Brief Summary of Work in Progress

(presented at the Surrogate Fuels Working Group meeting , Jan 6th 2008, Reno, NV)

posted on MURI Website – Jan 16, 2008

Principal Investigator: *Prof. Frederick L. Dryer*

Other Co-Investigators and Institutions:

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

Visiting Researchers:

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

Technical Management: *Dr. Julian Tishkoff, AFOSR*

AFOSR MURI FA9550-07-1-0515

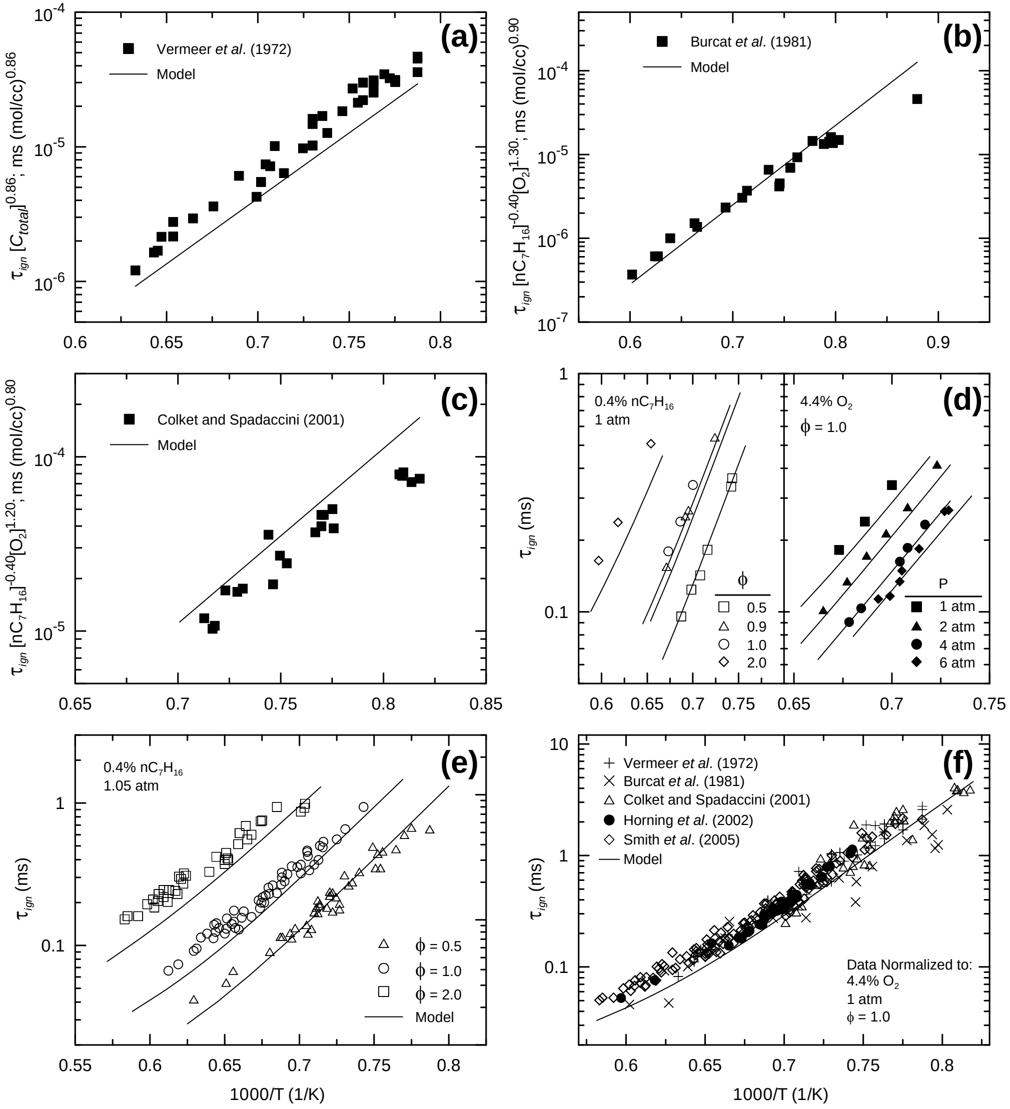
Objective

- Brief descriptive summary of some of the efforts underway over the period July 1 – December 31, 2007 on this program.

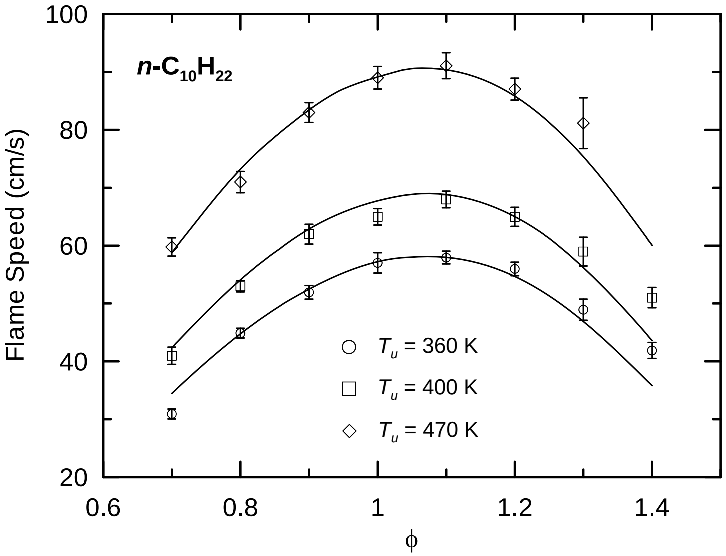
- Specifics will appear in preprints and publications as well as at the annual progress review being scheduled for early fall, 2008 (Date, Location to be determined)

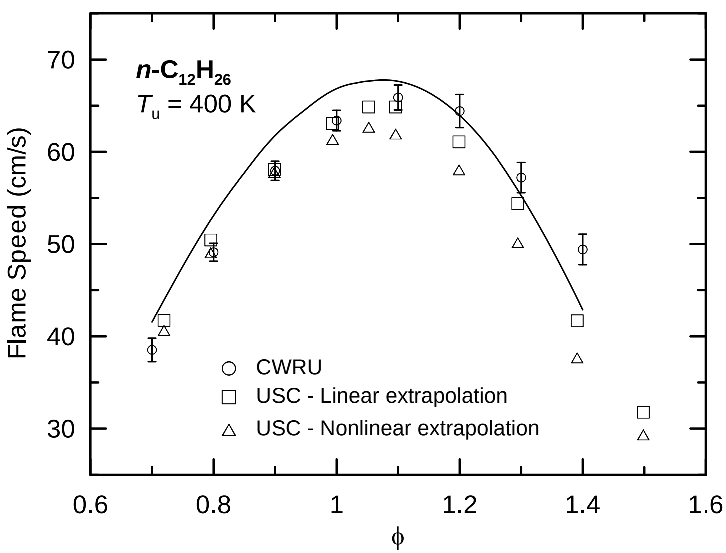
Current Large Molecule High Temperature Models (Dryer, PU)

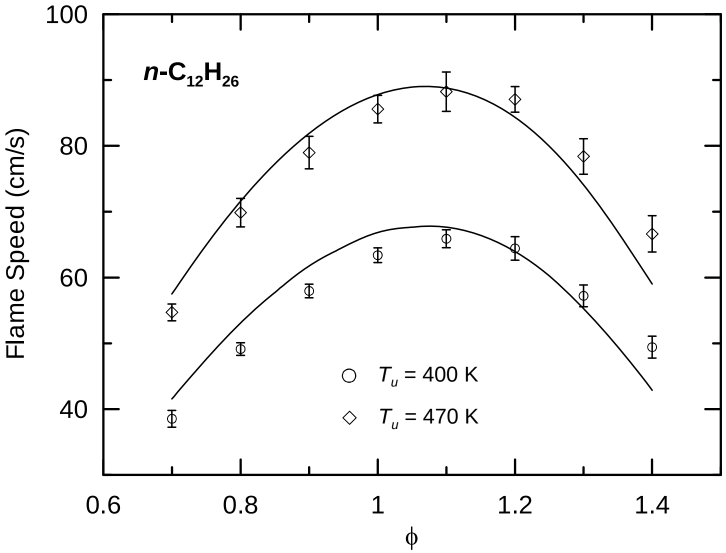
- **n-Decane**
    - Zhao et al. (2005), “Burning Velocities and a High Temperature Skeletal Kinetic Model for n-Decane”, Combust. Sci Tech. 177,89-106. (Updated model available by request; mchaos@princeton.edu)
- **Primary Reference Components**
    - Chaos et al. (2007) “A High-Temperature Chemical-Kinetic Model for Primary Reference Fuels”, Int. J. Chem Kin. 39, 399-414. (Model available in IJCK supplemental materials)
- **Primary Reference + 1 (Toluene)**
    - Full range and High T models completed and in use by HONDA, others (Model available on the PU (Dryer) website soon)
- **n-Nonane, n-Dodecane, n-Hexadecane**
    - High T Model developments complete, some validation (Models available by request; mchaos@princeton.edu)



Recent Flame Modeling (Dryer, PU)





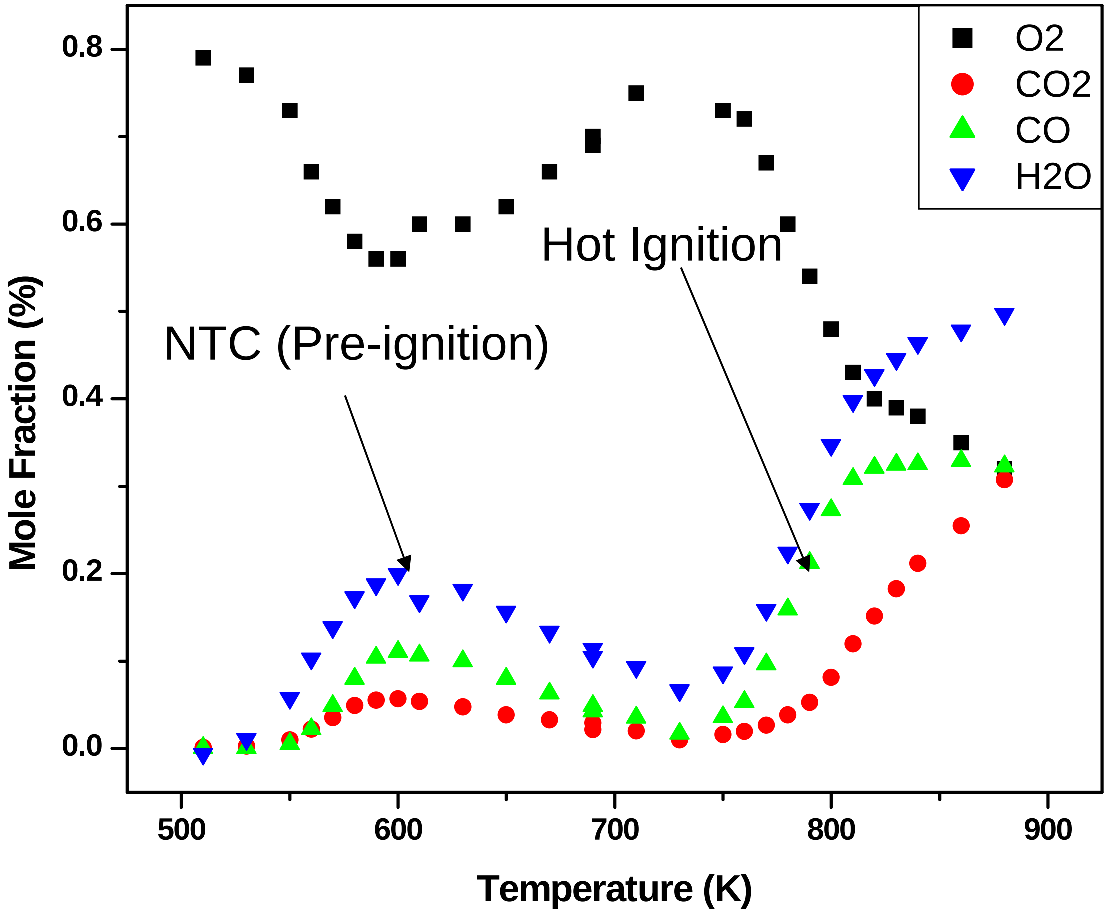


- Modeling of laminar flame speed data from CWRU (K. Kumar and C.-J. Sung, *Combust. Flame* 151, 2007, 209-224) using the PU high temperature models for n-decane and n-dodecane are encouraging; similar agreement with recent USC Data for n-dodecane (see AIAA-2008-0972).

n-Decane Reactivity – VPFR (Dryer, PU)

(Low/Int T models in Development)

Φ = 1.0; P = 12.5 atm; Res. Time = 1.8 s



n-Decane Reactivity – VPFR (Dryer, PU)

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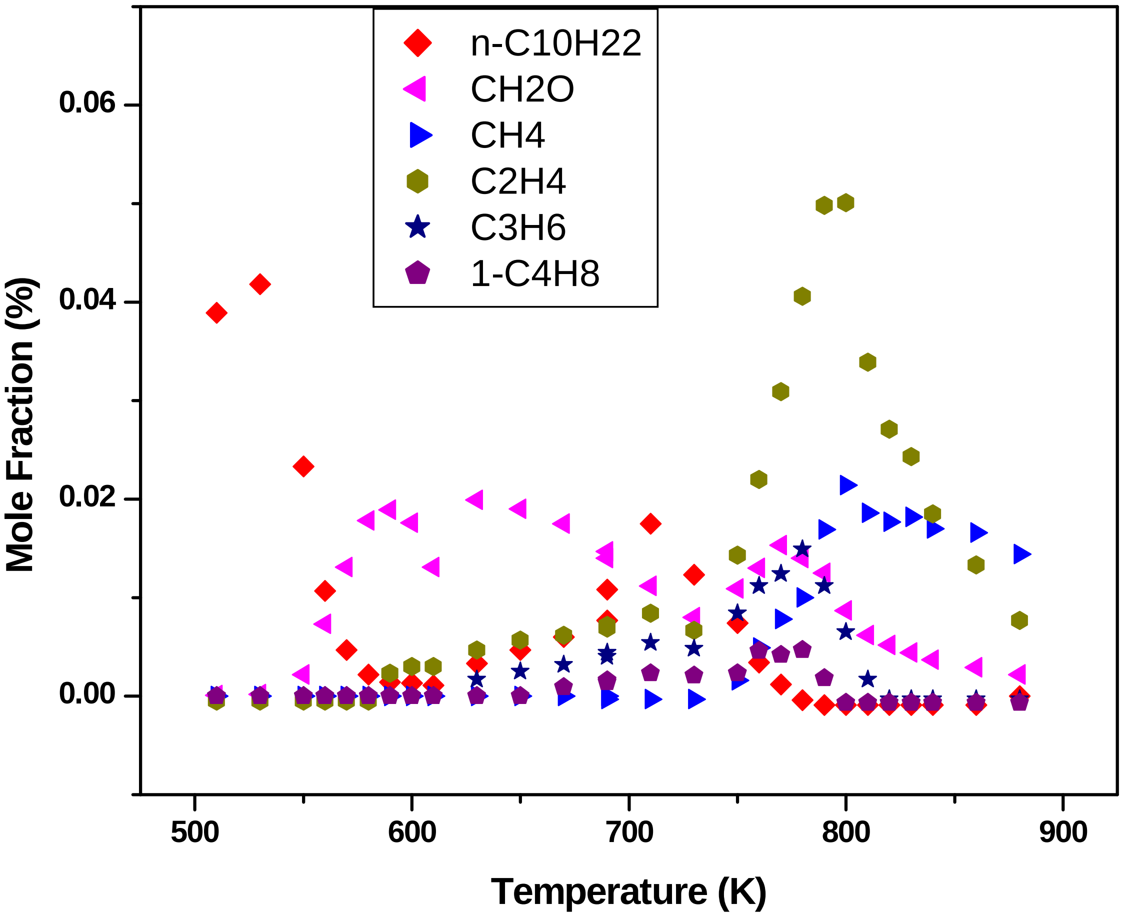
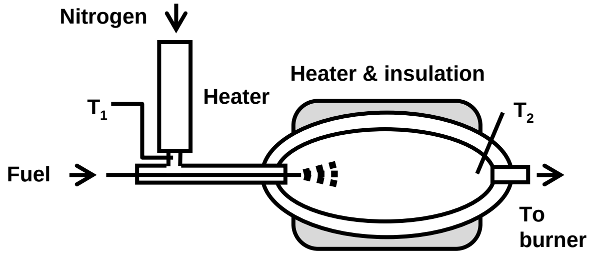
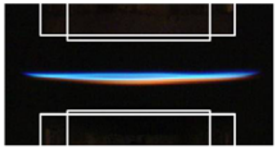


Generation of Comprehensive Surrogate Kinetic Models and Validation Databases for Simulating Large Molecular Weight Hydrocarbon Fuels (Ju, PU)

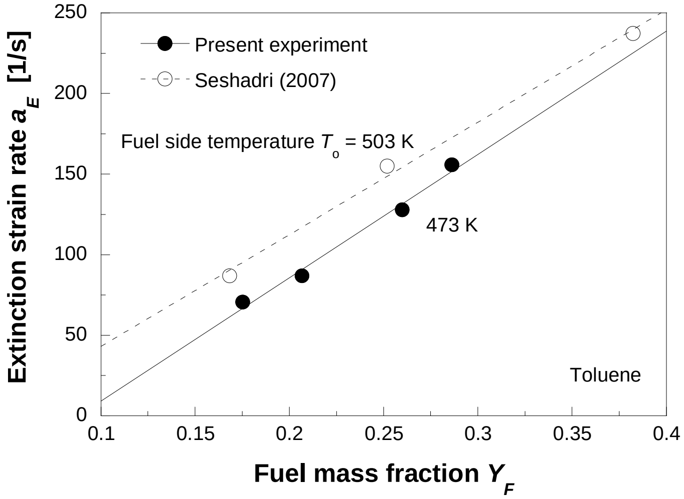
- Technical Accomplishments
  - Developing the evaporation systems for liquid fuels
    - Validation of evaporation with FTIR
      - Concentration fluctuation < 1%
  - Counterflow experiment for non-premixed flame extinction
    - Toluene, methane
    - Validation with previous experimental results
- Future Work
  - Observing extinction & ignition limits
    - For n-dodecane, 1,3,5 tri-methylbenzene
    - Effect of fuel blending on ignition & extinction
  - Concentration and temperature measurement
    - With Laser diagnostics (PLIF and Rayleigh scattering)
    - To provide experimental results of flame structure for the validation of kinetic model.



Schematics of evaporation system



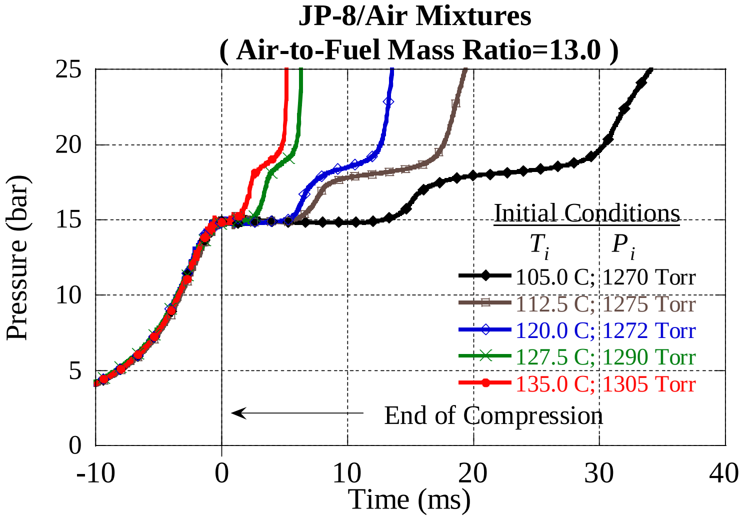
Direct photo of non-premixed flame In counterflow burner for toluene Y_F = 0.25, a = 76 s^{-1}, and T_o = 473 K



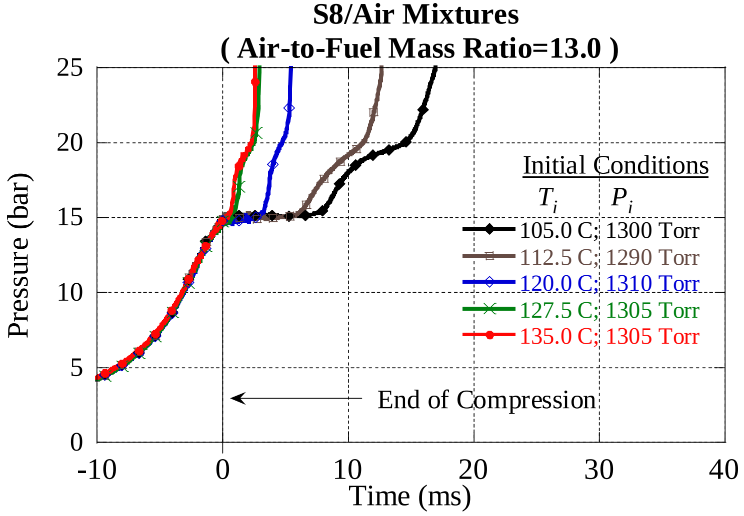
Comparison of extinction strain rate for toluene

Generation of Comprehensive Surrogate Kinetic Models and Validation Databases for Simulating Large Molecular Weight Hydrocarbon Fuels (Sung, CWRU)

- Technical Accomplishments (Highlights)
  - Autoignition experiments for two real jet fuels
    - JP-8 and S8
    - Compressed pressures of 15 and 30 bar
    - Two air fuel mass ratios of 19 (fuel lean) and 13 (fuel rich)
  - Autoignition experiments for three neat surrogate components
    - n-Decane, n-Dodecane, and Methyl Cyclohexane (MCH)
    - Obtained extensive experimental data and assessed model performances for n-decane autoignition
      - Compressed pressures of 7, 14.3, and 30 bar
      - Equivalence ratios from 0.5 to 2.2
- Future Work
  - Complete autoignition experiments of real jet fuels and neat fuels of n-dodecane and MCH
  - Measurement of atmospheric pressure laminar flame speeds of real jet fuels



JP-8/Air Mixtures
(Air-to-Fuel Mass Ratio=13.0)



S8/Air Mixtures
(Air-to-Fuel Mass Ratio=13.0)

Shock Tube and Modeling (Brezinsky, UIC)

- Researched available vaporizers for high molecular weight fuels
  - Concluded a nebulizer based vaporizer is best
    - Purchased the main component of the vaporizer
    - Aeroneb Lab Nebulizer from Aerogen
  - Designed the casing for the nebulizer
- Developed protocol for shock tube investigation of aromatic components of jet fuel
  - Purchased 1,2,4- and 1,3,5-trimethyl benzene and n-propylbenzene in preparation for experiments
- Acquired publicly available published literature models
  - Ran the available low-pressure xylene and propyl-benzene models for the conditions in High Pressure Single Pulse Shock Tube using CHEMKIN in order to establish expected species
- Planned out experiments on oxidation of m-, o-, and p-xylene using the High Pressure Shock Tube to begin soon
- Developing models using xylene mechanisms as a basis for extrapolation to 1,2,4- and 1,3,5-trimethyl benzene
  - Techniques: CHEMKIN, Gaussian, group additivity
- *High Pressure experiments and model comparisons for n-heptane and n-heptene oxidation (ESSCI, Paper A-18, 2007)*

Sooting and High Pressure Autoignition (Santoro/Litzinger, PSU)

- Two New Graduate Projects underway
  - Amy Mensch - TSI technique, application to determining Smoke Heights of surrogate fuel mixtures and real fuels
    - Measurements of the TSI values for n-decane, n-dodecane, n-propybenzene, 1,3,5 trimethylbenzene and 1-methylnaphthalene.
    - Check formulation rules for surrogate components and conversion of TSI measurements to Soot Points.
  - Venkatesh Lyer - high-pressure autoignition work and will start officially on January 2, 2008.

Surrogate Composition Effects: A Comparison of Surrogate Mixture Candidates with Combustion Targets (H/C, TSI, CN)

(Work in Progress)

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Mechanical and Aerospace Engineering
Princeton University

January 15, 2008

AFOSR MURI FA9550-07-1-0515

Objectives

- A comparison of surrogate mixtures of various components with combustion targets: overall H/C ratio, sooting characteristics, autoignition characteristics
  - Utilize mixture TSI, CN as representatives for sooting and autoignition
    - Experimental verification of these choices is required
    - Further refinements for diffusive ignition/extinction to be considered in future

Reference Information

- 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) were adopted for computing mixture values

$$\mathrm{TSI}_{\mathrm{mix}} = \sum x_i \mathrm{TSI}_i$$

$$\mathrm{CN}_{\mathrm{mix}} = \sum v_i \mathrm{CN}_i$$

- where x_i and v_i are the mole and volumetric fractions, respectively, of each species.
- Limits of H/C, TSI, CN, were estimated or taken from data listed in the Petroleum Quality Information System (PQIS) 2006 report: http://www.desc.dla.mil/DCM/Files/2006PQISreport.pdf

Jet Fuel Survey (2006 PQIS Report)

	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	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

(*) – TSI values are estimated here assuming $C_{11}H_{21}$ for JP-8 and $C_{12}H_{23}$ for Jet-A using TSI=3.18(MW/SP) (Yang et al., 2007), where MW is the molecular weight.

4- to 6-Component Surrogates

Violi et al. (2002a) Sur_1

- Objective: Match distillation curve and sooting propensity important for pool fire.
- H/C, TSI and CN of the jet fuel were not reported.
- ***All targets within listed ranges.***

	Mole fraction %	H/C	TSI	Cetane#
m-xylene	20.9	1.25	49	-13
iso-octane	10.4	2.25	6.4	15
n-dodecane	22.5	2.167	5.1	87
n-tetradecane	13.2	2.143	5.4	95
methylcyclohexane	26.8	2.0	4.9	22
tetralin	6.2	1.2	61	13
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	20.0%	1.91	17.88	49.45

Violi et al. (2002a) Sur_3

- Objective: Match distillation curve and sooting propensity important for pool fire.
- H/C, TSI and CN of the jet fuel were not reported.
- ***TSI and CN values significantly outside target ranges.***

	Mole fraction %	H/C	TSI	Cetane#
iso-octane	6.2	2.25	6.4	15
n-dodecane	59.8	2.167	5.1	87
methylcyclohexane	14.5	2.0	4.9	22
benzene	2.1	1.0	29	0
toluene	17.4	1.143	44	10.0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	11.0%	2.02	**12.43**	**67.85**

Violi et al. (2002b)

- H/C, TSI and CN of the jet fuel were not reported.
- ***CN value higher that target.***

	Mole fraction %	H/C	TSI	Cetane#
n-decane	22.4	2.2	4.2	76.73
iso-octane	5.3	2.25	6.4	15
n-dodecane	19.2	2.167	5.1	87
n-tetradecane	13.4	2.143	5.4	95
methylcyclohexane	6.8	2.0	4.9	22
toluene	32.9	1.143	44	10
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	20.0%	1.92	17.78	**63.72**

Montgomery et al. (2002)

- Objective: (unspecified)
- ***TSI and CN values significantly outside target ranges.***

	Mole fraction %	H/C	TSI	Cetane#
n-dodecane	34.7	2.167	5.1	87
methylcyclohexane	10	2.0	4.9	22
n-decane	32.6	2.2	4.2	77
butylbenzene	16	1.4	62	15
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	13.8%	2.03	**14.28**	**66.20**

Agosta et al. (2003) S1

- Objective: Match autoignition behavior of JP-8 in a flow reactor.
- The H/C, TSI and CN of the JP-8 in this work were not reported.
- ***Marginal TSI on high end.***

	Mole fraction %	H/C	TSI	Cetane#
iso-cetane	18.4	2.125	14.6	15
n-dodecane	37.2	2.167	5.1	87
methylcyclohexane	23.2	2.0	4.9	22
1-methylnaphthalene	21.2	0.91	91	0.0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	15.0%	1.87	25	44.57

Agosta et al. (2003) S5

- Objective: Match autoignition behavior of JP-8 in a flow reactor.
- The H/C, TSI and CN of the JP-8 in this work were not reported.
- ***Linear Cetane number prediction of the mixture is 33.***
  - ***Paper reports CN as 43 from nonlinear empirical blending rules based upon NTC kinetic comparisons***

	Mole fraction %	H/C	TSI	Cetane#
iso-cetane	24.1	2.125	14.6	15
n-dodecane	22.2	2.167	5.1	87
methylcyclohexane	21.3	2.0	4.9	22
decalin	7.4	1.8	15	33.0
1-methylnaphthalene	25	0.91	91	0.0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	18.0%	1.81	**29.57**	**32.91**

Cooke et al. (2005)

- Objective: Match temperature profile in OPPDIF.
- ***TSI and CN values significantly outside target ranges.***

	Mole fraction %	H/C	TSI	Cetane#
m-xylene	15	1.25	49	-13
iso-octane	10	2.25	6.4	15
n-dodecane	30	2.167	5.1	87
n-tetradecane	20	2.143	5.4	95
methylcyclohexane	20	2.0	4.9	22
tetralin	5	1.2	61	13
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	13.5%	1.99	**14.63**	**61.35**

Eddings et al. (2005) Hex-11

- Objective: Match distillation curve, burning rate, radiant heat flux, and sooting tendency in pool fire.
- TSI of the Jet-A fuel in this work is 26.7, CN not available.
- ***Marginal TSI on low end, high CN.***

	Mole fraction %	H/C	TSI	Cetane#
m-xylene	8.5	1.25	49	-13
n-dodecane	40	2.167	5.1	87
decalin	35	1.8	15	33
n-octane	3.5	2.25	3.2	64
n-hexadecane	5	2.125	6	100
tetralin	8	1.2	61	13
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	11.4%	1.92	16.75	**61.64**

Eddings et al. (2005) Hex-12

- Objective: Match distillation curve, burning rate, radiant heat flux, and sooting tendency in pool fire.
- TSI of the Jet-A fuel in this work is 26.7, CN not available.
- ***Marginal H/C on low end, high CN.***

	Mole fraction %	H/C	TSI	Cetane#
m-xylene	15	1.25	49	-13
n-dodecane	30	2.167	5.1	87
decalin	27	1.8	15	33
n-octane	3	2.25	3.2	64
n-hexadecane	12	2.125	6	100
tetralin	13	1.2	61	13
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	19.4%	1.86	21.68	**59.70**

Vasu et al. (2008) Stanford A

- Objective: Match ignition delay behind reflected shock wave of JP-8.
- The JP-8 in this work has a CN of 43.3.
- ***TSI and CN values significantly outside target ranges.***
- ***H/C close to the upper limits.***

	Mole fraction %	H/C	TSI	Cetane#
iso-octane	25	2.25	6.4	15
n-dodecane	54	2.167	5.1	87
methylcyclohexane	10	2.0	4.9	22
benzene	1	1.0	29	0
toluene	10	1.143	44	10.0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	6.1%	**2.09**	**9.5**	**62**

Vasu et al. (2008) Stanford B

- Objective: Match ignition delay behind reflected shock wave of JP-8.
- The JP-8 in this work has a CN of 43.3.
- ***Marginal TSI value***
- ***CN outside target ranges***

	Mole fraction %	H/C	TSI	Cetane#
iso-octane	5.5	2.25	6.4	15
n-dodecane	54	2.167	5.1	87
methylcyclohexane	10	2.0	4.9	22
benzene	1	1.0	29	0
toluene	29.5	1.143	44	10.0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	18.2%	1.93	16.87	**64.45**

3-Component Surrogates

Guéret et al. (1990)

- Objective: study species concentration in a jet-stirred reactor.
- ***TSI of the mixture is 11,***
- ***Cetane number is significantly higher than upper limit.***
- ***Marginal H/C***

	Mole fraction %	H/C	TSI	Cetane #
n-undecane	74.7	2.18	4.5	81
n-propylcyclohexane	11.7	2	4.9	52
1,2,4-trimethylbenzene	13.5	1.33	52	10
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	9.5%	2.07	**11**	**71.46**

Dagaut et al. (1990)

- Objective: match jet-stirred reactor species profile of Jet A1 fuel.
- ***TSI of the mixture is 10.8***
- ***Cetane number is significantly higher than upper limit.***

	Mole fraction %	H/C	TSI	Cetane#
n-decane	74	2.2	4.2	76.73
n-propylcyclohexane	11	2	4.9	52
n-propylbenzene	15	1.33	47	17
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	18.4%	2.06	**10.75**	**65.48**

SERDP Surrogates

(from the SERDP Website)

SERDP Soot Project – SERDP1

- Source: Med Colket 2007 SERDP Workshop presentation.
- Objective: development of surrogates matching engine soot emissions of jet fuels
- TSI computed using the relationship of Yang et al. (2007) with measured smoke point

	Mole fraction %	H/C	TSI	Cetane#
iso-cetane	23.9	2.125	14.6	15
n-decane	42.4	2.2	4.2	77
methylcyclohexane	15.4	2.0	4.9	22
n-propylbenzene	7	1.33	47	16
1,3,5-trimethylbenzene	7.1	1.33	52	2
1-methylnaphthalene	4.2	0.91	91	0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	13%	1.997	19.6	40.45

SERDP Soot Project – SERDP2

- Source: Med Colket 2007 SERDP Workshop presentation.
- Objective: development of surrogates matching engine soot emissions of jet fuels
- TSI computed using the relationship of Yang et al. (2007) with measured smoke point
- ***Marginal CN***

	Mole fraction %	H/C	TSI	Cetane#
iso-cetane	32.5	2.125	14.6	15
n-decane	32.5	2.2	4.2	77
methylcyclohexane	16	2.0	4.9	22
n-propylbenzene	7.3	1.33	47	16
1,3,5-trimethylbenzene	7.3	1.33	52	2
1-methylnaphthalene	4.4	0.91	91	0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	13%	1.991	20.9	33.66

SERDP Soot Project – SERDP3

- Source: Med Colket 2007 SERDP Workshop presentation.
- Objective: development of surrogates matching engine soot emissions of jet fuels
- TSI computed using the relationship of Yang et al. (2007) with measured smoke point

	Mole fraction %	H/C	TSI	Cetane#
iso-cetane	32.6	2.125	14.6	15
n-decane	39.7	2.2	4.2	77
methylcyclohexane	6.6	2.0	4.9	22
n-propylbenzene	6	1.33	47	16
1,3,5-trimethylbenzene	12.1	1.33	52	2
1-methylnaphthalene	3	0.91	91	0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	14%	2.000	21.5	36.77

Other Surrogates

Others (1 or 2 Components)

- The following models using 1 or 2 components (composition in mol %) all have some values outside target ranges.

	H/C	TSI	Cetane#
Goal	*1.84-2.07*	*22-30*	*32-57*
n-decane (100%); Dagaut et al. (1994)	**2.20**	**4.2**	**76.7**
n-decane (89%), ethylbenzene (11%); Lindstedt and Maurice (2000)	**2.12**	**9.7**	**71.8**
n-dodecane (46%), iso-cetane(54%); Agosta et al. (2004)	**2.14**	**10.2**	43.8
n-dodecane (25%), methylcyclohexane (75%); Agosta et al. (2004)	**2.06**	**5.0**	45.3
n-dodecane (39%), 1-methylnaphthalene (61%) Agosta et al. (2004)	**1.43**	**57.5**	44.4
n-decane (80%), n-propylbenzene (20%); Eberius et al. (2001)	2.04	**12.8**	**67.5**

Large Surrogates (> 10 components)

- Schulz (1991) 12-component surrogate matching chemical classes found in JP-8:
  - n-decane (15%), n-dodecane (20%), n-tetradecane (15%), n-hexadecane (10%), iso-octane (5%), MCH (5%), cyclooctane (5%), o-xylene (5%), butylbenzene (5%), tetramethylbenzene (5%), 1-methylnaphthalene (5%), tetralin (5%) – Note: mass fractions
    Aromatics (liq. vol.) – 21.5%; H/C – 1.87; TSI – 21.6; CN – **59.70**
- Wood et al. (1989) 14-component surrogate for JP-4, matching compound classes and distillation curve:
  - n-hexane (5.5%), n-heptane (8%), n-octane (8%), n-nonane (10%), n-decane (10%), n-dodecane (10%), n-tetradecane (10%), cyclohexane (8%), methylcyclohexane (8%), cyclooctane (8%), toluene (8%), decalin (5%), tetralin (1%), 1-methylnaphthalene(0.5%) – Note: liquid volume fractions
    Aromatics (liq. vol.) – 9.5%; H/C – 1.94; TSI – **10.28**; CN – 52.20
- *Comments: Choosing so many components is not warranted with current understanding of jet fuel surrogate properties, kinetic models, and available validation data.*

Matching Jet Fuel with Gasoline Surrogate Components

(Modified) Gasoline Surrogate Components (1)

- For the combination of n-C_7H_{16}/i-C_8H_{18}/toluene:
  - To match TSI first, i-C_8H_{18} is preferable over n-C_7H_{16}, the minimum amount of toluene needed is 25.5 mol% (18.1 vol%) in the i-C_8H_{18}/toluene mixture.
  - To match H/C first, i-C_8H_{18} is also preferable over n-C_7H_{16}, the highest amount of toluene allowed is 39.8 mol% (30 vol%).
  - ***It is possible to match TSI, H/C, and CN, as shown in the table.***
  - ***The highest possible CN is 42.7, the highest possible TSI is 19.4.***
  - ***Low average molecular weight (~100 g/mol)***

	Mole fraction	H/C	TSI	Cetane#
n-heptane	55%	2.29	2.6	54
iso-octane	10 %	2.25	6.4	15
toluene	35 %	1.143	44	10.0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	27.7%	1.89	17.5	37

(Modified) Gasoline Surrogate Components (2)

- For the combination of n-$C_{10}H_{22}$/i-C_8H_{18}/toluene:
  - To match TSI first, i-C_8H_{18} is preferable over n-$C_{10}H_{22}$, the minimum amount of toluene needed is 25.5 mol% (18.1 vol%) in the i-C_8H_{18}/toluene mixture
  - To match H/C first, n-$C_{10}H_{22}$ is preferable over i-C_8H_{18}, the highest amount of toluene allowed is 42.1 mol% (28.4 vol%).
  - ***It is possible to match TSI, H/C, and CN, as shown in the table.***
  - ***The highest possible CN is 56.2, the highest possible TSI is 21.2.***
  - ***Low average molecular weight (~125 g/mol)***

	Mole fraction	H/C	TSI	Cetane#
iso-octane	40.9 %	2.25	6.4	15
n-decane	31.6%	2.2	4.2	76.73
toluene	27.5 %	1.143	44	10.0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	18.5%	1.98	16.0	38.1

Match Species Classes

- Matching the species classes exactly using surrogate candidates
- ***Marginal CN values.***

	Mole fraction	H/C	TSI	Cetane#
n-decane	27.0%	2.2	4.2	76.73
i-cetane	28.3%	2.125	14.6	15
decalin	7.8%	1.8	15	46
methylcyclohexane	17.3%	2.0	4.9	22
n-propylbenzene	12.7%	1.33	47	17
1-methylnaphthalene	6.8%	0.91	91	0
Goal	*Aromatic (liq. vol. %)*	*1.84-2.07*	*16-26*	*32-57*
Actual	13.9%	1.94	19.44	32.71

Summary

- Most of the surrogate formulations in literature have TSI and cetane number significantly outside the range of average JP 8 fuels.

	Aromatic liq. vol. fraction	H/C *(1.84-2.07)*	TSI *(16-26)*	Cetane# *(32-57)*
Violi (2002a), Sur_1	20.0%	1.91	17.9	49.5
Violi (2002a), Sur_3	11.0%	2.02	**12.4**	**67.9**
Violi (200b)	20.0%	1.92	17.8	**63.7**
Cooke (2005)	13.5%	1.99	**15**	**61.4**
Eddings (2005), Hex_11	11.4%	1.92	16.8	**61.6**
Eddings (2005), Hex_12	19.4%	1.86	21.7	**59.7**
Agosta (2003), S5	18.0%	**1.81**	**29.6**	32.9
Vasu (2008), Stanford A	6.1%	**2.09**	**9.5**	**62.0**
Vasu (2008), Stanford B	18.2%	1.93	16.9	**64.5**

Target Issues

- Experimental verification of TSI for components and mixture predictions.
- Comparison of mixture and jet fuel TSIs.
- Experimental verification of CN blending rules for surrogate mixture candidates (investigating IQT as comparison method).
- Comparison of mixture and jet fuel CNs.
  - Verification of ignition qualities of surrogate mixtures and jet fuels using other merits (VPFR reactivity, RCM, Shock Tube Ignition delay measurements).

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Cetane Determination Methods

- Cetane Engine Testing (ASTM D-613) This method requires the use of an industry standard test engine equipped with accepted instrumentation and operated under specific conditions. In this test, the engine compression ratio is varied for the test sample and reference fuels of known cetane number to obtain a fixed ignition delay. The compression ratio of the sample is bracketed by those of two reference fuels. The cetane number of the sample fuel is determined by estimating between the two reference fuel points (iso-cetane (15) and n-hexadecane (100).
- Cetane Index (ASTM D-976 or D-4737) Often substituted for cetane number because D-613 is expensive and time-consuming. The calculated cetane index is derived from the fuel's density and boiling range. While useful for estimating the cetane number of distillate fuels, this technique can not be applied to fuels containing additives that raise cetane number. These additives do not change the fuel density or distillation profile, so they do not alter the calculated cetane index.
- IQT Ignition Quality Testing (ASTM D6890, IP 498) A rapid, constant volume combustion method based upon Southwest Research Institute apparatus development that determines the pressure- and temperature-dependent autoignition characteristics of fuels. Emerging as an internationally accepted testing method for fuel qualification. Can be easily applied to single components, mixtures, and real (both petroleum derived and alternative) fuels to determine CN and test CN emulations.