Computational and Experimental Study of the Structure of Diffusion Flames of Jet Fuel and its Surrogates at Pressures up to 40 atm

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Outline

• Overview of completed work 2/06-11/08
• Discussion of work during no-cost extension
• Brief description of current project
Objectives (1)

- Examine flame structure of single component, JP-8 surrogate and JP-8 flames in a counterflow configuration
- Determine extinction values
- Model the surrogate(s) with semidetailed chemical kinetics
- Reduce chemical kinetics
JP-8 Surrogate

- JP-8 is modeled as a six-component surrogate mixture (Violi, et al., 2001)
  - 10% Iso-octane (C\(_8\)H\(_{18}\)), 20% Methylcyclohexane (C\(_7\)H\(_{14}\)),
  - 5% Tetralin (C\(_{10}\)H\(_{12}\)), 30% Dodecane (C\(_{12}\)H\(_{24}\)),
  - 20% Tetradecane (C\(_{14}\)H\(_{30}\)), 15% m-Xylene (C\(_8\)H\(_{10}\))

- Surrogate kinetics are modeled using two semi-detailed mechanisms
  - Initial studies use a 221-species mechanism containing 5032 reactions
  - Selected flames are modeled with a 260-species mechanism containing 7001 reactions
3 hours of flame burning and 30 hours of off-line analysis
Results: Surrogate Flames
Comparison of Temperature Profiles

SU RR_0002:
Strain Rate = 95 s⁻¹
X_{Surr} = 1.40%, T_{F} = 394 K,
V_{F} = 35.28 cm/s
X_{O2} = 76.8%, T_{OX} = 306 K,
Results: JP-8 Flames
Comparison of Temperature Profiles

Predicted, 221 species
Predicted, 260 species
Measured T (JP-8, cyl. corr.)
Measured T (JP-8, sph. corr.)

SU RR_0001:
Strain Rate = 115 s⁻¹
\(X_{SU RR} = 1.56\%\), \(T_F = 387\) K,
\(V_F = 40.26\) cm/s
\(X_O2 = 76.8\%\), \(T_{OX} = 315\) K,
\(V_{OX} = 36.57\) cm/s
Results: JP-8 Surrogate Flames Comparison of Rich Extinction Limits

- Rich extinction limits have been determined for two surrogate flames via continuation methods.
- Extinction limits for JP-8 flames with the same fuel flow rate have been measured and are identical to the surrogate extinction limits.
- The effects of kinetic mechanism on the rich extinction limit are examined for each surrogate flame.

<table>
<thead>
<tr>
<th>Inlet Surrogate Mole Fraction</th>
<th>Inlet Oxygen Mole Fraction</th>
<th>Strain Rate (s(^{-1}))</th>
<th>Mechanism</th>
<th>Predicted Rich Extinction Limit (% O(_2) by mole)</th>
<th>Measured Rich Extinction Limit (% O(_2) by mole)</th>
<th>% Variation (relative to measurement)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0156</td>
<td>0.768</td>
<td>115</td>
<td>221 Species</td>
<td>0.5512</td>
<td>0.594</td>
<td>7.21</td>
</tr>
<tr>
<td>260 Species</td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>0.014</td>
<td>0.768</td>
<td>95</td>
<td>221 Species</td>
<td>0.6185</td>
<td>0.602</td>
<td>2.74</td>
</tr>
<tr>
<td>260 Species</td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>6.81</td>
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</table>
Summary of Completed Counterflow Work (1)

• Results were generated for lean, non-sooting counterflow diffusion flames with \( n \)-dodecane, methylcyclohexane, iso-octane, and the surrogate blend as fuels
• Single-solution methods provide computational temperature profiles for experimental comparison and a basis for future validation of velocity and species profiles
• Arc length continuation is used to predict rich extinction limits for each flame
• Predicted and measured temperature profiles and rich extinction limits are presented for each flame
  – Measurements are corrected for radiative losses
  – Especially good agreement is noted between computational results and experimental JP-8 flames
  – Rich extinction limits agree within 10%
Objectives (2)

- Examine flame structure of JP-8 doped flames
- Compare and contrast with promising surrogate candidates
- Model the surrogate(s) with semidetailed chemical kinetics
- Reduce chemical kinetics
Experimental System

- One-dimensional counterflow flame
- Perturbed baseline (methane/ethylene) flame
  - Use flame as a “controlled” reactor by maintaining a fixed time-temperature baseline and constant stoichiometric mixture fraction and add O(1000) ppm liquid fuel
- Liquid dispersion by the electrospray, followed by spray evaporation in the fuel line
- Flame burning ~3 hrs, off-line analysis at least 30 hrs
**Selection of Flames Spanning a Broad Range of Conditions**

<table>
<thead>
<tr>
<th>Non-sooting Flame Set</th>
<th>Sooting Flame Set</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Temp= 1750K</td>
<td>Max. Temp= 1989K</td>
</tr>
<tr>
<td>Strain Rate= 102 s⁻¹</td>
<td>Strain Rate= 69 s⁻¹</td>
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<tr>
<td>Stoich. mixture fraction $Z_f = 0.77$</td>
<td>$Z_f = 0.18$</td>
</tr>
<tr>
<td>Fixed temperature profile</td>
<td>Fixed temperature profile</td>
</tr>
<tr>
<td>Flame on fuel side of stagnation plane</td>
<td>Flame on oxidizer side of stagnation plane</td>
</tr>
</tbody>
</table>
# Experimental Conditions: Nonsooting Flames

<table>
<thead>
<tr>
<th></th>
<th>Molar Composition</th>
<th>Flame A</th>
<th>Flame B</th>
<th>Flame C</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fuel Side</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Molar Composition</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N₂</td>
<td>0.897</td>
<td>0.902</td>
<td>0.902</td>
<td></td>
</tr>
<tr>
<td>CH₄</td>
<td>0.103</td>
<td>0.097</td>
<td>0.097</td>
<td></td>
</tr>
<tr>
<td>C2-C5 alkane impurities</td>
<td>232 ppm</td>
<td>232 ppm</td>
<td>219 ppm</td>
<td></td>
</tr>
<tr>
<td>JP-8 (C₁₁H₂₁)</td>
<td></td>
<td>992 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methyl-Cyclohexane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Iso-Octane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>m-Xylene</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tetraline</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dodecane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tetradecane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mass Flux (g/min/cm²)</td>
<td>2.80</td>
<td>2.97</td>
<td>2.97</td>
<td></td>
</tr>
<tr>
<td>Temperature (K)</td>
<td></td>
<td>379</td>
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</tr>
<tr>
<td><strong>Oxidizer Side</strong></td>
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<td></td>
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</tr>
<tr>
<td>Molar Composition</td>
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<td></td>
</tr>
<tr>
<td>N₂</td>
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<td>0.227</td>
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</tr>
<tr>
<td>O₂</td>
<td></td>
<td>0.773</td>
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</tr>
<tr>
<td>Mass Flux (g/min/cm²)</td>
<td>3.19</td>
<td>3.42</td>
<td>3.42</td>
<td></td>
</tr>
<tr>
<td>Temperature (K)</td>
<td></td>
<td>340</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Strain Rate (s⁻¹)</td>
<td></td>
<td>110</td>
<td>117</td>
<td>117</td>
</tr>
<tr>
<td>z₀</td>
<td></td>
<td>0.76</td>
<td></td>
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</tbody>
</table>
# Experimental Conditions: Sooting Flames

<table>
<thead>
<tr>
<th></th>
<th>Flame A Baseline</th>
<th>Flame A\textsuperscript{*} Equal Carbon</th>
<th>Flame B Jet Fuel</th>
<th>Flame C Utah/Yale Surrogate</th>
<th>Flame D Aachen Surrogate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molar Composition</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N\textsubscript{2}</td>
<td>0.7278</td>
<td>0.7280</td>
<td>0.7340</td>
<td>0.7339</td>
<td>0.7339</td>
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<tr>
<td>C\textsubscript{2}H\textsubscript{4}</td>
<td>0.2722</td>
<td>0.2719</td>
<td>0.2641</td>
<td>0.2641</td>
<td>0.2641</td>
</tr>
<tr>
<td>C\textsubscript{2} (Ethane) impurities</td>
<td>637 ppm</td>
<td>636 ppm</td>
<td>618 ppm</td>
<td>618 ppm</td>
<td>618 ppm</td>
</tr>
<tr>
<td>Jet Fuel\textsuperscript{1} (C\textsubscript{11}H\textsubscript{22})</td>
<td></td>
<td></td>
<td>1953 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fuel Side</td>
<td></td>
<td>Methyl-cyclohexane</td>
<td>394 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Iso-Octane</td>
<td>197 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>m-Xylene</td>
<td>295 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Tetralin</td>
<td>98 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Dodecane</td>
<td>591 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Tetradecane</td>
<td>394 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Total=</td>
<td>1970 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1,2,4-trimethylbenzene</td>
<td></td>
<td>450 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>n-Decane</td>
<td></td>
<td>1520 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Total=</td>
<td></td>
<td>1970 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mass Flux (g/(cm\textsuperscript{2}.min))</td>
<td>1.619</td>
<td>1.683</td>
<td>1.684</td>
<td>1.683</td>
<td>1.682</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>407</td>
<td>407</td>
<td>407</td>
<td>407</td>
<td>407</td>
</tr>
<tr>
<td>Oxidizer side</td>
<td>Molar Composition</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N\textsubscript{2}</td>
<td>0.8070</td>
<td>0.8070</td>
<td>0.8070</td>
<td>0.8070</td>
<td>0.8070</td>
</tr>
<tr>
<td>O\textsubscript{3}</td>
<td>0.1843</td>
<td>0.1843</td>
<td>0.1843</td>
<td>0.1843</td>
<td>0.1843</td>
</tr>
<tr>
<td>Mass Flux (g/(cm\textsuperscript{2}.min))</td>
<td>1.891</td>
<td>1.925</td>
<td>1.925</td>
<td>1.925</td>
<td>1.925</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>370</td>
<td>370</td>
<td>370</td>
<td>370</td>
<td>370</td>
</tr>
<tr>
<td>Strain Rate (s\textsuperscript{-1})</td>
<td>89.9</td>
<td>85.2</td>
<td>97.3</td>
<td>97.3</td>
<td>97.3</td>
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<tr>
<td>z\textsubscript{f}</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
</tr>
</tbody>
</table>
Non-sooting Flames: Major Species and Temp

JP-8 doped - Full Symbols; Surrogate doped - Open Symbols; Line - computations
Non-sooting Flames: C7-C15 Alkanes

JP-8 doped

Surrogate doped (line-computational)
Sooting Flames: Benzene Profiles

- Blue: \( \text{C}_2\text{H}_4 \) Baseline (A)
- + Modified \( \text{C}_2\text{H}_4 \) Baseline (A*)
- Black: JP-8-doped (B)
- Open: Utah/Yale-doped (C)
- Red: Aachen-doped (D)
Sooting Flames: Toluene Profiles

Black  JP-8-doped (B)
Open   Utah/Yale-doped (C)
Red    Aachen-doped (D)
• Baseline flames were identified spanning a broad range of stoichiometric mixture fractions, including nonsooting and incipiently sooting conditions, to test the perturbation from the addition of O(1000) ppm JP-8 and surrogates.

• The addition of jet fuel to these flames flame leads to the fragmentation of heavier alkanes to smaller ones, down to C2-hydrocarbons and the appearance of peak aromatic concentrations surviving further into the high temperature region.

• A 6-component surrogate captures the pyrolysis and oxidation behavior of JP-8 reasonably well, with the most significant discrepancy for benzene, toluene and ethylene under non-sooting conditions.

• The computational results using a semi-detailed kinetic mechanism are in reasonably good agreement with the experiments.
Summary of Completed Counterflow Work (2)

- Experiments on an incipiently sooting doped flame show good agreement between surrogates and JP-8 even with respect to benzene and toluene, as soot precursors.
- A procedure was demonstrated to reduce the experimental time to operate the burner for a complete flame scan to approximately 4 hours, with 30 hours of automated off-line GC/MS/FID chemical analysis.
- The JP-8 chemical analysis is invariably incomplete and accounts for roughly only 15-20% of the overall carbon introduced as liquid fuel.
Freely Propagating Flames

- Freely propagating JP-8/Air premixed flames were computed for
  - Pressures ranging between 0.5 to 35 atmospheres
  - Equivalence ratios varying between 0.4 – 2.7
  - Inlet temperatures ranging from 300 K to 1000 K
  - Vitiation equivalence ratio ranging from 0.0 – 0.3
Variations in Flame Speed and Flame Thickness as a Function of Pressure

Flame speed (open symbols) and Flame Thickness (smaller solid symbols) at Stoichiometric Conditions. □ 400K, X 475K, ○ 600K, △ 700K, and ◇ 800K. Solid lines are correlations.
Flame speeds and Flame thickness as a Function of Temperature

Flame speeds (open symbols) and Flame thickness (closed symbols) as a Function of Temperature at Stoichiometric Conditions.

◇ 1 atm, □ 5 atm, ○ 10 atm, △ 20 atm. Solid lines are correlations.
Comparison of Flame Speeds as a Function of Equivalence Ratio

Comparison of Computations and Correlations of Flame Speeds for Selected Conditions as a Function of Equivalence Ratio. Symbols are computed flame speeds: □ 800K/10 atm, ○ 800K/35 atm, △ 572K/1 atm, X 600K/10 atm, ◇ 500K/5 atm. Solid lines are correlations.
Goal is to develop a parallel algorithm that solves axisymmetric coflow diffusion flame problems across a distributed-memory computing cluster.

Motivation is to speed the simulation of combustion problems that are already tractable on a single processor:
- *e.g.*, steady-state and transient simulations of sooting flames using simple hydrocarbon fuels

and to facilitate the simulation of complex combustion problems that were previously intractable on a single processor:
- *e.g.*, sooting, coflow/2-d counterflow diffusion flames using a six-component JP-8 surrogate blend.
Axisymmetric Coflow Diffusion Flame Model

- Cylindrical coordinates
- Unconfined flow at atmospheric pressure
- Steady-state, (sooting), lifted diffusion flame
- Burner dimensions:
  - $R_i = 0.2 \text{ cm}$
  - $R_O = 2.5 \text{ cm}$
  - $R_{\text{MAX}} = 7.5 \text{ cm}$
Parallel Coflow Diffusion Flame Model

Issues needed to be addressed by parallel flame model

⇒ Domain decomposition of the computational tensor-product grid
⇒ Parallel implementation of a damped, modified, Newton’s method
⇒ Parallel implementation of the block-line Gauss-Seidel preconditioned Bi-CGSTAB iterative solver
**Domain Decomposition Techniques**

**Strategy**

Uses a parallel computing model in which

- Master and local processors perform computations
- Master processor coordinates inter-processor communication and I/O
- Large data structures are decomposed onto each processor (e.g., Jacobian)
- Small data structures are stored on each processor (e.g., solution vector)

Simple, strip-domain decomposition techniques partition contiguous blocks of physical grid rows onto individual processors

- Evenly distribute the total number of $N_{PZ}$ grid rows across the $N_{PROC}$ processors of the cluster
- Remaining grid rows are distributed amongst all local processors
- Master processor receives fewest possible grid rows

Results in processor-specific subdomains each containing $N_{PZL}$ contiguous grid rows
Sooting ethylene-air diffusion flame

⇒ 66 chemical species
⇒ 20 soot sections
⇒ 476 reactions (Sun, Sung, Wang and Law, 1996)
⇒ Bridges gap between simple fuels and multicomponent surrogate blends
Results: Comparison of Serial and Parallel Solutions

$N_{PROC} = 1$  $N_{PROC} = 16$

Predicted Temperature

Predicted $H_2O$ Mass Fraction

Predicted $CO_2$ Mass Fraction
Results: Reduction in Computational Time

Serial Computational Time
- Residual Formation 11.4 sec.
- Jacobian Formation 722.6 sec.
- Bi-CGSTAB Solution 21.8 sec.
- Total 833.7 sec

16-Processor Computational Time
- Residual Formation 0.30 sec.
- Jacobian Formation 47.5 sec.
- Bi-CGSTAB Solution 1.56 sec.
- Total 55.6 sec
• JP-8 is modeled as a six-component surrogate mixture (Violi, et al., 2001)

10% Iso-octane ($\text{C}_8\text{H}_{18}$), 20% Methylcyclohexane ($\text{C}_7\text{H}_{14}$), 5% Tetralin ($\text{C}_{10}\text{H}_{12}$), 30% Dodecane ($\text{C}_{12}\text{H}_{24}$), 20% Tetradecane ($\text{C}_{14}\text{H}_{30}$), 15% m-Xylene ($\text{C}_8\text{H}_{10}$)

• Surrogate kinetics are modeled using a 221-species mechanism containing 5032 reactions

• $\text{VF} = 35$ cm/sec (average)  \hspace{1cm} \text{VOX}=35$ cm/sec (plug)

• $\text{TF} = 480$ K  \hspace{1cm} \text{TOX} = 480$ K
Temperature and Major Species
Surrogate Components
Soot Related Species

- $C_2H_2$ mass fraction
- Benzene mass fraction
- Naphthalene mass fraction
- Pyrene mass fraction
- Coronene mass fraction
High Pressure Flames

• Examine systematically individual components of surrogate(s) and model their chemical kinetics (collaboration with Charlie Westbrook);
• Design and test a high-pressure chamber to perform similar work at high pressures (up to 40 atm);
• Model two-dimensional flame configurations using parallel methodology
  - Coflow flames
  - Counterflow
• Employ various chemistry reduction techniques
System Overview

- Fuel: fuel flow controller, O2: oxygen flow controller,
Burner and Flame

System Overview (2)
System Overview

• The chamber is an 8x8x8 in³ stainless steel cube bored with 6 in holes
• The system is controlled by a Labview interface to ease the monitoring of safe chamber operation
• Chamber pressure and wall temperature are automatically checked for anomalous values
• Visual interface controls the mass flow controllers to set automatically the experimental conditions (strain rate, fuel mass fraction and stoichiometric mixture fraction)
• A glow coil allows flame ignition at high pressure
• 20 different flow controllers are necessary to set accurately the flow rates in the pressure range 1 to 40 atm. A system of valves controls the switching between the set of flow controllers depending on pressure range
Scaling Considerations

The selection of the counterflow configuration was based upon

- the anticipated suppression of buoyancy instabilities at elevated pressures compared to coflow flames
- the use of the temperature-time history to control soot formation by strain rate and dilution
- the use of an inert such as helium to maintain the Reynolds number within the laminar range and to compensate for the pressure-induced reduction in flame thickness by stretching the Convective-Diffusive and Reactive-Diffusive zones.
## Computational Estimates

<table>
<thead>
<tr>
<th>$P$ (atm)</th>
<th>Inert</th>
<th>$\delta$ (mm)</th>
<th>$a$ (s$^{-1}$)</th>
<th>Re</th>
<th>Gr/Re$^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>N$_2$</td>
<td>4</td>
<td>95</td>
<td>2.0 $10^2$</td>
<td>0.15</td>
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<tr>
<td>10</td>
<td>He</td>
<td>3.3</td>
<td>95</td>
<td>2.8 $10^2$</td>
<td>0.15</td>
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<tr>
<td>20</td>
<td>He</td>
<td>2.4</td>
<td>95</td>
<td>5.6 $10^2$</td>
<td>0.15</td>
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<tr>
<td>40</td>
<td>He</td>
<td>1.7</td>
<td>95</td>
<td>1.1 $10^3$</td>
<td>0.15</td>
</tr>
</tbody>
</table>
Preliminary Results

• Preliminary testing demonstrated that stable flames could be established at pressures up to 25 atm without any buoyancy instability or turbulence. The flames were operated under either nonsooting or lightly sooting conditions at stoichiometric mixture fractions between 0.24 and 0.5 and strain rates between 20 s\(^{-1}\) and 150 s\(^{-1}\), regardless of pressure.

• Scaling considerations suggest that by experimenting with a high-diffusivity diluent such as Helium, sufficiently thick flames can be stabilized, despite the high-pressure conditions, for subsequent probing of the flame structure with adequate resolution.

• Future work includes
  - Implementing optical diagnostics (OH LIF) to check the thickness of the reacting layer (Lewis number effect);
  - Gas sampling by ultrafine quartz microprobes for off-line GC/MS analysis.
Acknowledgements

- Luca Tosatto, Hugo Bufferand and Saeed Jahangirian performed the bulk of the experiments; Lorenzo Figura designed and tested the high-pressure chamber; and Bruno Coriton helped with OH LIF experiments.
- Research supported also by
  - ARO DURIP (Grant # W911NF-07-1-0231, Dr. Ralph Anthenien, Program Manager)