Computational and Experimental Studies of Jet Fuel Combustion

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Objectives

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

- One-dimensional counterflow flame
  - complex kinetics but simple fluids
- Liquid dispersion by the electrospray, followed by spray evaporation in the fuel line
- Perturbed baseline methane flame
  - Use flame as a “controlled” reactor by maintaining a fixed time-temperature baseline
  - Avoid condensation problems and “cooking” the fuel in the transfer lines
Microprobe Details

- 30µm tip size 100µm body (but 3X probe maintains comparable spatial resolution at atmospheric pressure)
- SiO$_2$ for high temperature tolerance
- Small sampling flow rate ($\approx$ 50µ l/min)
4 hours of flame burning and .....30 hours of off-line analysis!
Experimental Conditions (non-Sooting Flames)

- **Baseline Flame**
  - Fuel stream: $X_{N_2} = 0.935$, $X_{CH_4} = 0.065$
  - Oxidizer stream: $X_{N_2} = 0.74$, $X_{O_2} = 0.26$

- **Dopant perturbation**
  - $4.2 \times 10^3$ ppm of either JP-8 or surrogate

- **Additional Conditions**
  - Max. Temp $= 1750K$
  - Strain Rate $= 102 \text{ s}^{-1}$
  - $Z_f$ (stoich. mixture fraction) = 0.77
  - Flame on **fuel** side of stagnation plane

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Numerical Simulations

• 1D Simulation using self-similar transformation
• Dirichlet conditions imposed at the inlet
• 221 Species $\times$ 5032 reactions
  

• Pseudo-time stepping + Newton’s Method

Experimental results have been shifted by 1.0mm to account for probe intrusiveness and other effects
Surrogate Formulation

From [Violi et al., Comb. Sci. Tech., 2002], designed to match distillation properties, smoke point behavior, laminar flame speed and validated for extinction limits in (Cooke et al., 2005)

- 10% iso-Octane
- 30% n-Dodecane
- 20% n-Tetradecane
- 20% Methylcyclohexane
- 15% o-Xylene
- 5% Tetralin

……but ready to test other promising alternatives
(e.g., Aachen, SERDP, MURI, etc.)
Results

• Measured and computed mole fractions for
  • Large alkanes
  • Ethane, ethylene, acetylene, methane
  • Major species (CO, CO\textsubscript{2} and O\textsubscript{2})
  • Aromatics
  • Temperature measurements corrected for radiation losses
  • Zoom in on fuel side of the domain
  • \(x = \) distance from fuel inlet
Major Species and Temperature

- CH4
- CO
- CO2
- Temperature [K]

JP-8 doped-
Symbols/continuous line
Surrogate-doped (exp)-
Symbols/dashed line
Surrogate-doped (comp)-
Continuous thick line
JP-8 vs. Surrogate: Large Alkanes

![Graph showing comparison between JP-8 and surrogate Large Alkanes](image_url)
Surrogate- Experiments vs. Computation: Large Alkanes

- Methylcyclohexane
- Isooctane
- Dodecane
- Tetradecane
- Tetraline
- Xylene

Surrogate-doped (exp)- Symbols/dashed line
Surrogate-doped (comp)- Continuous thick line

Distance from fuel inlet [mm]

ppm
JP-8 vs. Surrogate: C4-C6 Species

- JP-8 doped-
  - Symbols/continuous line
- Surrogate-doped (exp)-
  - Symbols/dashed line

- Propane
- Butane
- Pentane
- 1-Hexene

Distance from fuel inlet [mm]

ppm
Aromatics

- Benzene
- Toluene
- Xylene

Surrogate-doped (exp)-
Symbols/dashed line
Surrogate-doped (comp)-
Continuous thick line

Distance from fuel inlet [mm]

ppm
Aromatics (close-up)

Distance from fuel inlet [mm]

JP-8 doped-
Symbols/ continuous line
Surrogate-doped (exp)-
Symbols/ dashed line
Surrogate-doped (comp)-
Continuous thick line

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Conclusions (Part 1)

- The addition of jet fuel to a nonsooting baseline methane 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.

- The computational results using a semi-detailed kinetic mechanism are in reasonably good agreement with the experiments.
More flames?

With what feed stream composition?

Objective: span a broad range of $Z_f$, from non-sooting flames to sooting ones
Non-sooting Flames

- Max. Temp = 1750K
- Strain Rate = 102 s\(^{-1}\)
- \(Z_f\) (stoich. mixture fraction) = 0.77
- Flame on fuel side of stagnation plane

Sooting Flames

- \(\uparrow\) Max. Temp
- \(\downarrow\) Strain Rate
- \(\downarrow\) \(Z_f\)
- Flame on oxidizer side of stagnation plane
2. Experimental Conditions (Incipiently Sooting Flames)

- **Baseline Flame #2**
  - Fuel stream
    \[ X_{N_2} = 0.728 \]
    \[ X_{C_2H_4} = 0.272 \]
  - Oxidizer stream
    \[ X_{N_2} = 0.807 \]
    \[ X_{O_2} = 0.184 \]

- **Dopant perturbation**
  - \( 2 \times 10^3 \) ppm of either JP-8 or surrogate

- **Max. Temp** = 1989 K
- **Strain Rate** = 67.8 s\(^{-1} \)
- **\( Z_f \)** = 0.18
- **Flame on oxidizer side of stagnation plane**
Major Species and Temperature

- JP-8 doped-
  Symbols/ continuous line
- Surrogate-doped (exp)-
  Symbols/ dashed line
- Baseline (exp)-
  small dash line

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Surrogate Components

- Methylcyclohexane
- Isooctane
- Dodecane
- Tetradecane
- Tetraline
- Xylene

JP-8 Alkanes

- Meth.Cyc.Hex
- Heptane
- Isooctane
- Octane
- Nonane
- Decane
- Undecane
- Dodecane
- Tridecane
- Tetradecane
- Pentadecane

Distance from fuel inlet [mm]

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C$_1$ and C$_2$ Species

![Graph showing mole fraction of C$_1$ and C$_2$ species versus distance from fuel inlet in mm.]

- **Ethane** (△)
- **Methane** (•)
- **Acetylene** (□)

**Legend:**
- **JP-8 doped:**
  - Symbols/ continuous line
- **Surrogate-doped (exp):**
  - Symbols/ dashed line
- **Baseline (exp):**
  - Small dash line

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Aromatics

JP-8 doped-
  Symbols/ continuous line
Surrogate-doped (exp)-
  Symbols/ dashed line
Baseline (exp)-
  small dash line

Soot band

ppm

Distance from fuel inlet [mm]

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Chromatogram Comparison

Surrogate

- Clean distinct peaks
- Possibility to track minor species

JP-8

- Grassy background
- Overlapping peaks
- 30 species identified and measured
- 20 species identified but not quantified
Carbon Count Problem

Methane baseline flames (exp 1)
CO and CO$_2$ excluded from count

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Perturbation of Sampling Probe

- The objective is to assess the probe perturbation in terms of flame displacement by OH PLIF
- A potentially useful byproduct is the concurrent PLIF from PAH blends in the JP-8
<table>
<thead>
<tr>
<th>Probe position above fuel outlet</th>
<th>OH PLIF image</th>
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<tbody>
<tr>
<td>2.8 mm</td>
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<td>9.8 mm</td>
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Flame shift $\leq 0.6$ mm
Conclusions (Part 2)

• Experiments on an incipiently sooting ethylene flame show good agreement between surrogate and JP-8 even with respect to benzene and toluene, suggesting that the surrogate may capture even the sooting behavior of JP-8, as intended by the matching of the smoke point in the surrogate design.

• 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 20% of the overall carbon introduced as liquid fuel.

• OH PLIF showed a modest perturbation by the sampling probe.
Future Work (pending renewal)

• Examine systematically other surrogate candidates and their individual components (e.g., Aachen, MURI, SERDP);
• Tweak the chemical kinetic mechanism in the computational model to improve agreement with experiments (in collaboration with Ranzi’s group in Milan);
• Use sensitivity tests in the chemical kinetic model for guidance in the chemical analysis;
• Design and test a high pressure chamber to perform similar work at high pressures (up to 40 atm);
• Implement a reduced kinetics strategy.
References

• Bufferand et al., submitted to C&F, 2008
• Jahangirian et al., in preparation, 2008

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Back up
From JP8: aliphatics

- toluene, xylene, ethylbenzene, n-alkylbenzenes, etc.
- isopropylbenzene etc.

- benzene
- benzyl
- styrene

- naphthalene
- soot

Courtesy of Charles McEnally
C2 Hydrocarbons in a JP-8-doped hydrogen flame (full symbols) and a surrogate-doped hydrogen flame (open symbols).
## Sooting Flames B.C.

In the surrogate-doped flame, B, $1.42 \times 10^3$ ppm of C as C$_2$H$_4$ in the baseline flame, A, are replaced with $1.10 \times 10^3$ ppm of C as JP-8.