Fuels Summit 2009

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Outline of Presentation

- Background and general considerations of flame speed determination
  - Development of experimental apparatus
  - Further considerations of extrapolation accuracy
- Flame speeds of gaseous fuels
- Flame speeds of liquid fuels
- Reduced mechanism of JetSurf
- Hydrogen addition
Progress in the Determination of Laminar Flame Speeds

Reported Experimental Measurements of the Maximum Burning Velocity for Methane/Air Flames at 1 atm, 298K
Experimental Apparatus (Princeton Counterflow)
Dual Chamber Design for Constant & High Pressure Combustion
Experimental Apparatus (Princeton - MKII)
Experimental Apparatus (Princeton - MKII)
Extrapolation to Eliminate Stretch Effects

- **Linear Extrapolation**
  \[ s_b = s_b^o - L_b \kappa \]

- **Nonlinear Extrapolation (General)**
  \[
  \left( \frac{s_b}{s_b^o} + \frac{2 \ell_T}{r_f} \right) \ln \left( \frac{s_b}{s_b^o} + \frac{2 \ell_T}{r_f} \right) = -\frac{2}{r_f} (L_b - \ell_T)
  \]

- **Nonlinear Extrapolation (Large radius limit)**
  \[
  \left( \frac{s_b}{s_b^o} \right)^2 \ln \left( \frac{s_b}{s_b^o} \right)^2 = -2 \frac{L_b \kappa}{s_b^o}
  \]
Gaseous Fuels

- n-Butane
- iso-Butane
- iso-Butene
- 1-Butene
- 2-Butene
Additional Data Presented

- n-Butane; 298K; 1, 2, 5, and 10 atm. pressure
- Iso-Butane; 298K; 1, 2, 5, and 10 atm. pressure
- 1-Butene; 298K; 1, 2, 5, and 10 atm. pressure;
  - Also comparison with USC Mech II and updated version
- 2-Butene; 298K; 1, 2, 5, and 10 atm. pressure
- Also comparison with USC Mech II and updated version
Liquid Fuels

• n-Pentane
• n-Hexane
• cyclo-Hexane
• n-Heptane
Data Presented

- n-Pentane; 353K; 1, 2, 5, and 10 atm. pressure
- n-Pentane/15%O2:85%He; 353K; 10 and 20 atm. pressure
- n-Hexane; 353K; 1 and 2 atm. pressure
- cyclo-Hexane, 353K; 1 and 2 atm. pressure
- N-Heptane; 353K; 1 atm. pressure
Mechanism Reduction of JetSurf

Reduction performed by Tianfeng Lu, University of Connecticut
Reduction Method, Targets & Parametric Ranges

- JetSurf (Mech 1): 194 species and 1,459 reactions
- Reduced JetSurf (Mech 2): 123 species & 977 reactions
- Present reduction through Directed Relation Graph
- Targets:
  - Low-temperature chemistry: auto-ignition delay
  - High-temperature chemistry: perfectly-stirred reactor
  - n-Dodecane, n-nonane, & n-heptane
- Parametric ranges
  - p: 1-20 atm; T₀: 1,000 – 1,800K; φ: 0.5 – 1.5
- Reduced Mech (sk96): 96 species & 758 reactions
n-Dodecane (PSR & Autoignition)

- n-dodecane/air, $\phi=0.5$
- n-dodecane/air, $\phi=1$
- n-dodecane/air, $\phi=1.5$
n-Nonane (PSR & Autoignition)

n-nonane/air, $\phi=0.5$

n-nonane/air, $\phi=1$

n-nonane/air, $\phi=1.5$
n-Heptane (PSR & Autoignition)

- n-heptane/air, $\phi=0.5$
- n-heptane/air, $\phi=1$
- n-heptane/air, $\phi=1.5$

Graphs showing temperature, residence time, and ignition delay for different equivalence ratios and pressures.
Hydrogen addition to n-Butane

Experiments performed at Xian Jiaotung University, China
Hydrogen addition

- Define hydrogen addition parameter as:

\[
R_H = \frac{C_H + C_H / (C_H / C_A)_{stoic}}{C_F + [C_A - C_H / (C_H / C_A)_{stoic}]} 
\]

- Fuel equivalence ratio:

\[
\phi_F = \frac{C_F / [C_A - C_H / (C_H / C_A)_{stoic}]}{(C_F / C_A)_{stoic}} 
\]
Lean n-Butane/Hydrogen

\[ S_0^0 / \text{cm.s}^{-1} \]

\[ R_H \]

Symbol: Measurement
Line: Calculated

\[ \phi_F = 0.6 \]

\[ \phi_F = 0.7 \]

\[ \phi_F = 0.8 \]

\[ \phi_F = 0.9 \]

\[ \phi_F = 1.0 \]

\[ \phi_F = 1.1 \]
Rich \( n \)-Butane/Hydrogen

\[ \phi_F = 1.2 \]

\[ \phi_F = 1.3 \]

\[ \phi_F = 1.4 \]

\[ \phi_F = 1.5 \]

\[ \phi_F = 1.6 \]

\[ \phi_F = 1.7 \]

\[ \phi_F = 1.8 \]
Lean Flame Temperature

\[ T_{ad} / K \]

\[ R_H \]

\( \phi_F = 0.6 \)

\( \phi_F = 0.7 \)

\( \phi_F = 0.8 \)

\( \phi_F = 0.9 \)

\( \phi_F = 1.1 \)
Rich Flame Temperature

![Graph showing Rich Flame Temperature with temperature (T_ad / K) on the y-axis and R_H on the x-axis, with different lines for φ_F values of 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, and 1.8.](image)
Accomplishments this year

- Flame speed measurements using outwardly propagating flames
  - $C_4$: n-Butane, iso-Butane, iso-Butene, 1-Butene, 2-Butene
  - $C_5$: n-Pentane
  - $C_6$: n-Hexane, cyclo-Hexane
  - $C_7$: n-Heptane
- Extensively investigated data accuracy & consistency
  - Various methods of liquid fuel filling – same results
  - Various linear & nonlinear extrapolations
  - Flame configurations; computation vs experiment
- Effects and correlation of hydrogen addition
Plan for next year

- Flame speed measurements of pure fuels
  - n-Pentane (30 atm); n-Hexane (5, 10, 20, 30 atm)
  - cyclo-Hexane (5, 10, 20, 30 atm)
  - methyl-Cyclohexane (1, 2, 5 atm)
  - n-butyl-Cyclohexane (1, 2, 5 atm)
  - n-Heptane (2, 5, 10 atm); n-Octane (1, 2, 5 atm)
- Flame speed measurements of fuel mixtures
- Further reconciliation of data and calculation “discrepancy”
- Further reduction of JetSurf
Thank You!