs to be scrutinized for non-idealities so that proper interpretation can be applied to modeling

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Comparison of Property Targets of Published Surrogate Mixtures with Jet Fuel Ranges

Reference Information for next Chart

- TSI values are obtained from Olson et al. (1985)
- CN numbers are taken from Santana et al. (2006)
- Linear relationships for TSI (Yang et al., 2007) and CN (Murphy et al., 2004) adopted for computing mixture values
  - $TSI_{mix} = \Sigma x_i TSI_i$
  - $CN_{mix} = \Sigma v_i CN_i$
    - x_i and v_i are the mole and volumetric fractions, respectively, of each species.
    - Experimental Validation of functional relationships underway for both TSI and Cetane number as part of this MURI

Highlighted values in following chart represent projected surrogate mixture parameters that do not fall within those found for real fuels

Mixture Make-up (vol%); Sample Compositions from the Literature

Component	Schulz	Mont-gomery	Violi Sur_3	Agosta S5	Agosta M2	Cooke	Eddings Hex-11	Stanford Mix A
iso-cetane				36.0%				
n-hexadecane	10.2%						7.8%	
n-tetradecane	15.5%					27.7%		
n-dodecane	21.1%	41.8%	73.5%	26.0%	37.0%	36.4%	48.5%	65.2%
1-methylnaphthalene	3.9%			18.0%				
n-decane	16.2%	33.6%						
decalin				6.0%			29.2%	
tetramethylbenzene	4.4%							
n-butylbenzene	4.6%	13.8%						
tetralin	4.1%					3.6%	5.8%	
n-octane							3.0%	
iso-octane	5.7%		5.5%			8.8%		21.9%
m-xylene	4.6%					9.8%	5.6%	
cyclooctane	4.7%							
methylcyclohexane	5.1%	10.8%	10.0%	14.0%	63.0%	13.6%		6.8%
toluene			10.0%					5.6%
benzene			1.0%					0.5%
Aromatics (vol. %)	21.5%	13.8%	11.0%	18.0%	0.0%	13.5%	11.4%	6.1%
H/C	1.866	2.034	2.015	**1.807**	2.060	1.990	1.919	**2.093**
H (wt %)	13.54%	14.58%	14.46%	**13.17%**	14.74%	14.31%	13.87%	**14.94%**
MW (g/mol)	147.284	143.620	140.861	159.120	116.066	144.379	151.448	140.357
CN	**60.36**	**66.20**	**67.49**	32.91	45.26	**62.75**	**62.44**	**61.61**
TSI	21.64	**14.28**	**12.43**	**29.57**	**4.95**	**14.63**	16.75	**9.53**
Density (g/ml)	0.79218	0.76383	0.76462	0.82487	0.76562	0.77358	0.81132	0.74882

MURI Accomplishment Highlights

Surrogate Mixture formulation

- Determined specific surrogate component for forming mixtures
- Evaluating matching H/C ratio, threshold sooting index (TSI), and derived cetane number (DCN) rather than matching the molecular class composition.
- Developed reference database of TSI's from component smoke point measurements
  - Calculated TSI's of mixtures based upon a new database of component
  - TSI values derived from smoke point measurements compare favorably with real fuel experimental data.
  - Simulation of real fuel TSI using surrogate mixture candidates shows promise.
- 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 compared with real fuel DCN using simple efficient methods
  - New element of program initiated on DCN investigations using Ignition Quality Testing (IQT) Methods
  - Numerical model predictions of ignition delay for simple component mixtures with matching H/C, DCN with those of real jet fuels show promise.

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.
- 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 Contributions

- 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 alylated single ring aromatics (with UIC) underway.
- Re-discovery of non-ideal fluid dynamic and localized ignition effects on modeling assumptions for shock tube ignition delay measurements investigated (may affect prior model validation and developments)
- Dynamic multi-scale method for detailed kinetic model reduction was developed.

Publications/Presentations/Preprints

Archival publications

•G. Mittal and C. J. Sung, "Homogeneous Charge Compression Ignition of Binary Fuel Blends," *Combustion and Flame*, in press.

•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*, in press.

Non-Archival Preprints and Presentations

•M. Chaos and F.L. Dryer, "Chemical-kinetic Modeling of Ignition Delays: Considerations in Interpreting Shock Tube Data", Int. J. Chem. Kin. (2008) Submitted.

•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, 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. 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.

•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.

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