Flame Studies of Jet Fuels and Surrogate-Related Neat Hydrocarbons

Chunsheng Ji, Yang Lee Wang, Ning Liu, Fokion N. Egolfopoulos

Department of Aerospace and Mechanical Engineering
University of Southern California

MULTI AGENCY COORDINATION COMMITTEE
FOR COMBUSTION RESEARCH (MACCCR)
FUELS RESEARCH REVIEW

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Period of performance: 3/1/08 – 11/30/10
Technical Monitor: Dr. Julian M. Tishkoff

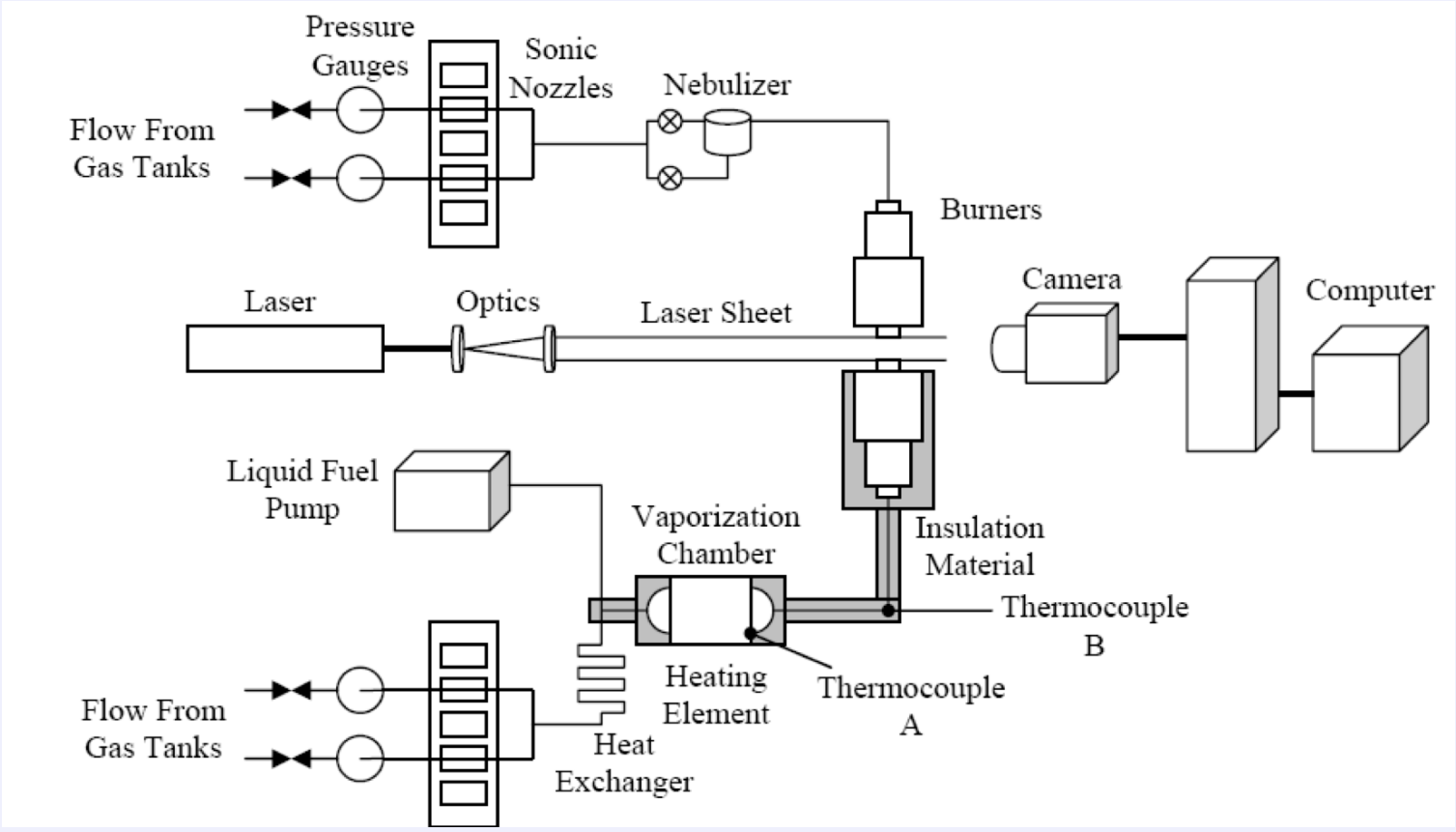
General Objectives

1. To determine experimentally archival fundamental flame properties (ignition, propagation, extinction) for:
   - Selected jet fuels
   - Single-component hydrocarbons
   - Mixtures of chosen hydrocarbons

2. To model experiments using detailed description of chemical kinetics and molecular transport.

3. To provide insight into the chemical and physical mechanisms that control the oxidative characteristics of large (liquid) hydrocarbon flames.

Experimental Approach (1)



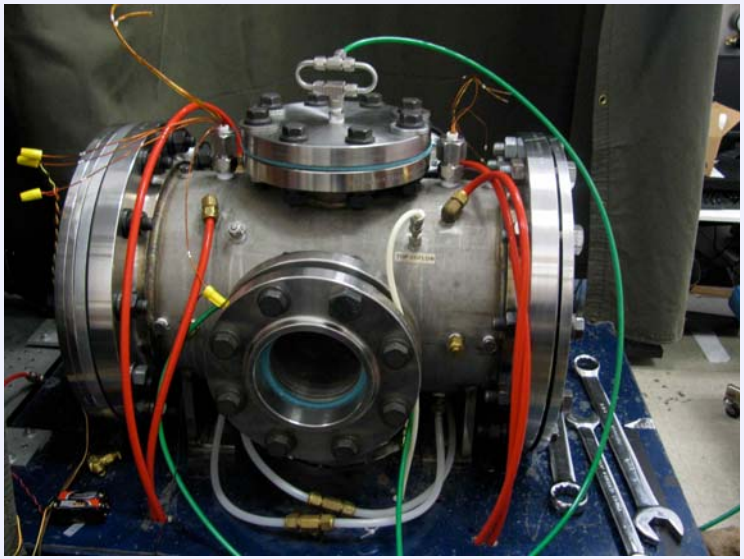
- **Flame stability has improved notably through extensive revisions of:**
  - **Liquid fuel injection**
  - **Silicon oil droplets injection, to perform DPIV measurements**

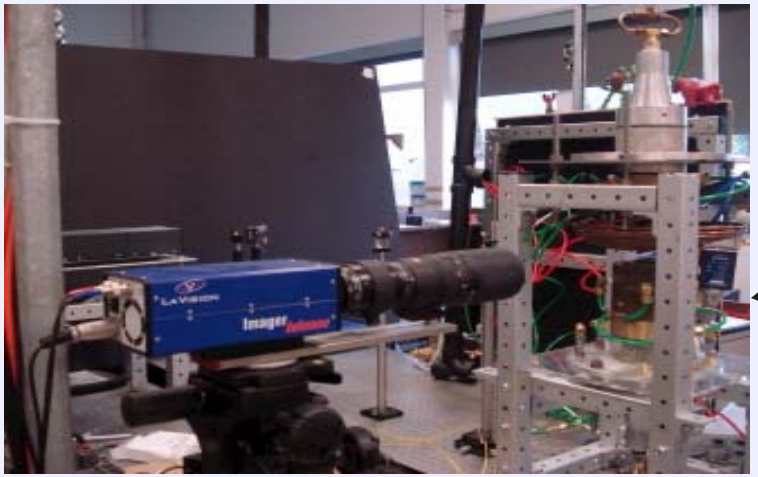
Experimental Approach (2)

- Use of counterflow technique

Twin premixed flames

Single premixed / non-premixed flame

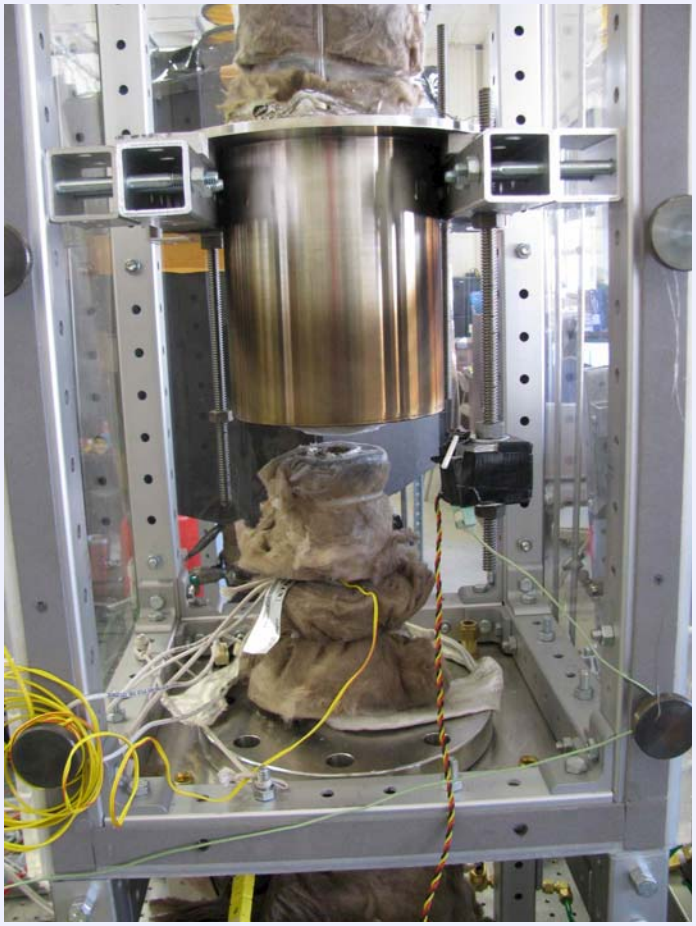




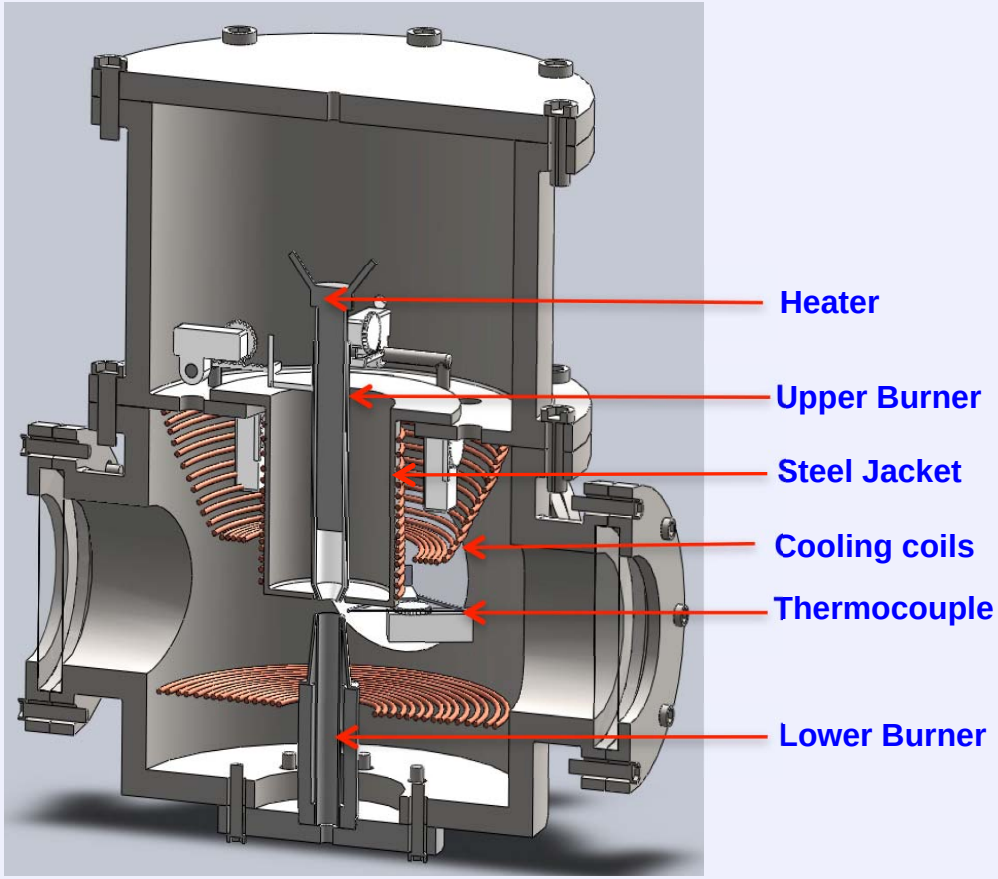
- Pressure chamber:
  - Pressure range 0.1-10 atm
- Diagnostics:
  - Digital Particle Image Velocimetry (DPIV)
  - Thermocouples
  - Intrusive NO_x sampling
  - Laser extinction

Experimental Approach (3)

- **Use of counterflow technique**

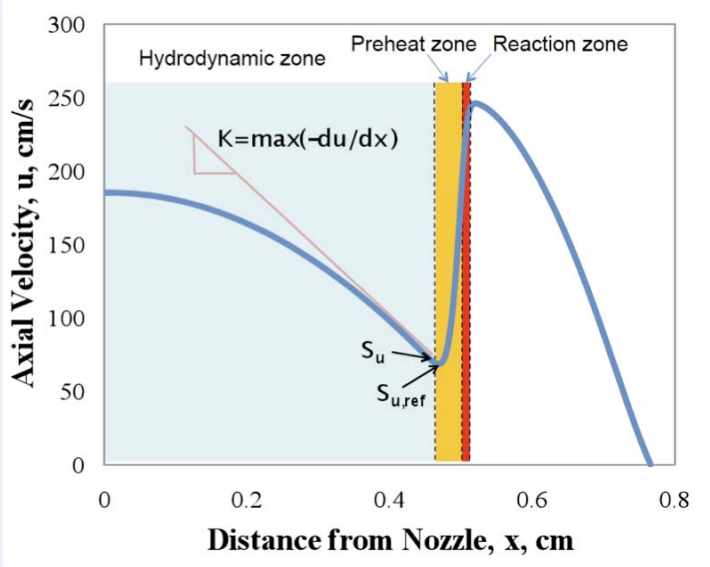


Flame ignition facility, p = 1 atm

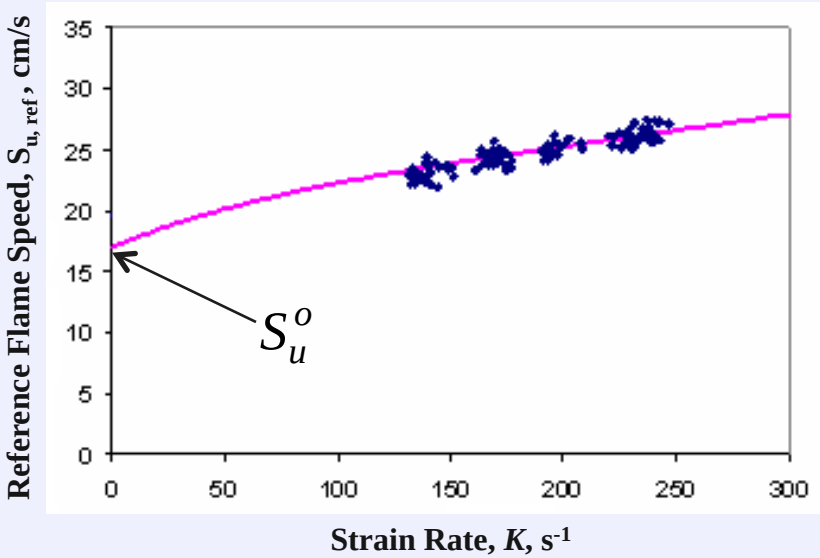


Flame ignition facility, $0.1 \leq p \leq 15$ atm (under construction)

Experimental Approach (4)

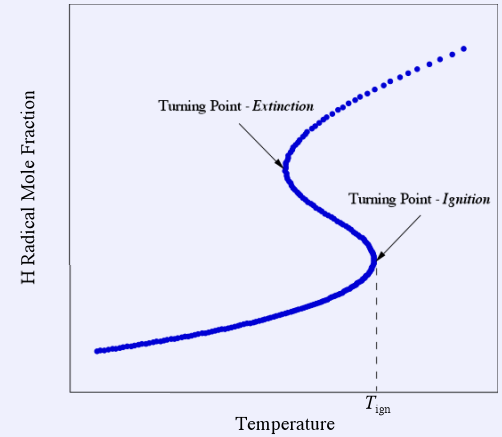


- **Laminar flame speeds, S_u^o :**
  - **Monitor $S_{u,ref}$ vs. K**
  - **Non-linear extrapolations**
- **Extinction strain rate, K_{ext}:**
  - **K at the state of extinction**
- **Ignition temperature, T_{ign}:**
  - **T at the hot boundary resulting in ignition**



Numerical Approach

- Use of CHEMKIN-based codes
- Proper description of "turning-point" behavior



- Mathematically rigorous determination of logarithmic sensitivity coefficients: $\partial(\ln Y)/\partial(\ln X)$
  - Y: laminar flame speed / extinction strain rate / ignition temperature
  - X: A-factor / $D_{i\text{-}N2}$
- Use of JetSurF (http://melchior.usc.edu/JetSurF) kinetic model(s) developed by Wang and coworkers.

- ***All numerical results have been produced by solutions that:***
  - ***Were properly converged, i.e. in highly resolved grids***
  - ***Included the effects of thermal radiation and Soret***
  - ***Included full multi-component transport formulation***
  - ***Included all pertinent experimental boundary conditions***

Challenges

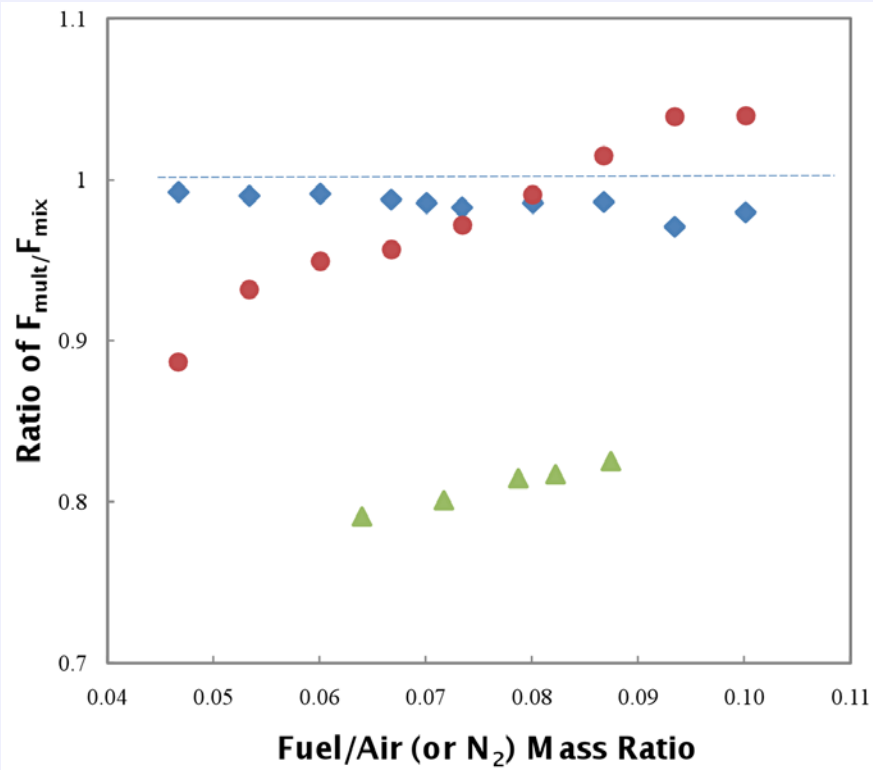
1. **Low fuel vapor pressure:**
   - **fuel heating**
   - **fuel cracking**
   - **fuel condensation**
   - **final mixture composition needs to be tested independent using, e.g., gas chromatography.**

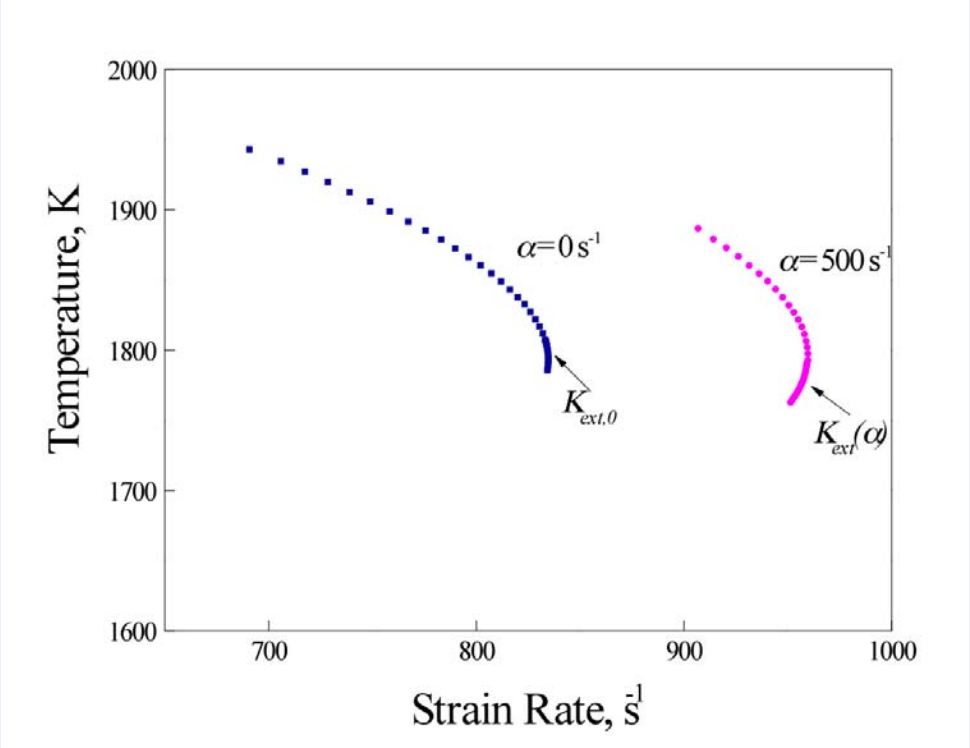
2. **Experiments can be further complicated as pressure increases.**

3. **The large molecular weight discrepancy between fuel and oxidizer can complicate experimental data interpretation.**

4. **Computed results can be compromised by:**
   - **using simplifying assumptions for transport due to the size of kinetic models**
   - **not accounting properly for the experimental boundary conditions**

Two Potential Sources of Error





Computed S_u^o (◆) and K_{ext} for premixed (●) and non-premixed (▲) flames using the multi-component transport formulation and scaled by the attendant values obtained using the mixture-averaged transport formulation.

Computed responses of the extinction strain rate on the velocity gradient at the burner exit *a*. The computations were carried out for a stoichiometric *n*-$C_{12}H_{26}$/air flame at T_u = 403 K.

Accomplishments During Years 1-3

	C_4-C_{12} *n*-alkanes	cycloalkanes	*iso*-alkanes	aromatics	fuel mixtures	jet fuels
Laminar flame speeds	C_4, C_5, C_6, C_7, C_8, C_9, C_{10}, C_{12} at 1 atm	cyclohexane (CHX) methyl-CHX ethyl-CHX *n*-propyl-CHX *n*-butyl-CHX at 1 atm		benzene (B) toluene *n*-propyl-B 1,2,4-TMB 1,3,5-TMB *o*-xylene *m*-xylene *p*-xylene at 1 atm	*n*-C_{12}+MCHX *n*-C_{12}+toluene at 1 atm	JP-7 JP-8 S-8 R-8 Shell-GTL at 1 atm
Flame ignition	C_3, C_5, C_6, C_7, C_8, C_9, C_{10}, C_{12} at 1 atm					
Flame extinction	C_5, C_6, C_7, C_8, C_9, C_{10}, C_{12} at 1 atm	CHX methyl-CHX *n*-butyl-CHX at 1 atm		benzene toluene *n*-propyl-B 1,2,4-TMB 1,3,5-TMB *o*-xylene *m*-xylene *p*-xylene at 1 atm		JP-7 JP-8 S-8 R-8 Shell-GTL at 1 atm

Progress During Year 3

1. **Propagation of cyclohexane and monoalkylated cyclohexane flames:**
   - **cyclohexane**
   - **methyl-cyclohexane**
   - **ethyl--cyclohexane**
   - ***n*-propyl-cyclohexane**
   - ***n*-butyl-cyclohexane**

   (*33rd Combustion Symposium, 2010*)
2. **Propagation of aromatics flames**
   - **benzene**
   - **toluene**
   - ***n*-propyl-benzene**
   - ***1,2,4*- and *1,3,5*-trimethyl-benzene**
   - ***o*-, *m*-, and *p*-xylene**

   (*in preparation*)
3. **Propagation and extinction of jet-fuel flames**
   - **JP-7, JP-8, S-8, Shell-GTL, R-8** (*Journal of Propulsion and Power, 2010*)
4. **Ignition of flames of C_3-C_{12} hydrocarbons**
   - **propane**
   - **C_5-C_{12} n-alkanes**

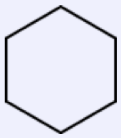
   (*in preparation*)
5. **Propagation of flames of binary fuel mixtures**
   - **methyl-cyclohexane + *n*-C_{12}**
   - **toluene + *n*-C_{12}**

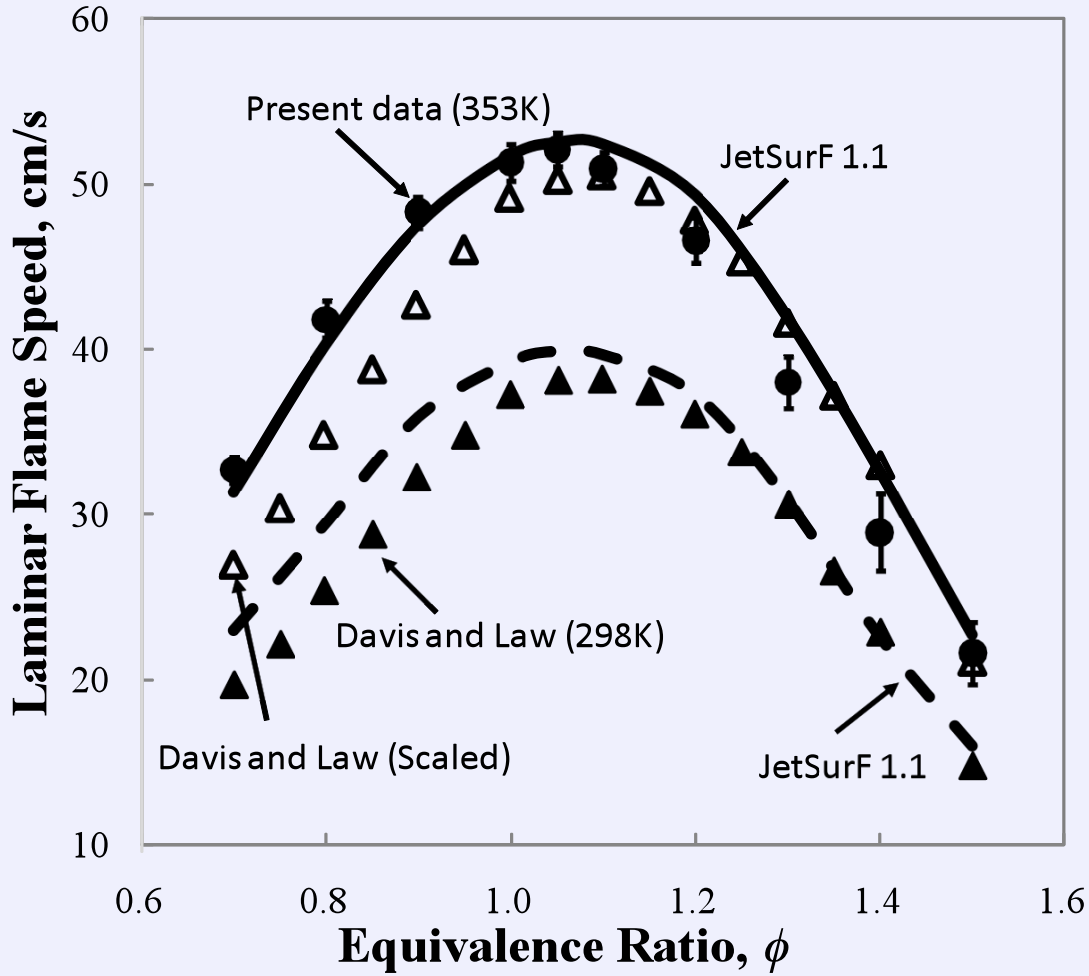
   (*33rd Combustion Symposium, 2010*)

Propagation of Cyclohexane and Monoalkylated Cyclohexane Flames

Laminar Flame Speeds of Cyclohexane/Air Flames[1]

Cyclohexane:



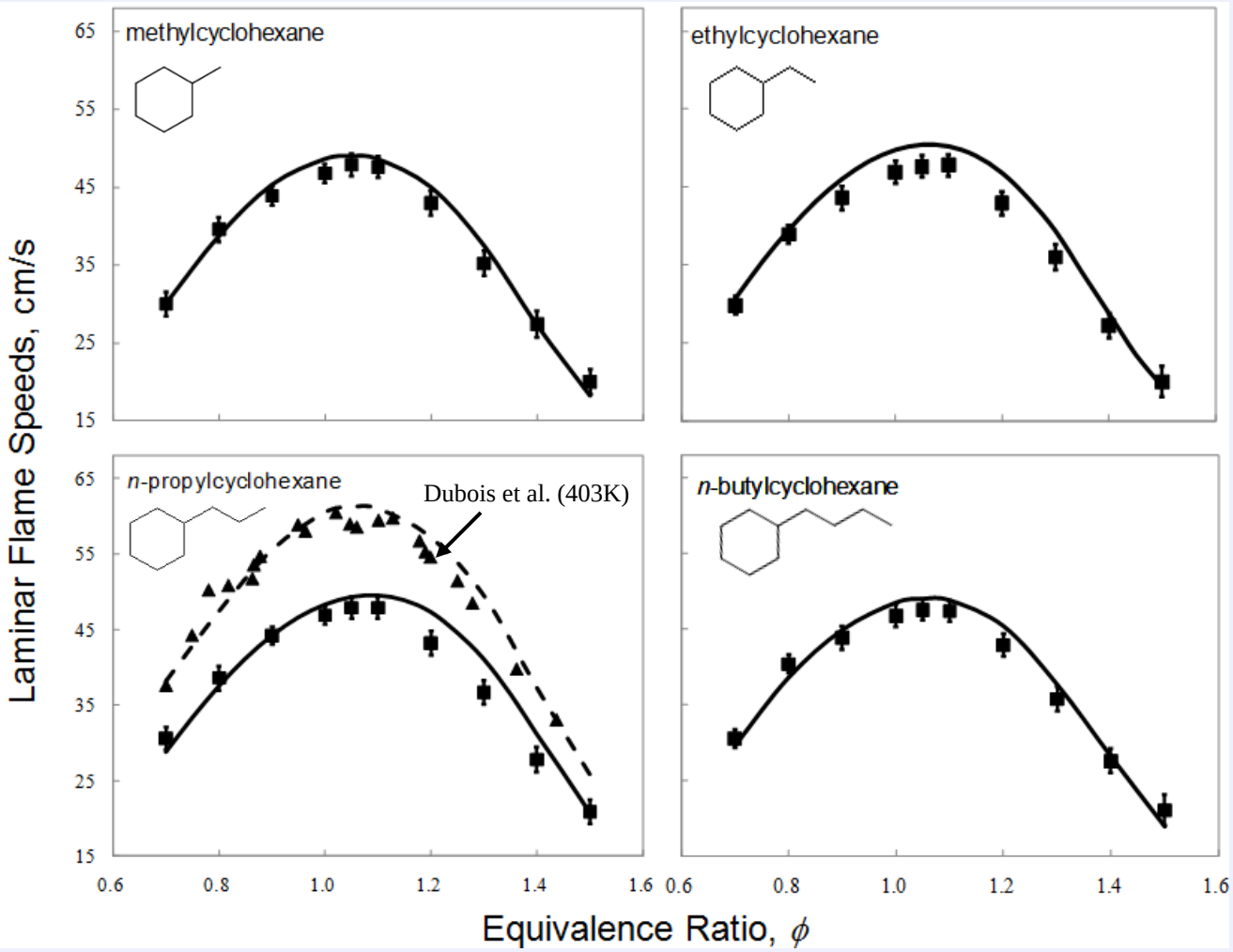


[1]C. Ji, E. Dames, B. Sirjean, H. Wang, F. N. Egolfopoulos, "An Experimental and Modeling Study of the Propagation of Cyclohexane and Mono-alkylated Cyclohexane Flames," Proc. Combust. Inst. 33 (2010) doi:10.1016/j.proci.2010.06.099.

[2]S.G. Davis, C.K. Law, "Determination of and fuel structure effects on laminar flame speeds of C_1 to C_8 hydrocarbons," Combust. Sci. Technol. 140 (1998) 427-499.

Laminar Flame Speeds of Methyl-, Ethyl-, n-Propyl-, and n-Butyl-Cyclohexane/air Flames[1]

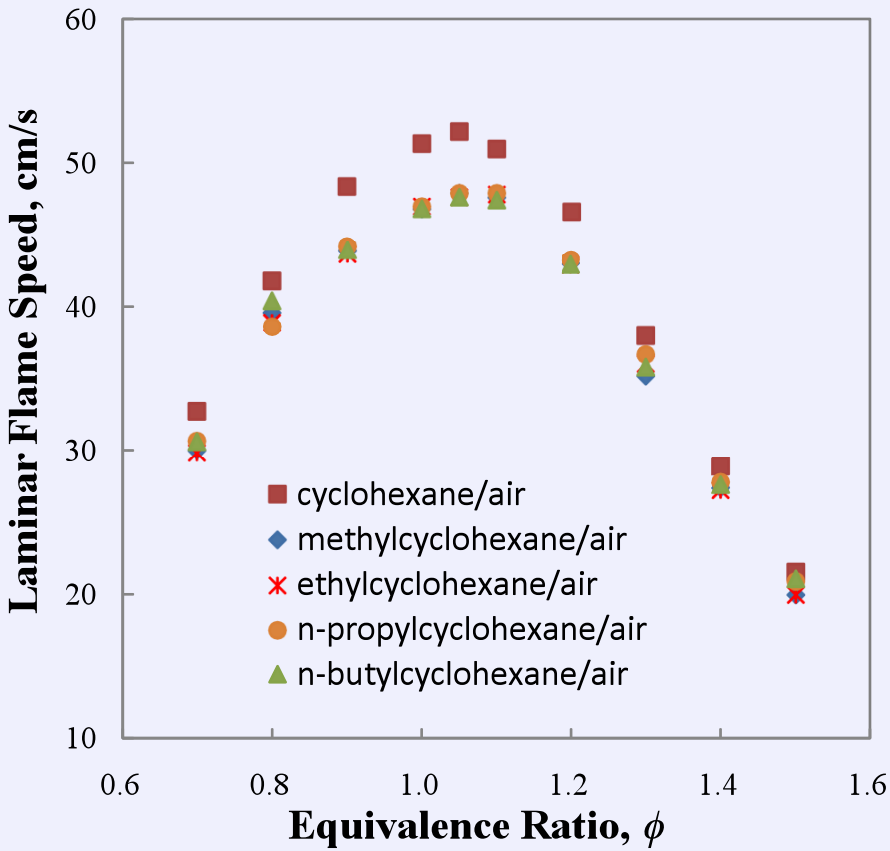
p = 1 atm
T_u = 353 K
JetSurF 1.1

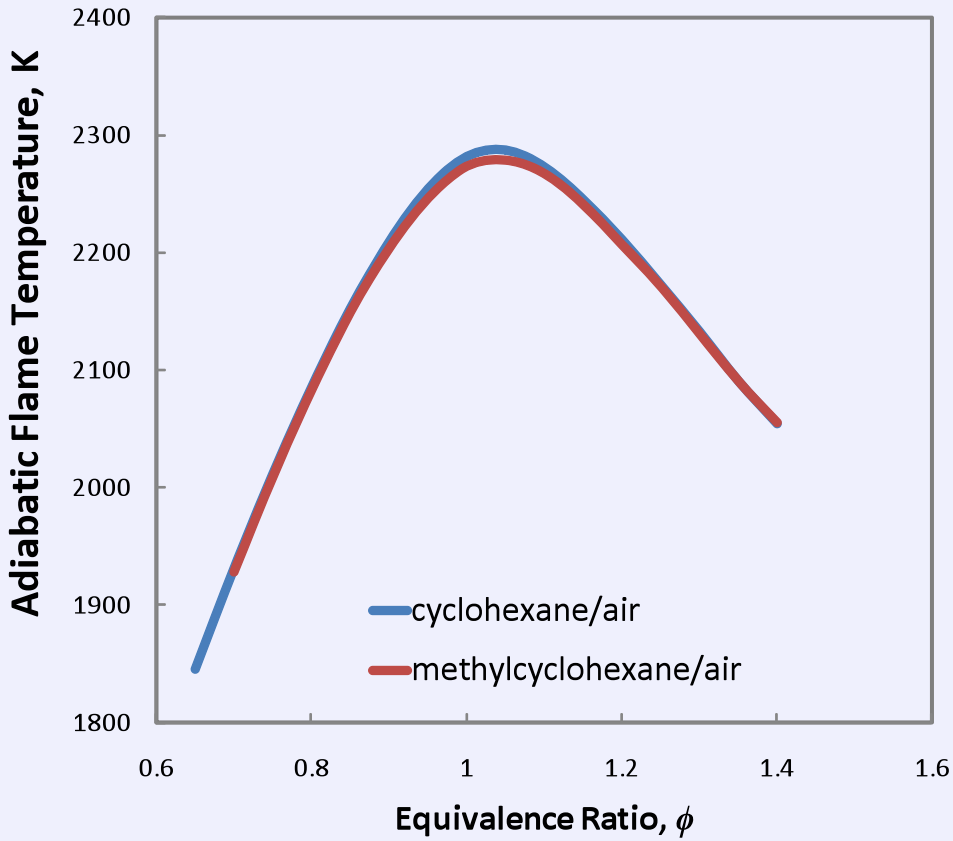


[1]C. Ji, E. Dames, B. Sirjean, H. Wang, F. N. Egolfopoulos, "An Experimental and Modeling Study of the Propagation of Cyclohexane and Mono-alkylated Cyclohexane Flames," Proc. Combust. Inst. 33 (2010) doi:10.1016/j.proci.2010.06.099.
[3]T. Dubois, N. Chaumeix, C. Paillard, "Experimental and Modeling Study of n-Propylcyclohexane Oxidation under Engine-relevant Conditions," Energy Fuels 23 (2009) 2453-2466.

Comparison of Experimentally Determined Laminar Flame Speeds[1]

p = 1 atm
T_u = 353 K





[1]C. Ji, E. Dames, B. Sirjean, H. Wang, F. N. Egolfopoulos, "An Experimental and Modeling Study of the Propagation of Cyclohexane and Monoalkylated Cyclohexane Flames," Proc. Combust. Inst. 33 (2010) doi:10.1016/j.proci.2010.06.099.

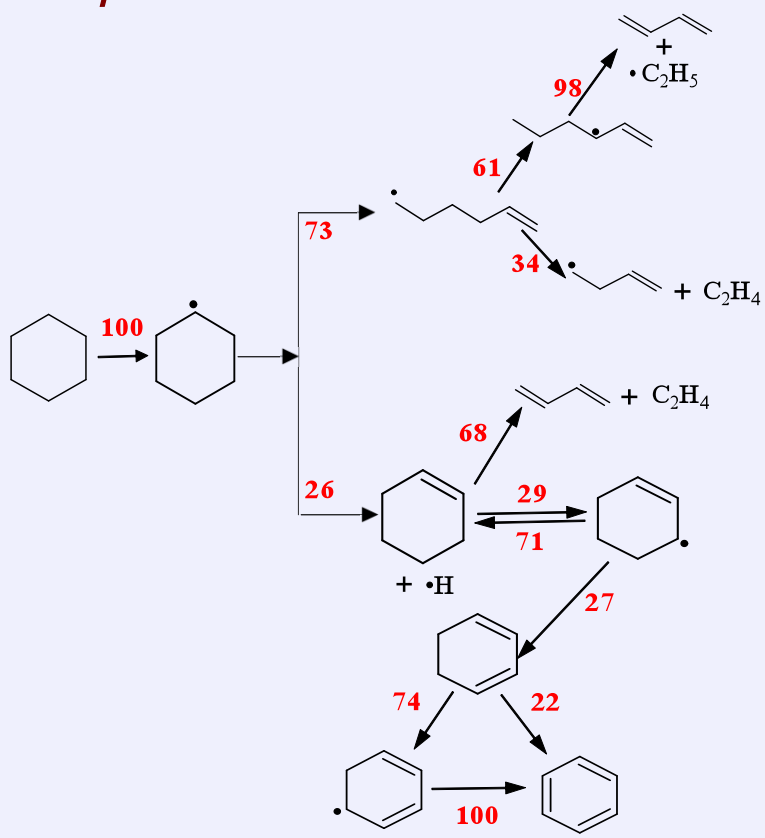
Reaction Path Analysis of Cyclohexane/Air and Methyl-Cyclohexane/Air Flames

cyclohexane/air

p = 1 atm

T_u = 353 K

ϕ = 1.0

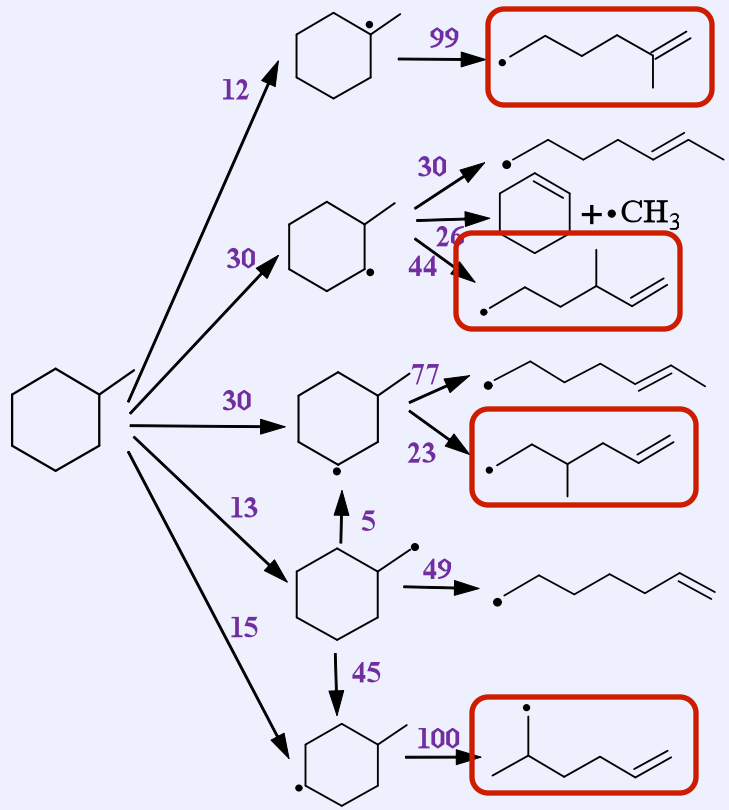


methyl-cyclohexane/air

p = 1 atm

T_u = 353 K

ϕ = 1.0



[1]C. Ji, E. Dames, B. Sirjean, H. Wang, F. N. Egolfopoulos, "An Experimental and Modeling Study of the Propagation of Cyclohexane and Mono-alkylated Cyclohexane Flames," Proc. Combust. Inst. 33 (2010) doi:10.1016/j.proci.2010.06.099.

Main Intermediates Production from Cyclohexane/Air and n-Propyl-Cyclohexane/Air Flames[1]

(---) cyclohexane/air flames

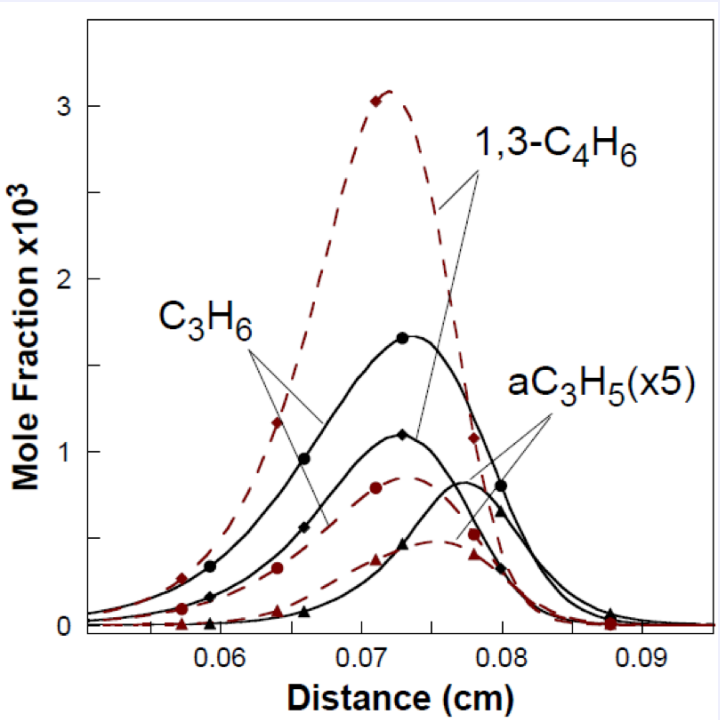
$1,3\text{-}C_4H_6 + H \rightarrow C_2H_4 + C_2H_3$;

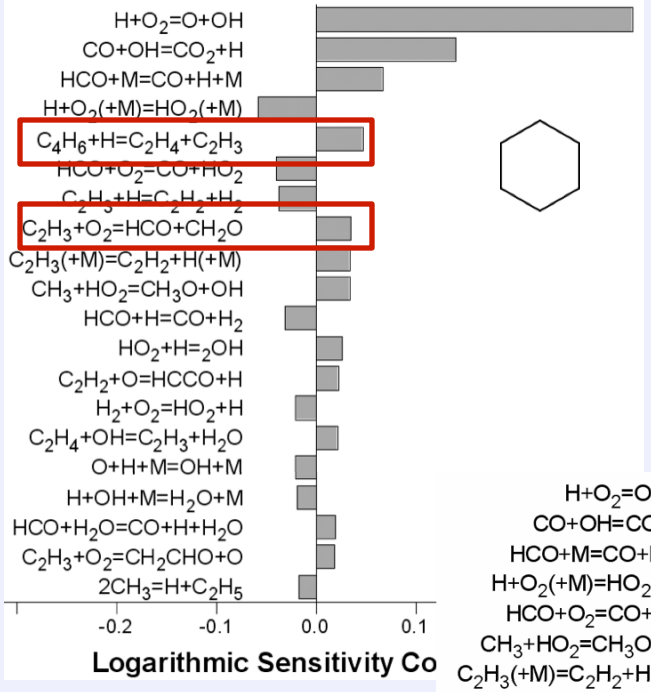
$C_2H_3 + O_2 \rightarrow HCO + CH_2O$

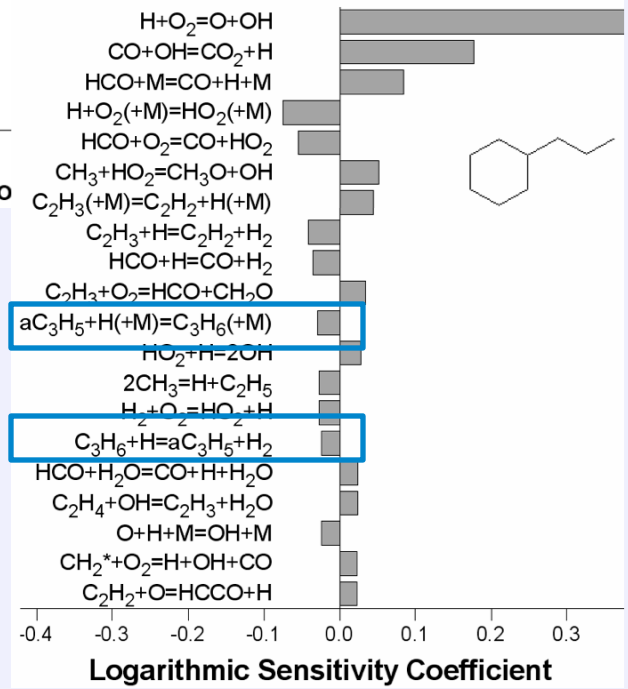
(—) *n*-propylcyclohexane/air flames

$aC_3H_5 + H + M \rightarrow C_3H_6 + M$

$C_3H_6 + H \rightarrow aC_3H_5 + H_2$







[1]C. Ji, E. Dames, B. Sirjean, H. Wang, F. N. Egolfopoulos, "An Experimental and Modeling Study of the Propagation of Cyclohexane and Mono-alkylated Cyclohexane Flames," Proc. Combust. Inst. 33 (2010) doi:10.1016/j.proci.2010.06.099.

Propagation and Extinction of

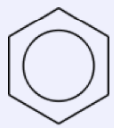
Benzene and Alkylbenzene Flames/Air Flames

Laminar Flame Speeds of Benzene/Air, Toluene/Air, and n-Propyl-Benzene/Air Flames

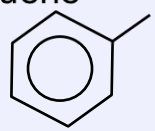
p = 1 atm

T_u = 353 K

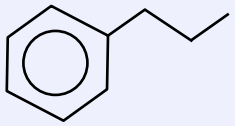
benzene

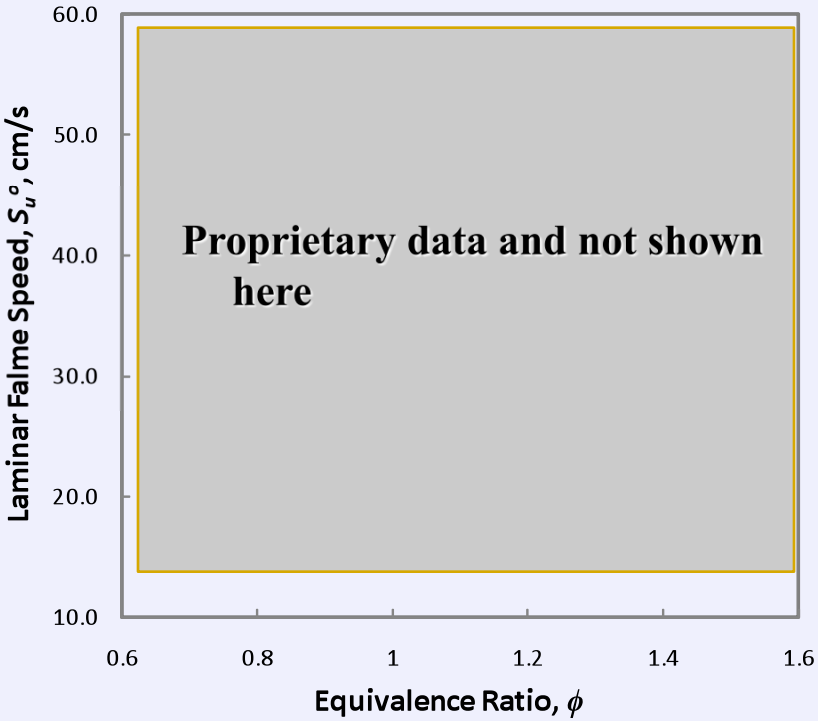


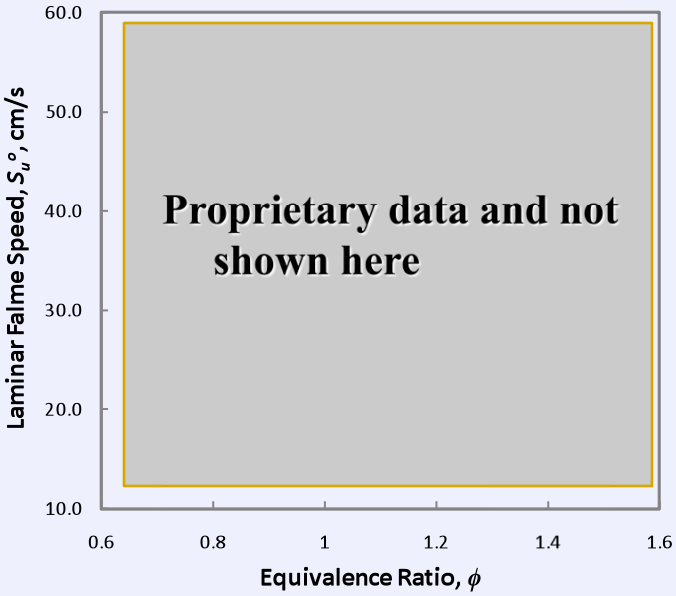
toluene

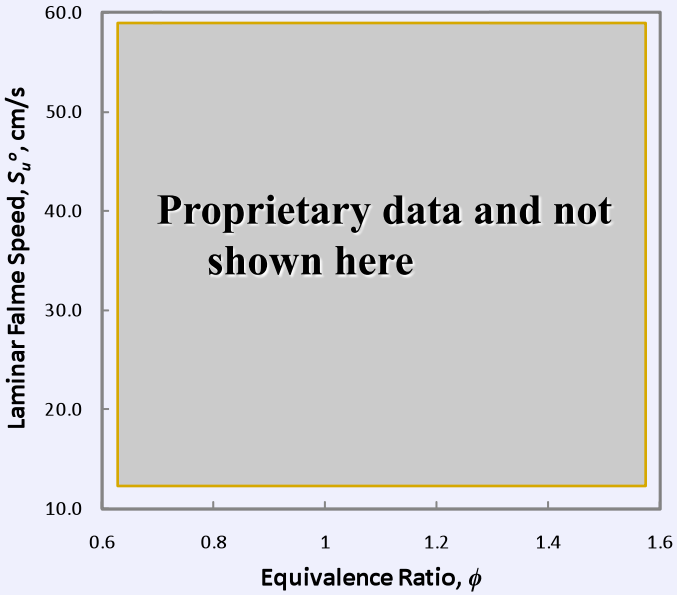


n-propylbenzene









Model I: H. Wang, X. You, A. V. Joshi, S. G. Davis, A. Laskin, F. Egolfopoulos and C. K. Law, USC Mech Version II. High-Temperature Combustion Reaction Model of H2/CO/C1-C4 Compounds. http://ignis.usc.edu/USC_Mech_II.htm, May 2007.

Model II: S. Dooley, S. H. Won, M. Chaosa, J. Heynea, Y. Jua, F. L. Dryer, K. Kumar, C-J. Sung, H. Wang, M. A. Oehlschlaegerc, R. J. Santorod and T. A. Litzinger, "A jet fuel surrogate formulated by real fuel properties ," Combust. Flame In press. doi:10.1016/j.combustflame.2010.07.001.

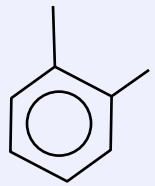
Model III: F. Battin-Leclerc, R. Bounaceur, N. Belmekki, and P. A. Glaude, "Experimental and modeling study of the oxidation of xylenes," Int. J. Chem. Kinet. 38 (2006) 284-302.

Model IV: K. Narayanaswamy , G. Blanquart, and H. Pitsch, "A consistent chemical mechanism for oxidation of substituted aromatic species," Combust. Flame 157 (2010) 1879-7898

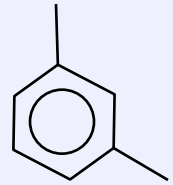
Laminar Flame Speeds of o-, m-, and p-Xylene/Air Flames

p = 1 atm
T_u = 353 K

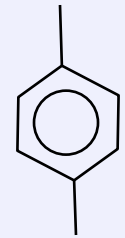
o-xylene

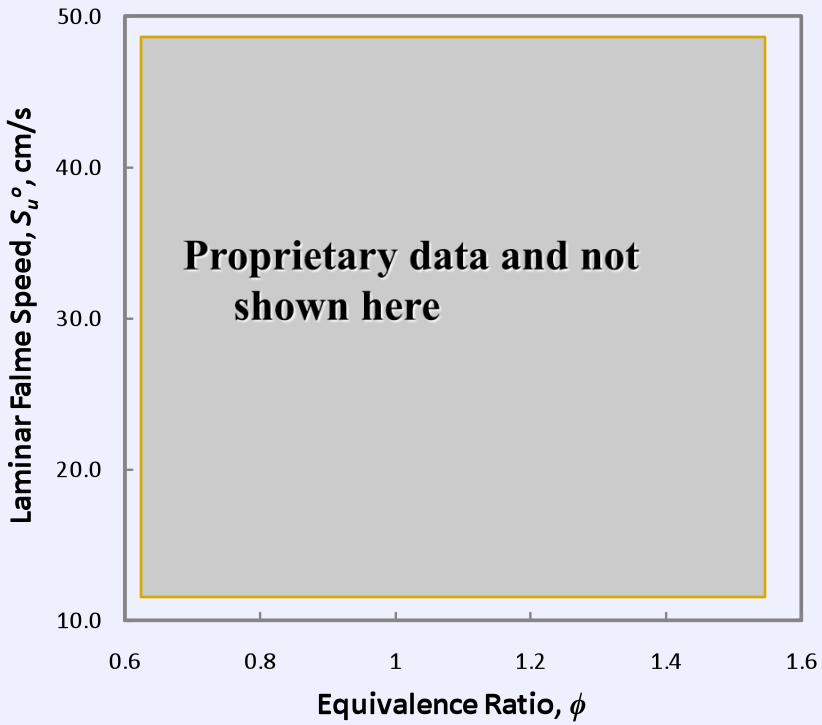


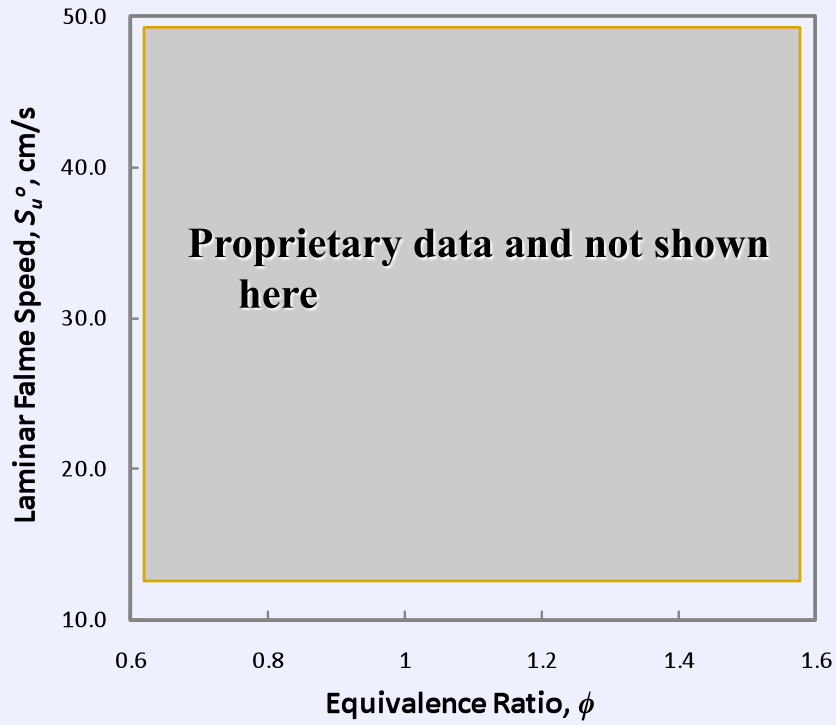
m-xylene



p-xylene







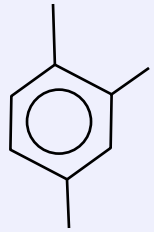
Model III: F. Battin-Leclerc, R. Bounaceur, N. Belmekki, and P. A. Glaude, "Experimental and modeling study of the oxidation of xylenes," Int. J. Chem. Kinet. 38 (2006) 284-302.

Model IV: K. Narayanaswamy , G. Blanquart, and H. Pitsch, "A consistent chemical mechanism for oxidation of substituted aromatic species," Combust. Flame 157 (2010) 1879-7898

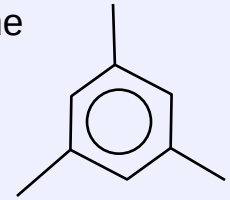
Laminar Flame Speeds of 1,2,4- and 1,3,5-Trimethyl-Benzene/Air Flames

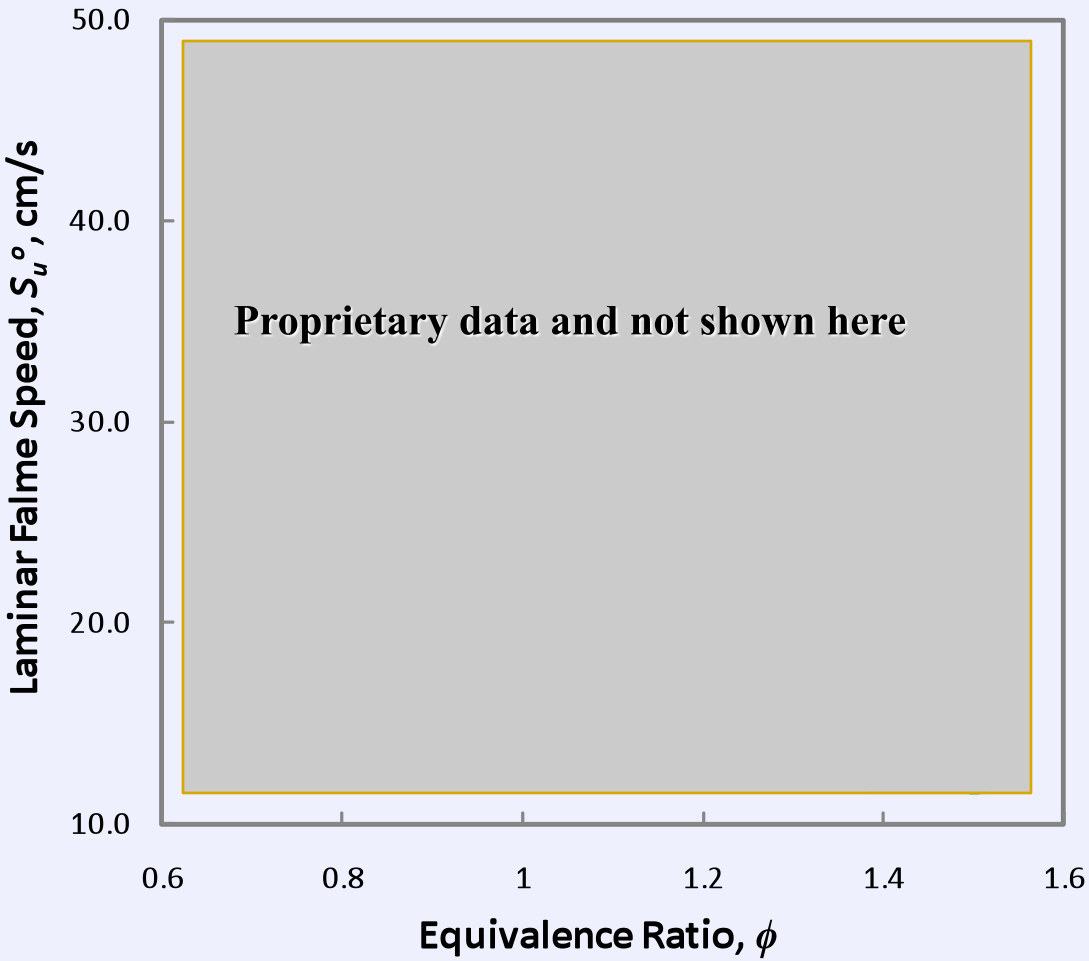
p = 1 atm
T_u = 353 K

1,2,4-trimethylbenzene



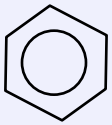
1,3,5-trimethylbenzene

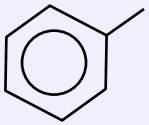


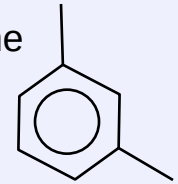


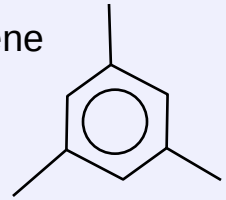
Comparison of Experimentally Determined Laminar Flame Speeds

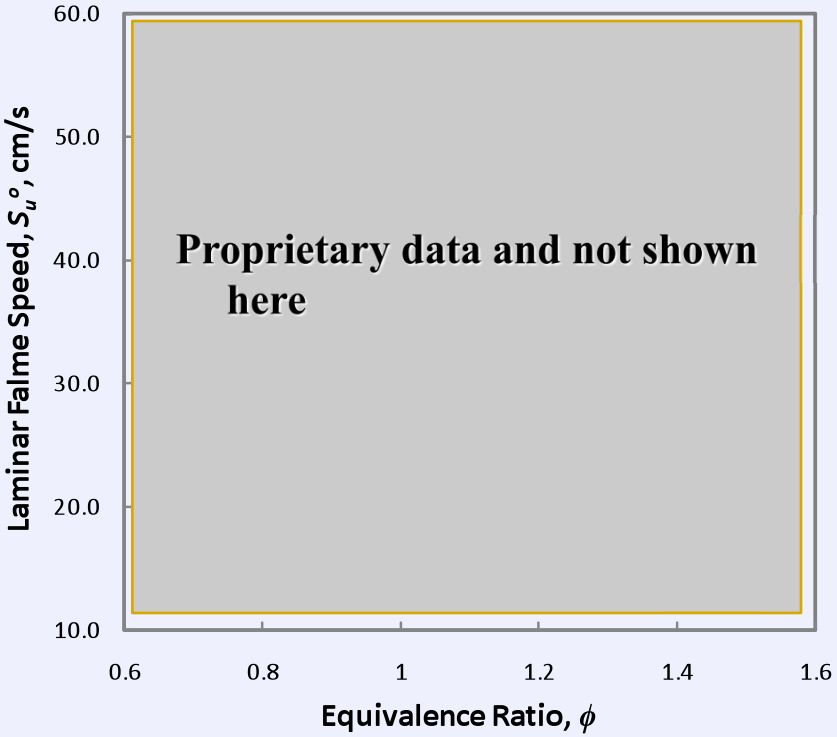
p = 1 atm
T_u = 353 K

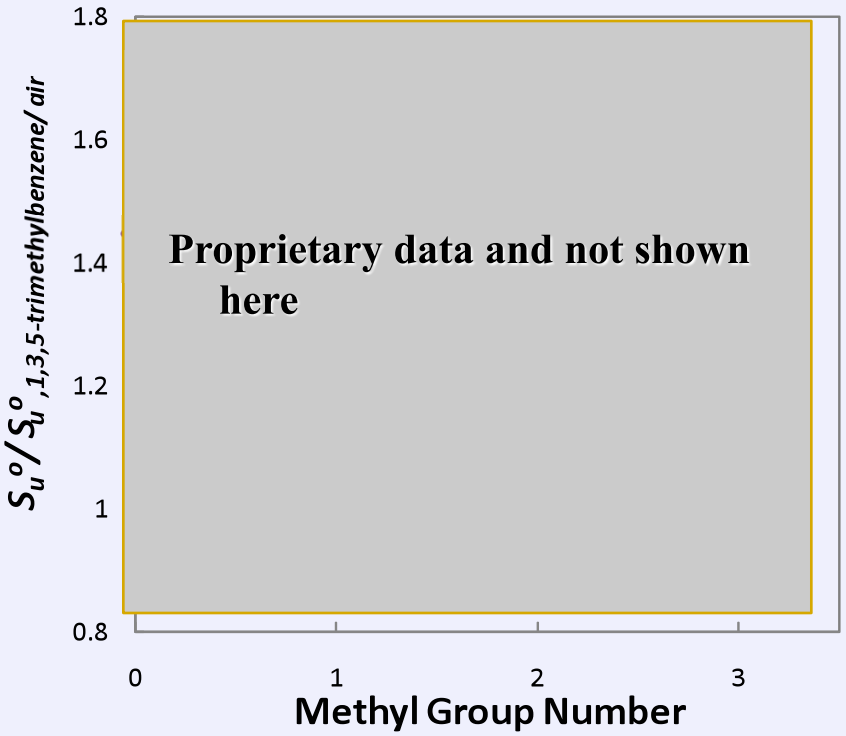
benzene 

toluene 

m-xylene 

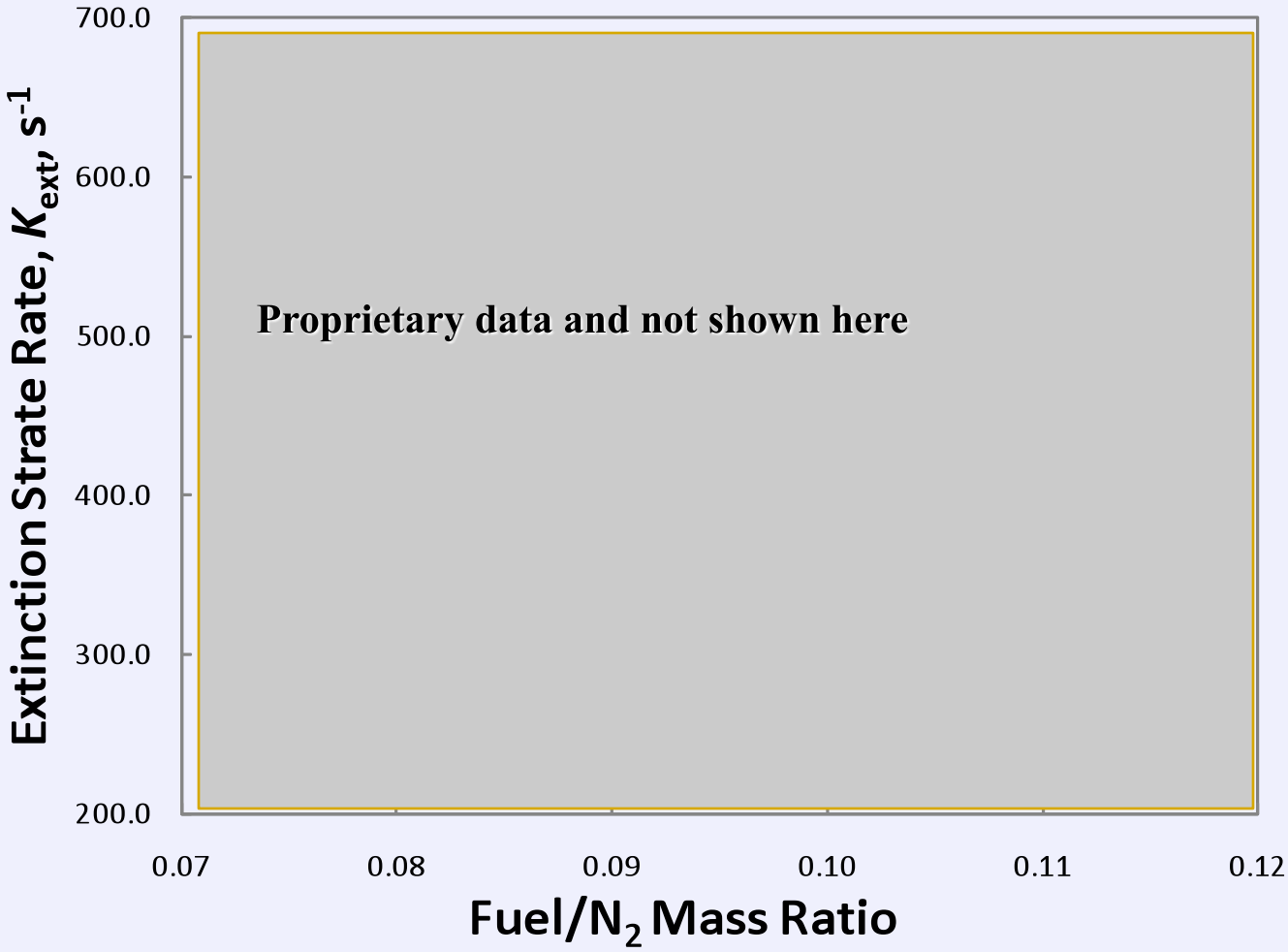
1,3,5-trimethylbenzene 





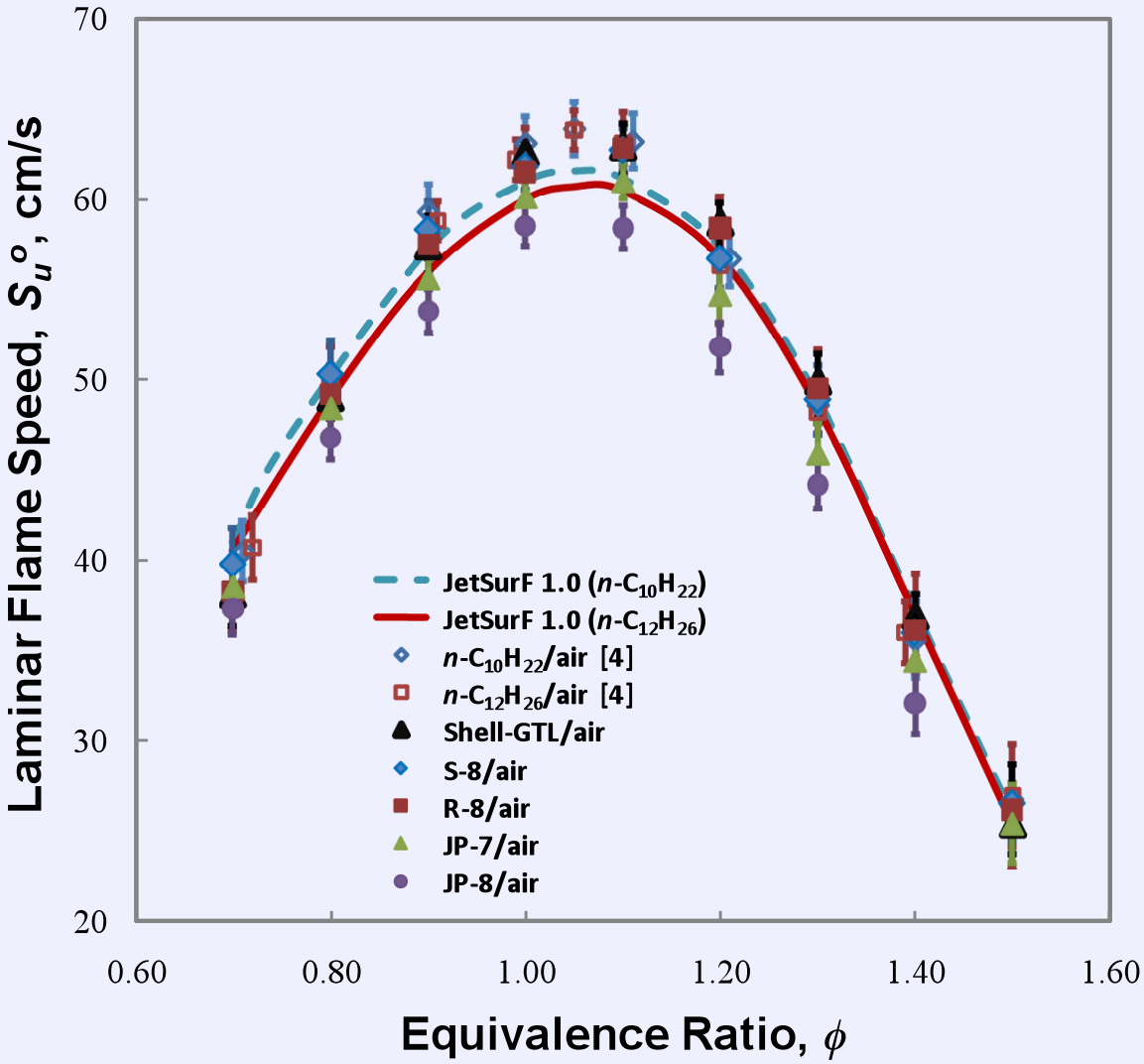
Extinction Strain Rates of Non-premixed Benzene/N_2 and Alkylbenzene/N_2 against O_2 Flames

***p* = 1 atm**
T_u = 353 K



Propagation and Extinction of Conventional and Alternative Jet Fuels

Laminar Flame Speeds Conventional and Alternative Jet Fuels Flames[5]



p = 1 atm
T_u = 403 K

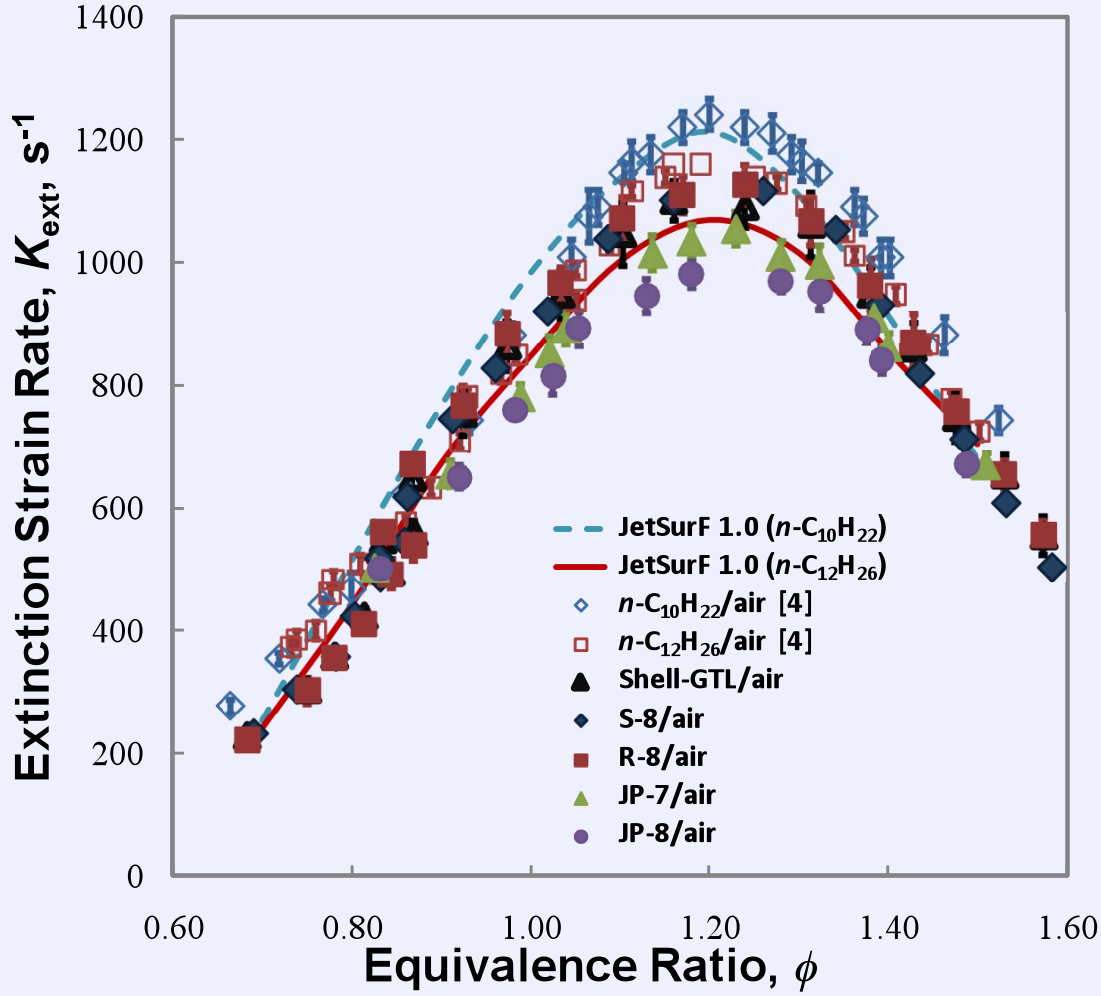
Shell GTL	(PSOF-5172)
S-8	(PSOF-4734)
R-8	(POSF-5469)
JP-7	(POSF-3327)
JP-8	(POSF-3373)

[4]C. Ji, E. Dames, Y.L. Wang, H. Wang, and F.N. Egolfopoulos, "Propagation and Extinction of Premixed C_5-C_{12} n-Alkane Flames," Combust. Flame 157(2) (2010) 277-287.

[5]C. Ji, Y.L. Wang, and F.N. Egolfopoulos, "Flame Studies of Conventional and Alternative Jet Fuels," J. Propul. Power Submitted.

Extinction Strain Rates of Conventional and Alternative Jet Fuels Flames[5]

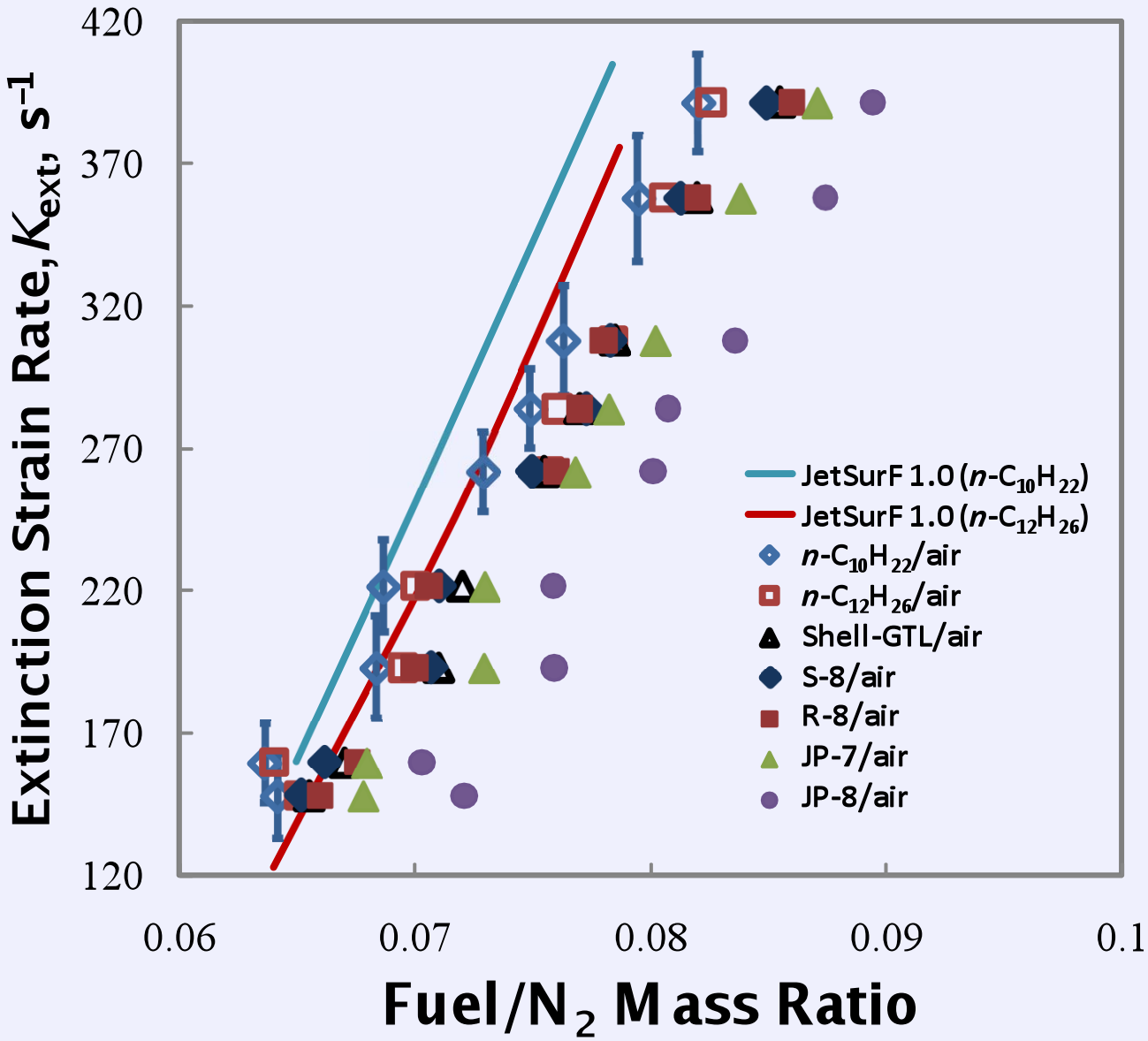
p = 1 atm
T_u = 403 K



[4]C. Ji, E. Dames, Y.L. Wang, H. Wang, and F.N. Egolfopoulos, "Propagation and Extinction of Premixed C_5-C_{12} *n*-Alkane Flames," Combust. Flame 157(2) (2010) 277-287.
[5]C. Ji, Y.L. Wang, and F.N. Egolfopoulos, "Flame Studies of Conventional and Alternative Jet Fuels," J. Propul. Power Submitted.

Extinction Strain Rates of Non-Premixed Flames[5]

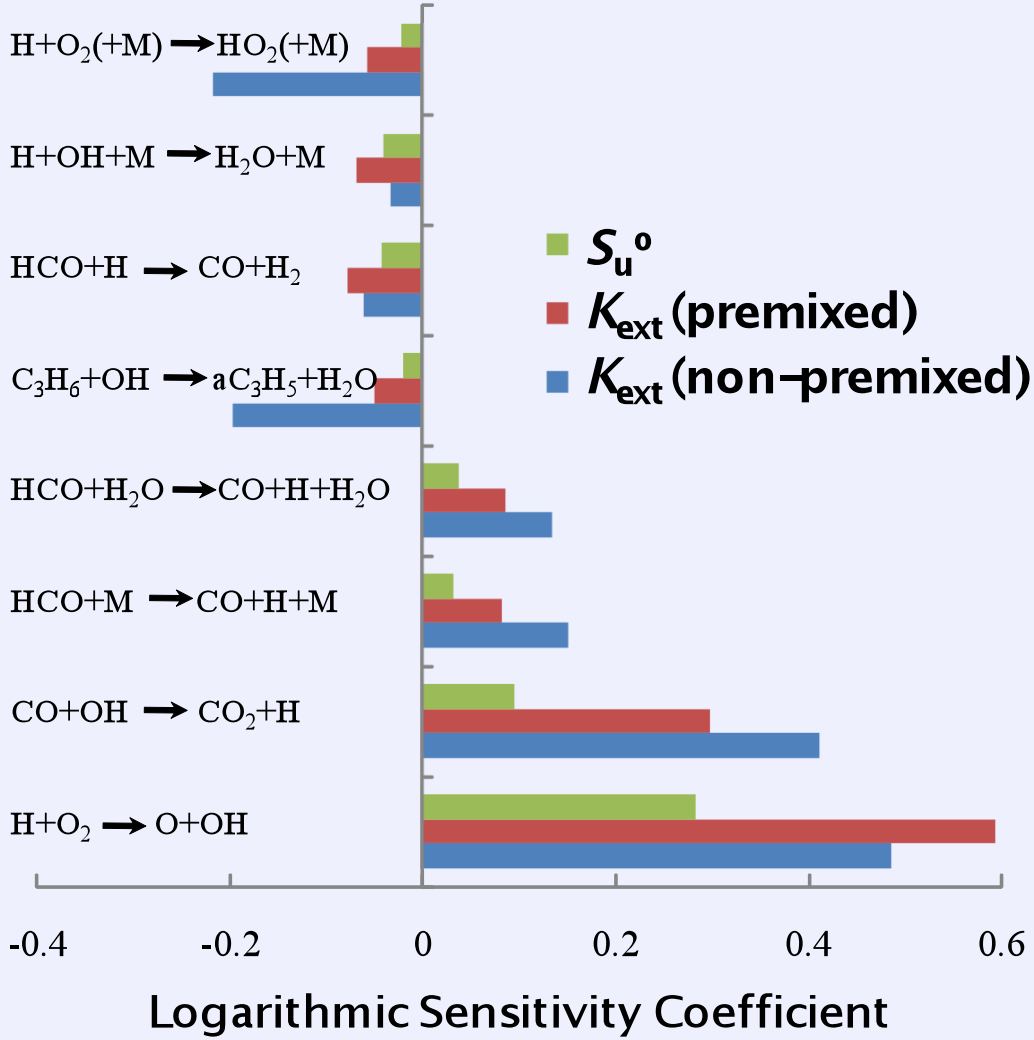
p = 1 atm
T_u = 403 K



[5]C. Ji, Y.L. Wang, and F.N. Egolfopoulos, "Flame Studies of Conventional and Alternative Jet Fuels," J. Propul. Power Submitted.

Kinetic Effects on the Propagation and Extinction of Conventional and Alternative Jet Fuels Flames[5]

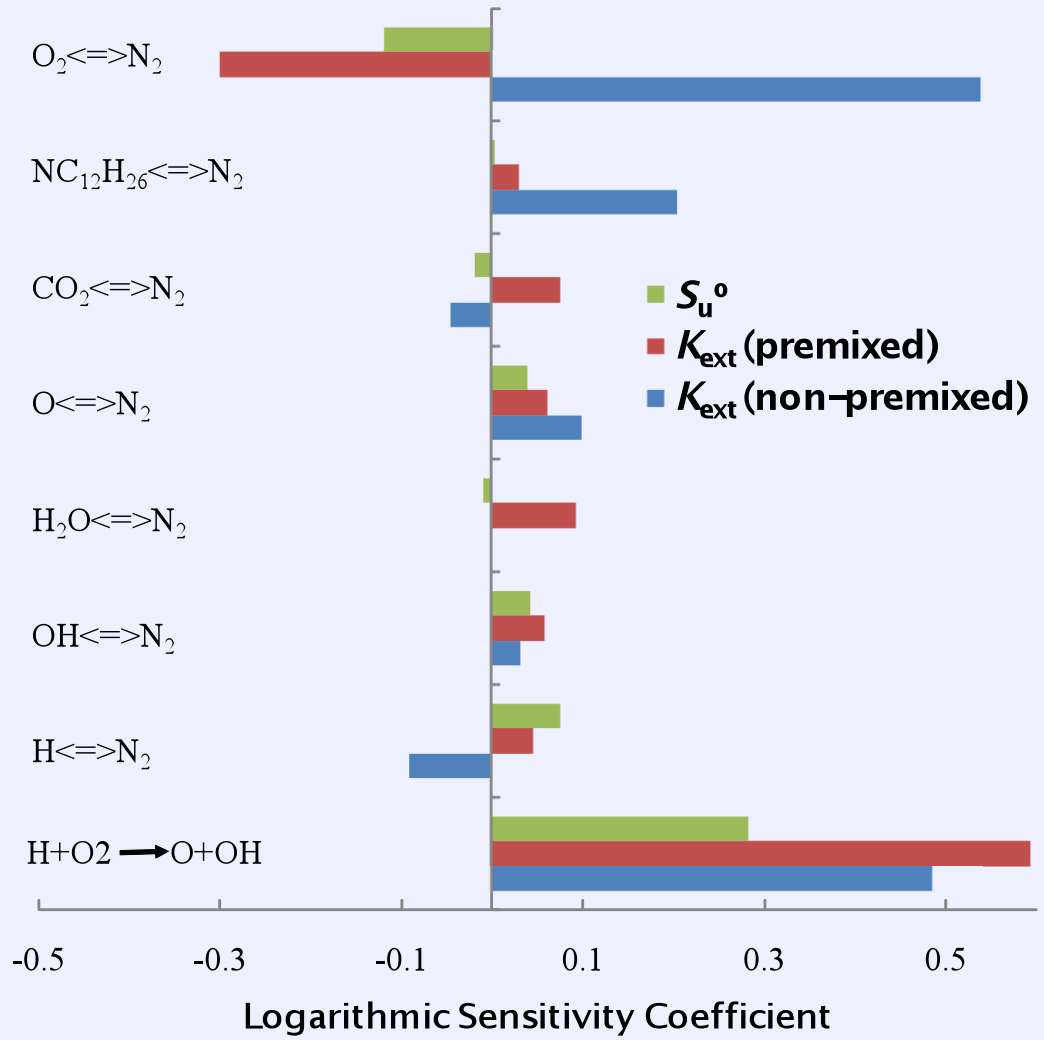
***n*-dodecane**
***p* = 1 atm**
T_u = 403 K
ϕ = 1.0; F/N_2=0.066



[5]C. Ji, Y.L. Wang, and F.N. Egolfopoulos, "Flame Studies of Conventional and Alternative Jet Fuels," J. Propul. Power Submitted.

Binary Diffusion Effect on the Propagation and Extinction of Conventional and Alternative Jet Fuels Flames[5]

***n*-dodecane**
p = 1 atm
T_u = 403 K
ϕ = 1.0; F/N_2=0.066

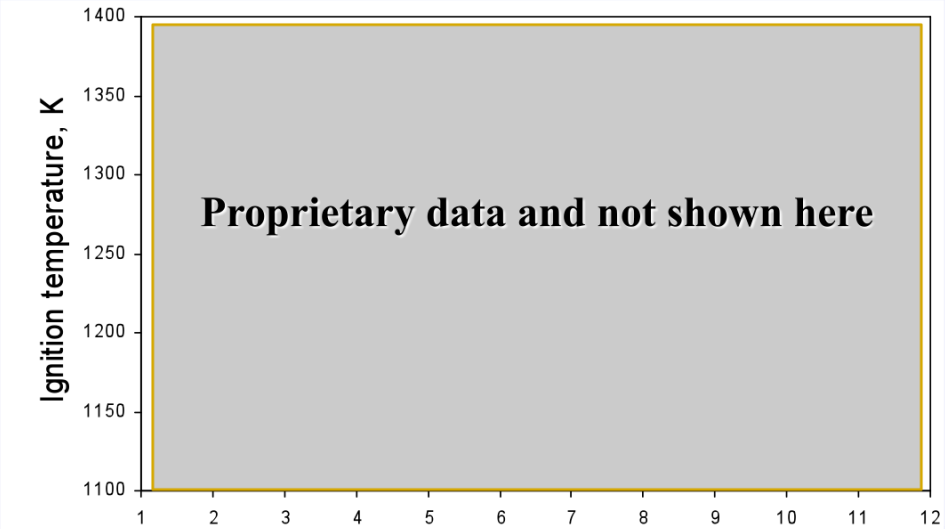


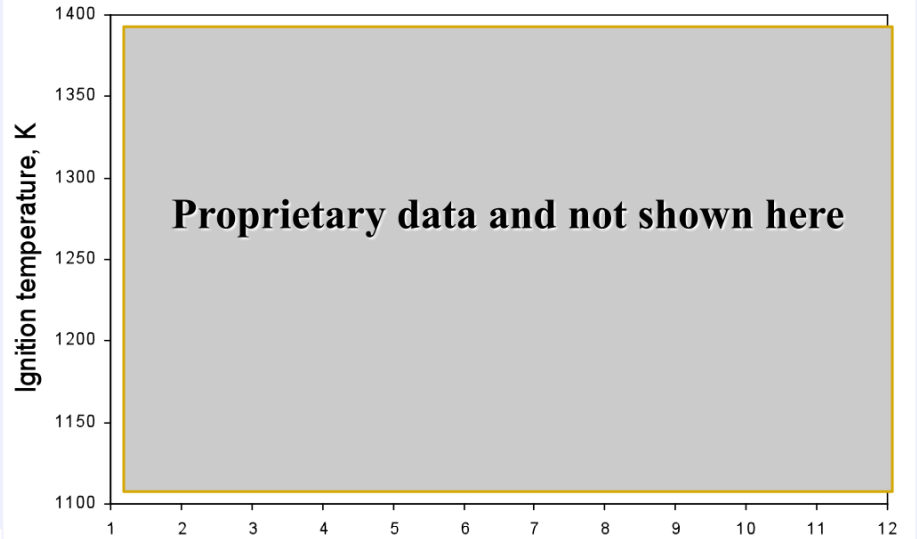
[5]C. Ji, Y.L. Wang, and F.N. Egolfopoulos, "Flame Studies of Conventional and Alternative Jet Fuels," J. Propul. Power Submitted.

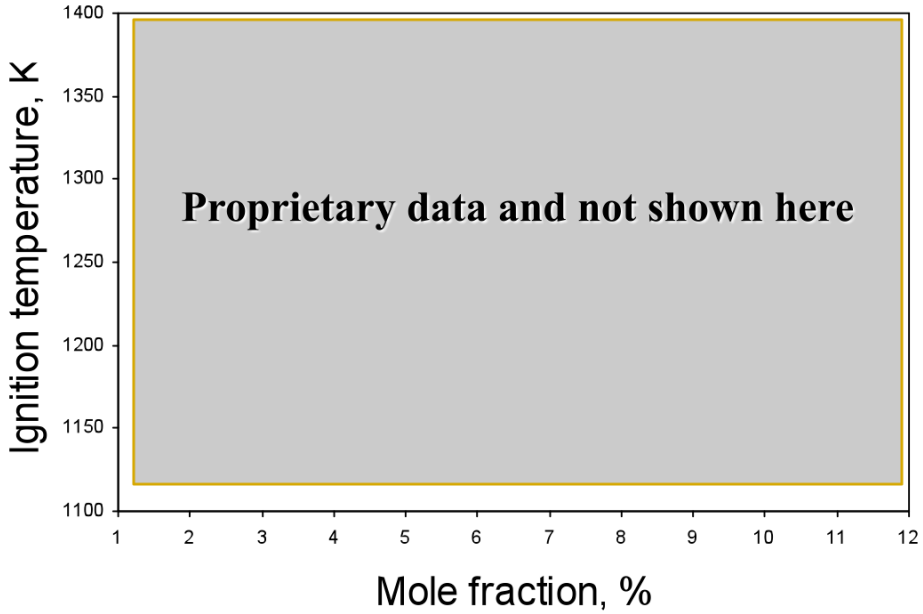
Ignition of Non-premixed Flames of n-Alkanes

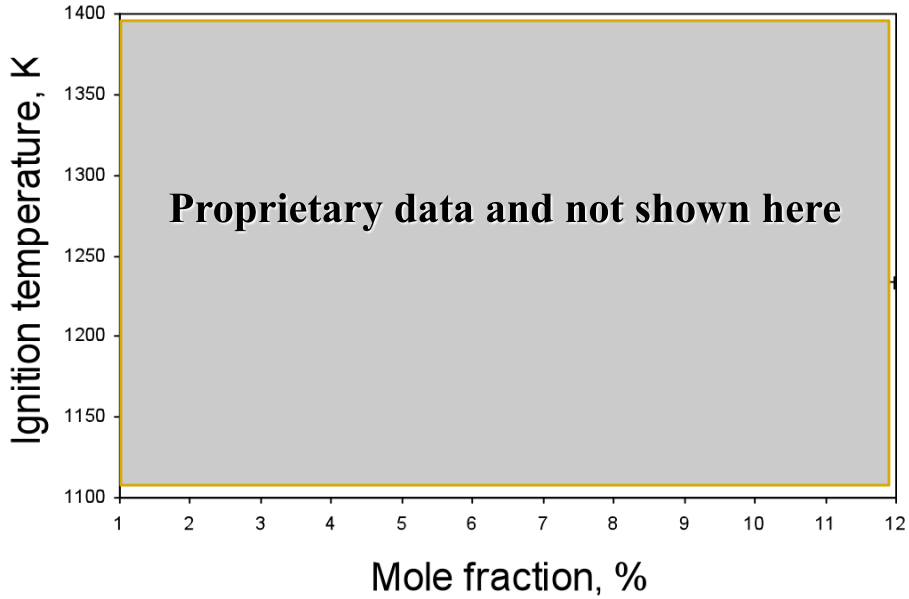
Ignition Temperatures of Non-premixed Flames of propane, n-Pentane, n-Hexane, and n-Heptane

p=1 atm, T_u=448K, Local strain rate K=140s^{-1},
Symbols: Experimental data; Lines: Numerical results using JetSurF 1.1



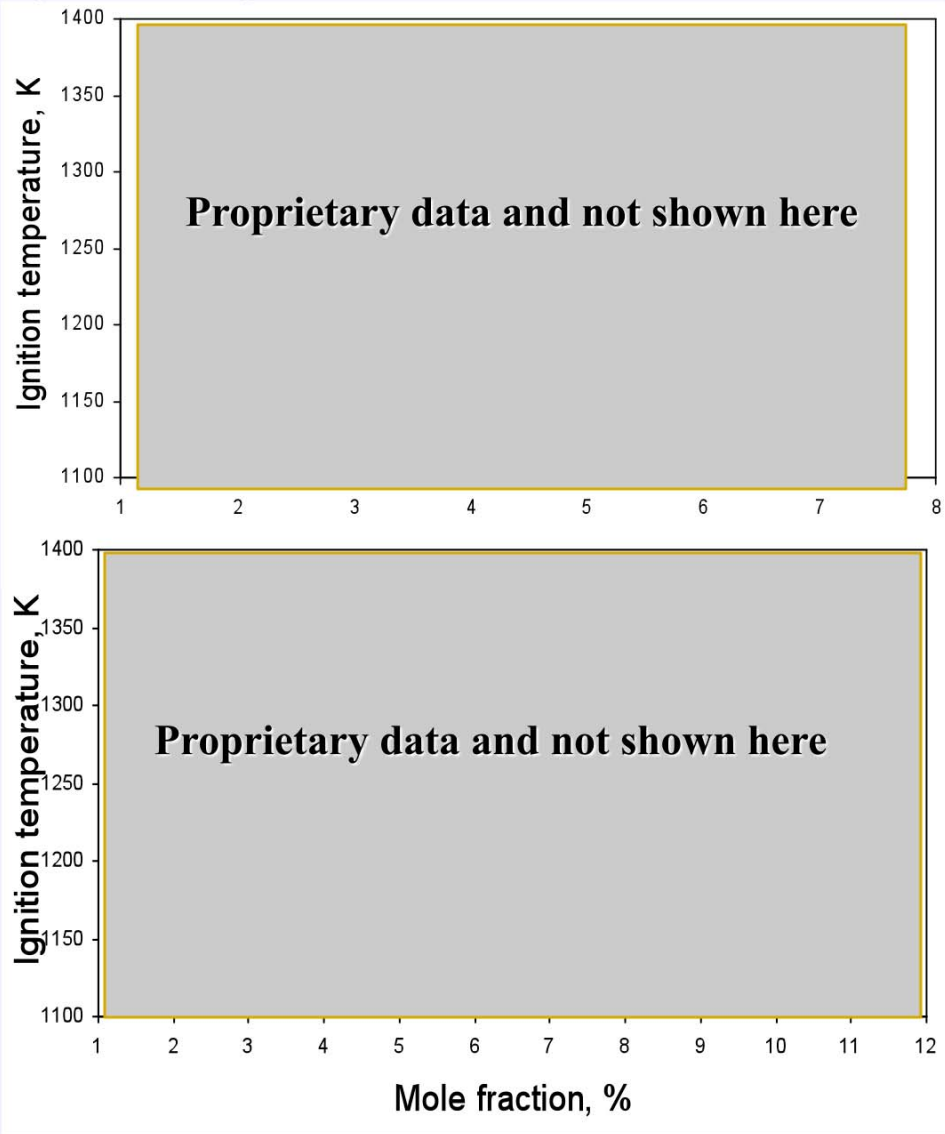


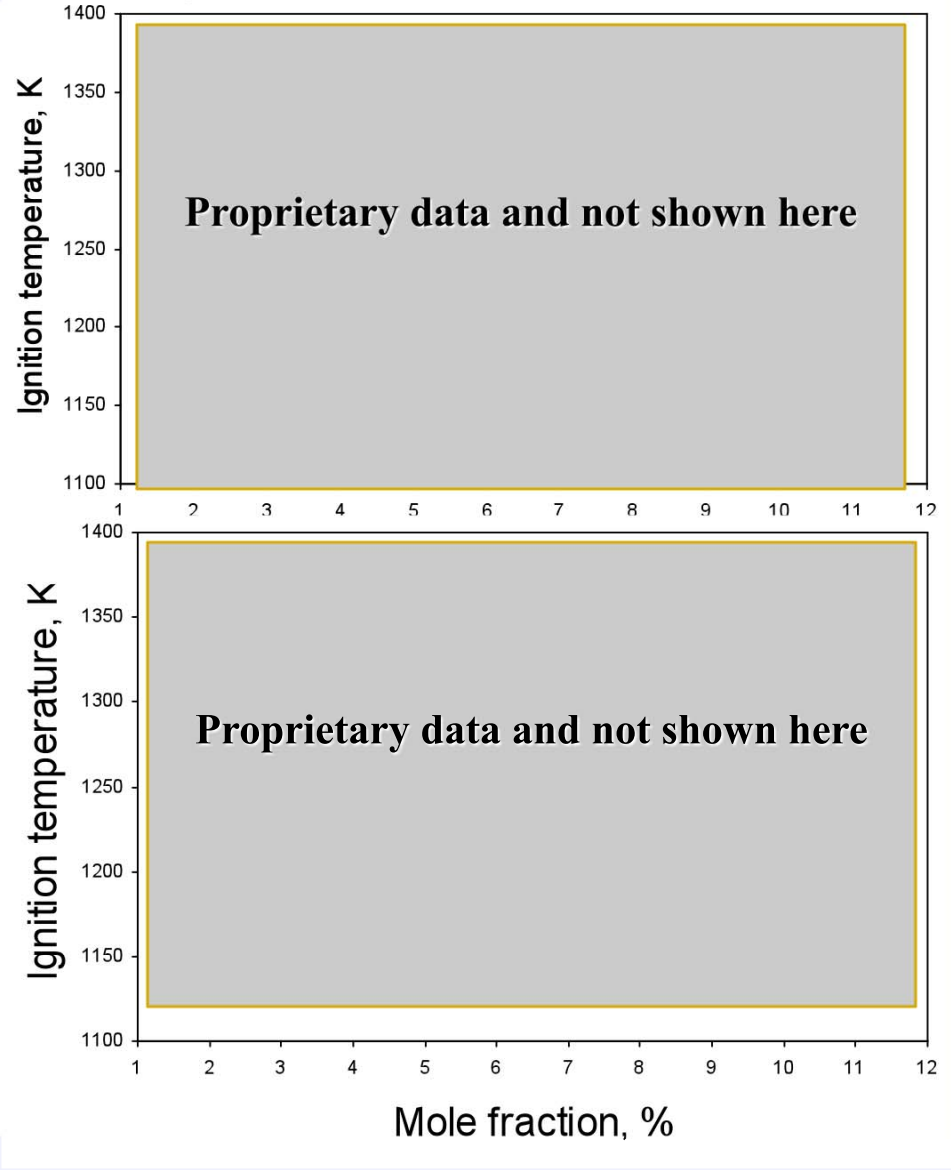




Ignition Temperatures of Non-premixed Flames of n-Octane, n-Nonane, n-Decane, and n-Dodecane

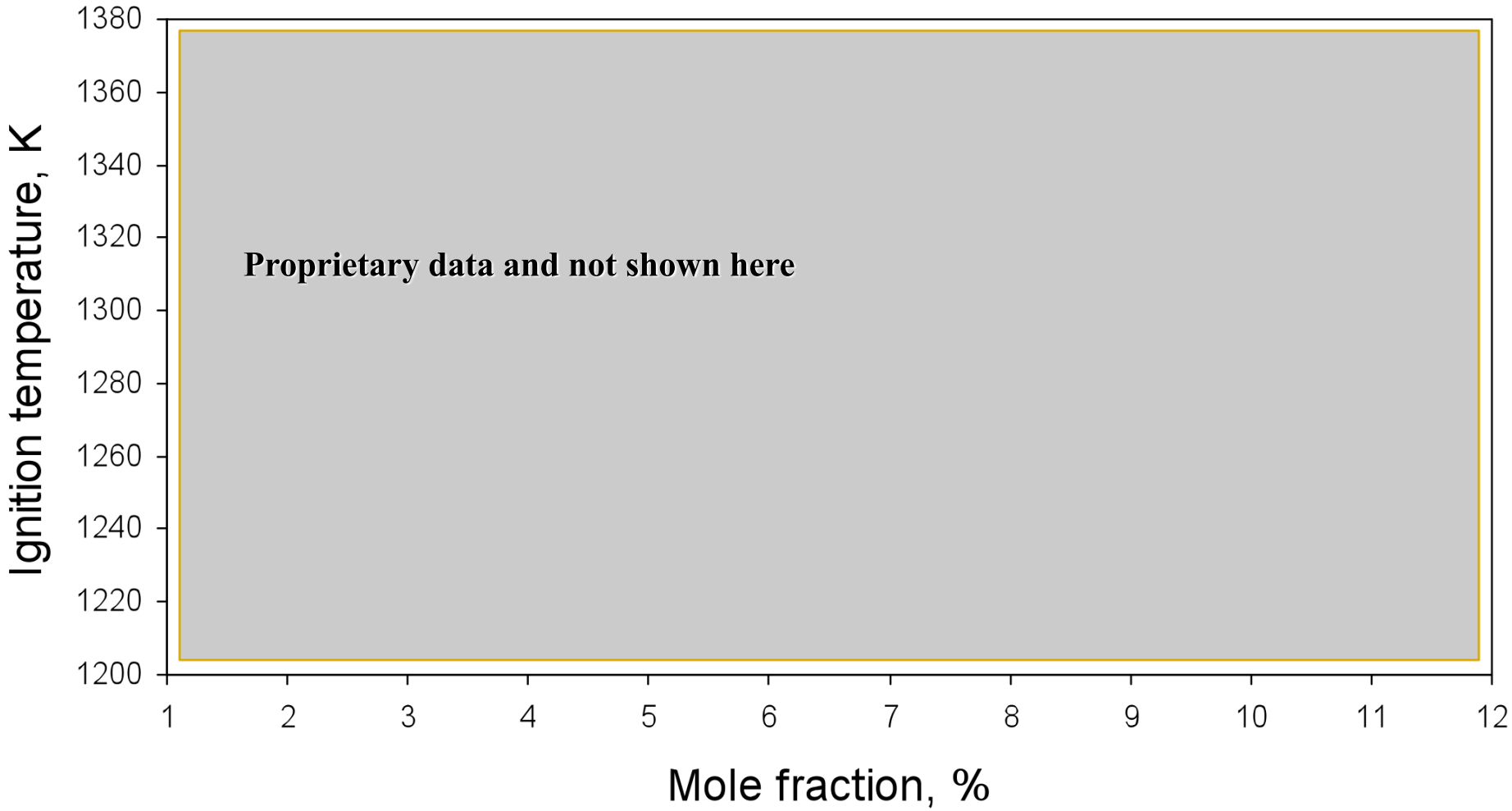
p=1 atm, T_u=448K, Local strain rate K=140s^{-1},
Symbols: Experimental data; Lines: Numerical results using JetSurF 1.1





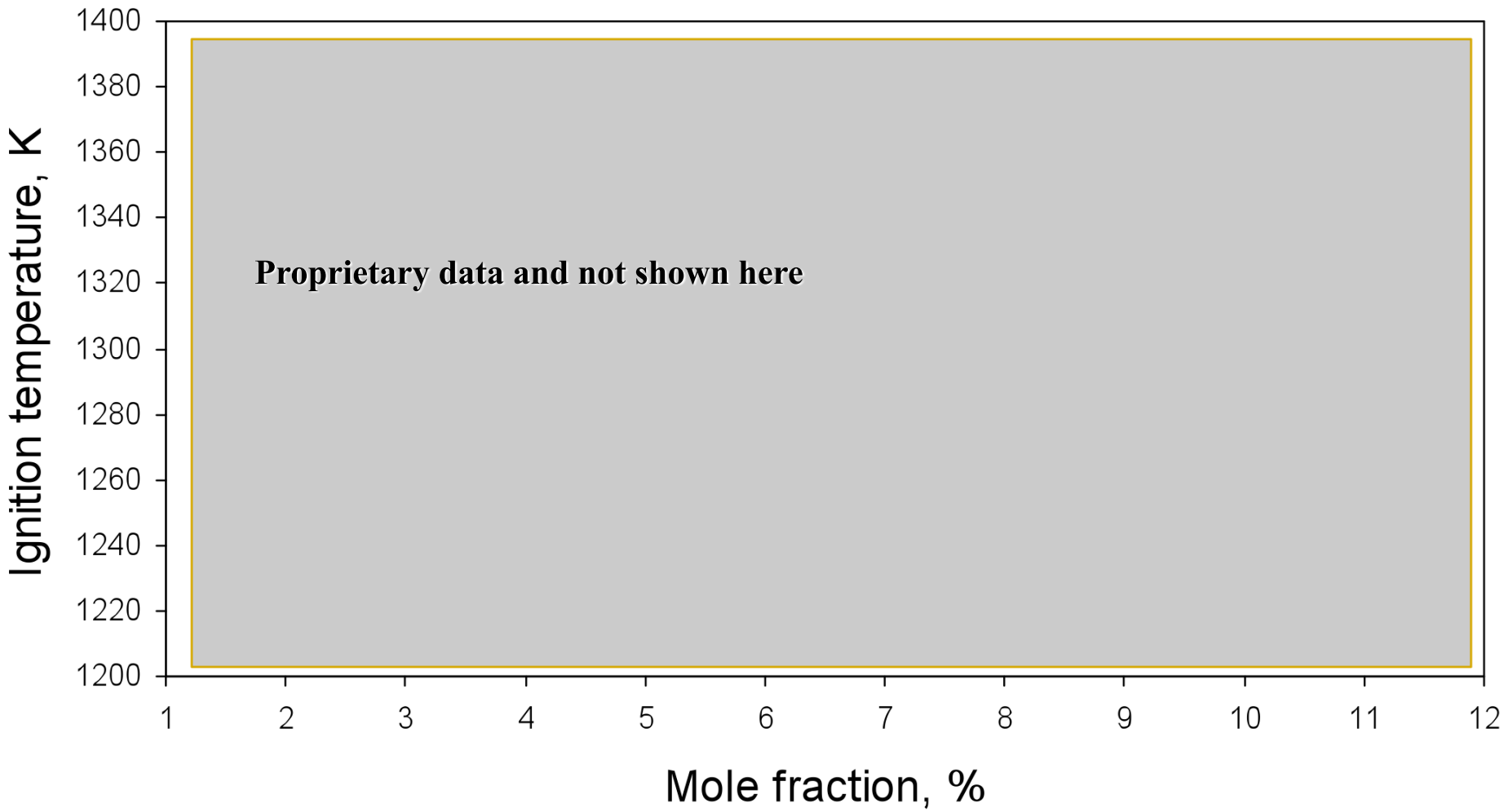
Comparison of Experimentally Determined Ignition Temperatures

p=1 atm, T_u=448K, Local strain rate K=140s^{-1}



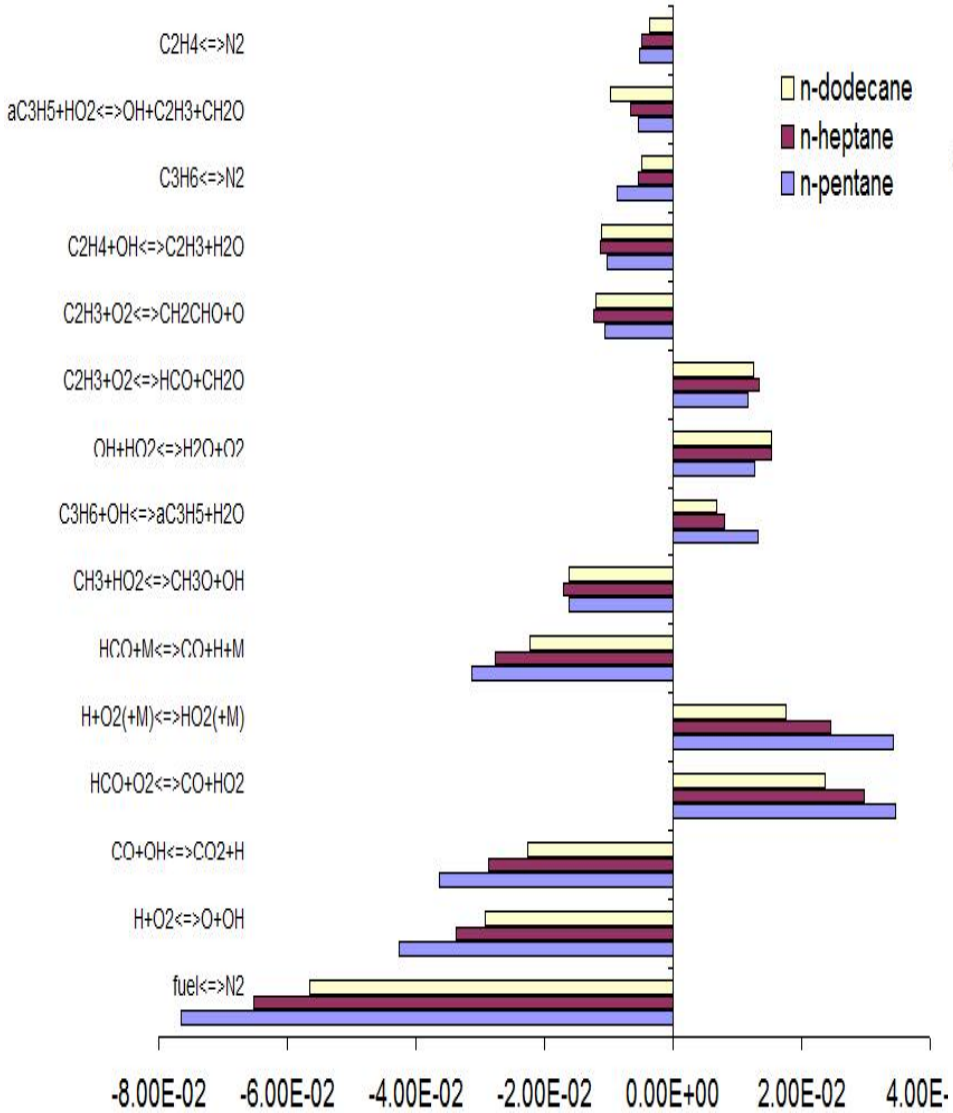
Comparison of Experimentally and Numerically Determined Ignition Temperatures for n-Pentane, n-Heptane, and n-Dodecane

p=1 atm, T_u=448K, Local strain rate K=140s^{-1},
Symbols: Experimental data; Lines: Numerical results using JetSurF 1.1

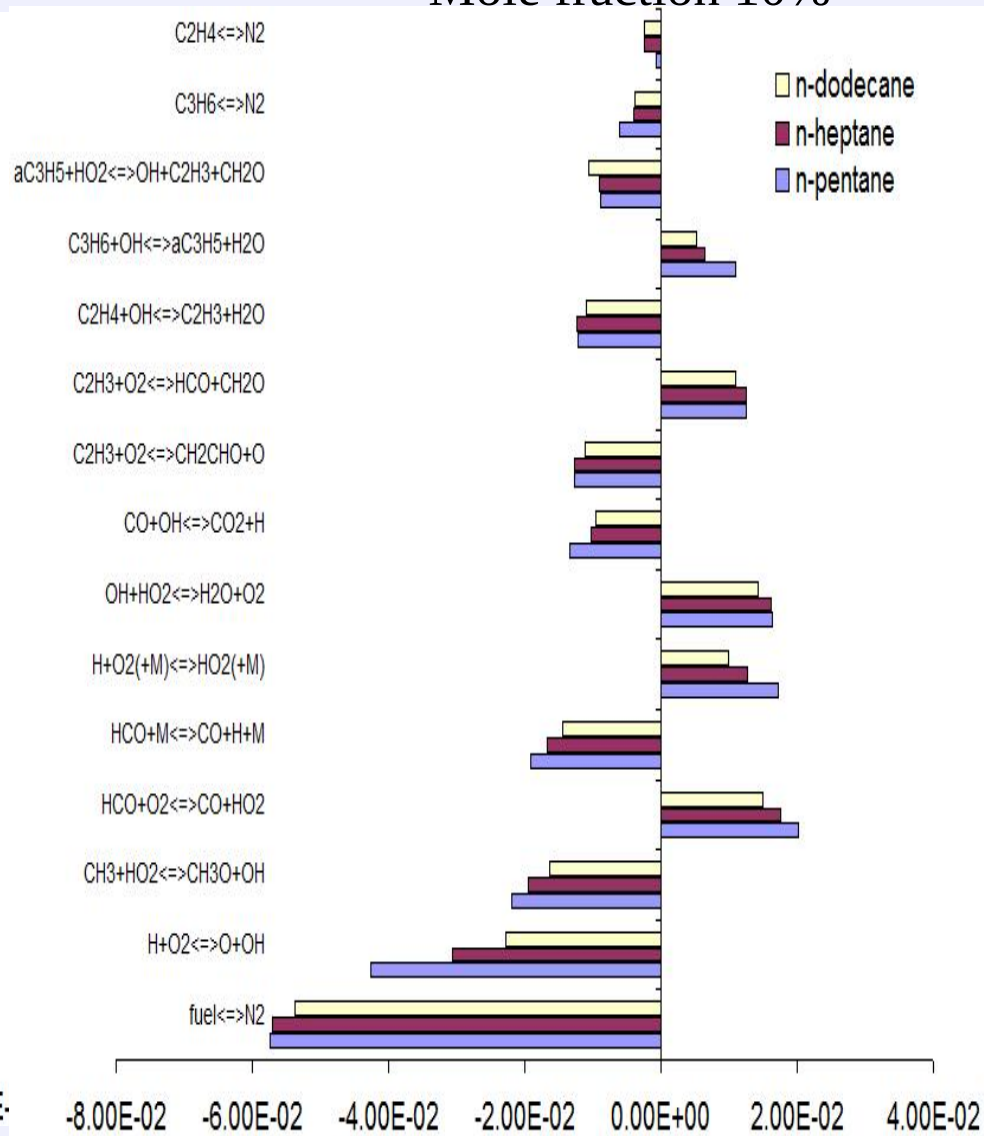


Kinetic and Diffusion Effects on the Ignition Temperatures of Non-premixed Flames

Mole fraction 2%

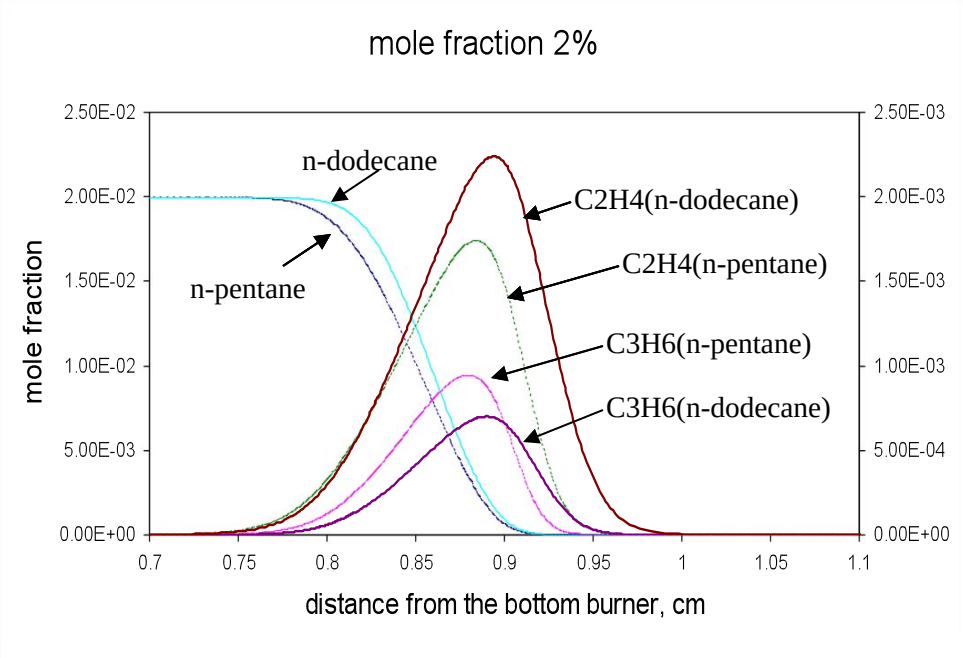


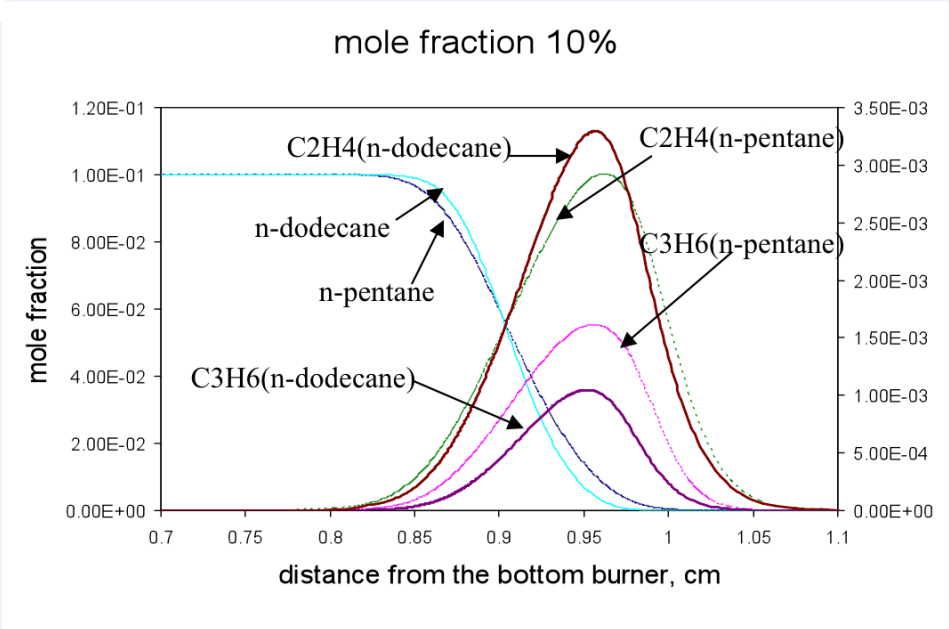
Mole fraction 10%



logarithmic sensitivity coefficient

Concentration Profiles of Fuels and Selected Intermediates





Concluding Remarks

1. **The phenomena of flame propagation and extinction of cyclo-alkanes, aromatics, jet fuels, and binary fuel mixtures were studied.**
2. **The reactivity of monoalkylated cyclohexane flames was determined to be reduced compared to cyclohexane due to the production of branched hydrocarbon intermediates.**
3. **The reactivity of alkylbenzene flames was determined to be reduced compared to benzene. This reduction is more profound as the number of methyl radicals in the fuel molecule increases.**
4. **It was determined that kinetic couplings have a minor effect on the the propagation of flames of binary fuel mixtures such as *n*-dodecane/toluene and *n*-dodecane/methyl-cyclohexane.**
5. **Ignition studies of non-premixed *n*-alkane flames revealed that in the diffusion-controlled regime, the extent of fuel decomposition and the diffusivities of the decomposition products control the ignition behavior.**