Flame Studies of Jet Fuels and Surrogate-Related Neat Hydrocarbons

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FUELS RESEARCH REVIEW

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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.
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](image1)

![Single premixed / non-premixed flame](image2)

- Pressure chamber:
  - Pressure range 0.1-10 atm

- Diagnostics:
  - Digital Particle Image Velocimetry (DPIV)
  - Thermocouples
  - Intrusive NO\textsubscript{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)
- Laminar flame speeds, $S_u^O$:
  - Monitor $S_{u,\text{ref}}$ vs. $K$
  - Non-linear extrapolations
- Extinction strain rate, $K_{\text{ext}}$:
  - $K$ at the state of extinction
- Ignition temperature, $T_{\text{ign}}$:
  - $T$ 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 / \( D_{i-N_2} \)
- 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
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

<table>
<thead>
<tr>
<th></th>
<th>C₄-C₁₂ n-alkanes</th>
<th>cycloalkanes</th>
<th>iso-alkanes</th>
<th>aromatics</th>
<th>fuel mixtures</th>
<th>jet fuels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laminar flame speeds</td>
<td>C₄, C₅, C₆, C₇, C₈, C₉, C₁₀, C₁₂ at 1 atm</td>
<td>cyclohexane (CHX) methyl-CHX ethyl-CHX n-propyl-CHX n-butyl-CHX at 1 atm</td>
<td>benzene (B) toluene n-propyl-B 1,2,4-TMB 1,3,5-TMB o-xylene m-xylene p-xylene at 1 atm</td>
<td>n-C₁₂+MCHX n-C₁₂+toluene at 1 atm</td>
<td>JP-7 JP-8 S-8 R-8 Shell-GTL at 1 atm</td>
<td></td>
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<tr>
<td>Flame ignition</td>
<td>C₃, C₅, C₆, C₇, C₈, C₉, C₁₀, C₁₂ at 1 atm</td>
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<tr>
<td>Flame extinction</td>
<td>C₅, C₆, C₇, C₈, C₉, C₁₀, C₁₂ at 1 atm</td>
<td>CHX methyl-CHX n-butyl-CHX at 1 atm</td>
<td>benzene toluene n-propyl-B 1,2,4-TMB 1,3,5-TMB o-xylene m-xylene p-xylene at 1 atm</td>
<td></td>
<td>JP-7 JP-8 S-8 R-8 Shell-GTL at 1 atm</td>
<td></td>
</tr>
</tbody>
</table>
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 C₃-C₁₂ hydrocarbons
   - propane
   - C₅-C₁₂ n-alkanes
   (in preparation)

5. Propagation of flames of binary fuel mixtures
   - methyl-cyclohexane + n-C₁₂
   - toluene + n-C₁₂
   (33rd Combustion Symposium, 2010)
Propagation of Cyclohexane and Monoalkylated Cyclohexane Flames
Laminar Flame Speeds of Cyclohexane/Air Flames¹

Cyclohexane:

![Cyclohexane structure](image)

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

\[ p = 1 \text{ atm} \]
\[ T_u = 353 \text{ K} \]

JetSurF 1.1

\[ \text{Dubois et al. (403K)} \]

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Comparison of Experimentally Determined Laminar Flame Speeds

$p = 1$ atm  
$T_u = 353$ K

![Graph showing laminar flame speed and adiabatic flame temperature as functions of equivalence ratio for different fuels.]

cyclohexane/air
$p = 1\ \text{atm}$
$T_u = 353\ \text{K}$
$\phi = 1.0$

methyl-cyclohexane/air
$p = 1\ \text{atm}$
$T_u = 353\ \text{K}$
$\phi = 1.0$

(**---**) cyclohexane/air flames

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

$$C_2H_3 + O_2 \rightarrow HCO + CH_2O$$

(**—**) n-propylcyclohexane/air flames

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

$$C_3H_6 + H \rightarrow aC_3H_5 + H_2$$

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Propagation and Extinction of
Benzene and Alkylbenzene Flames/Air Flames
\( p = 1 \text{ atm} \)
\( T_u = 353 \text{ K} \)

$p = 1 \text{ atm}$
$T_u = 353 \text{ K}$

Model III: F. Battin-Leclerc, R. Bounaceur, N. Belmekki, and P. A. Glaude,

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

\[ p = 1 \text{ atm} \]
\[ T_u = 353 \text{ K} \]

1,2,4-trimethylbenzene

1,3,5-trimethylbenzene

Proprietary data and not shown here
Comparison of Experimentally Determined Laminar Flame Speeds

$p = 1 \text{ atm}$
$T_u = 353 \text{ K}$

benzene  toluene  $m$-xylene  1,3,5-trimethylbenzene

Proprietary data and not shown here

Proprietary data and not shown here
Extinction Strain Rates of Non-premixed Benzene/N\textsubscript{2} and Alkylbenzene/N\textsubscript{2} against O\textsubscript{2} Flames

$p = 1 \text{ atm}$
$T_u = 353 \text{ K}$

Proprietary data and not shown here.
Propagation and Extinction of
Conventional and Alternative Jet Fuels
$p = 1 \text{ atm}$

$T_u = 403 \text{ K}$


Extinction Strain Rates of Conventional and Alternative Jet Fuels Flames

\[ p = 1 \text{ atm} \]
\[ T_u = 403 \text{ K} \]

\[
\text{Extinction Strain Rate, } K_{\text{ext}}, \text{ s}^{-1}
\]

\[
\text{Equivalence Ratio, } \phi
\]

\[\begin{align*}
\text{JetSurF 1.0 (n-C_{16}H_{32})} \\
\text{JetSurF 1.0 (n-C_{12}H_{26})} \\
n-C_{10}H_{22}/\text{air} [4] \\
n-C_{12}H_{26}/\text{air} [4] \\
\text{Shell-GTL/air} \\
\text{S-8/air} \\
\text{R-8/air} \\
\text{JP-7/air} \\
\text{JP-8/air}
\end{align*}\]


Extinction Strain Rates of Non-Premixed Flames

$p = 1 \text{ atm}$

$T_u = 403 \text{ K}$

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

*n*-dodecane

\( p = 1 \text{ atm} \)

\( T_u = 403 \text{ K} \)

\( \phi = 1.0; \ F/N_2=0.066 \)

**Binary Diffusion Effect on the Propagation and Extinction of Conventional and Alternative Jet Fuels Flames**

$n$-dodecane

$p = 1$ atm

$T_u = 403$ K

$\phi = 1.0; F/N_2=0.066$

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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

Proprietary data and not shown here

Proprietary data and not shown here

Proprietary data and not shown here

Proprietary data and not shown here
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

$\rho=1$ atm, $T_u=448\text{K}$, Local strain rate $K=140\text{s}^{-1}$

Proprietary data and not shown here
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

Proprietary data and not shown here
Kinetic and Diffusion Effects on the Ignition Temperatures of Non-premixed Flames

Mole fraction 2%

- $C_2H_4 \leftrightarrow N_2$
- $aC_3H_5H_2O \leftrightarrow OH + C_2H_3 + CH_2O$
- $C_3H_6 \leftrightarrow N_2$
- $C_2H_4 + OH \leftrightarrow C_2H_3 + H_2O$
- $C_2H_3 + O_2 \leftrightarrow CH_2CO + O$
- $C_2H_3 + O_2 \leftrightarrow HCO + CH_2O$
- $OH + H_2O \leftrightarrow H_2O + O_2$
- $C_3H_6 + OH \leftrightarrow aC_3H_5 + H_2O$
- $CH_3 + OH_2 \leftrightarrow CH_3 + OH$
- $HCO + H \leftrightarrow CO + H_2$
- $H + O_2 + H_2 \leftrightarrow H_3O^+$
- $HCO + OH_2 \leftrightarrow CO + OH_2 + O$
- $CO + OH_\leftrightarrow CO + O_2$
- $H_2O \leftrightarrow O + OH$
- $fuel \leftrightarrow N_2$

Mole fraction 10%

- $C_3H_6 \leftrightarrow N_2$
- $aC_3H_5H_2O \leftrightarrow OH + C_2H_3 + CH_2O$
- $C_3H_6 + OH \leftrightarrow aC_3H_5 + H_2O$
- $C_2H_4 + OH \leftrightarrow C_2H_3 + H_2O$
- $C_2H_3 + O_2 \leftrightarrow HCO + CH_2O$
- $C_2H_3 + O_2 \leftrightarrow CH_2CO + O$
- $CO + OH \leftrightarrow CO_2 + H$
- $OH + H_2O \leftrightarrow H_2O + O_2$
- $H + O_2 + H_2 \leftrightarrow H_3O^+$
- $HCO + H \leftrightarrow CO + H_2$
- $HCO + OH_2 \leftrightarrow CO + OH_2 + O$
- $CH_3 + OH_2 \leftrightarrow CH_3O + OH$
- $H + O_2 \leftrightarrow O + OH$
- $fuel \leftrightarrow N_2$

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 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.