Flame and Droplet Processes in Combustion

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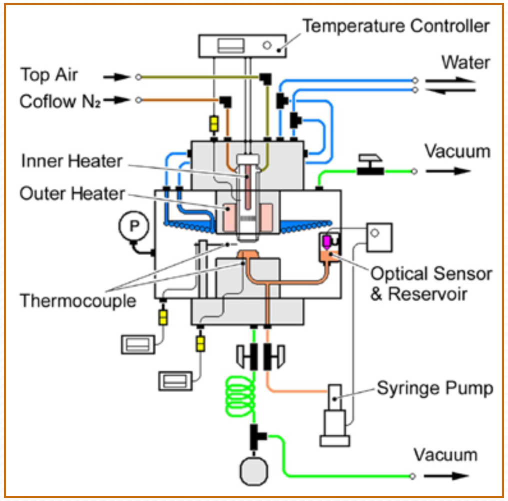
Outline of Presentation

1. Nonpremixed ignition, laminar flame propagation, and mechanism reduction of butanols
2. Effects of hydrogen addition on flame speeds of hydrocarbon fuels
3. Soot formation and explosive gasification in burning droplets of diesel/biodiesel/ethanol blends

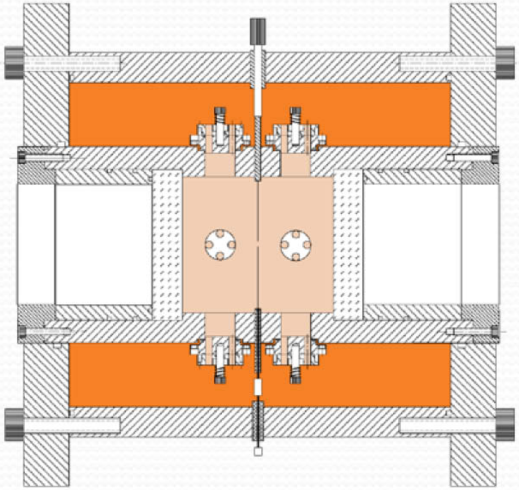
Ignition, Flame Propagation and Mechanism Reduction of Butanols

Experimental

- Nonpremixed ignition temperature and flow strain rate determined using variable pressure stagnating heated air over fuel pool



- Laminar flame speeds at elevated pressures determined from expanding spherical flames in heated constant-pressure bomb

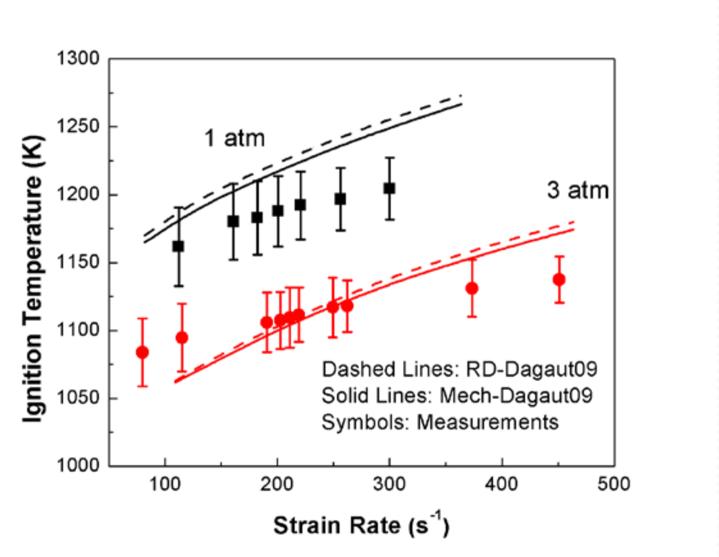


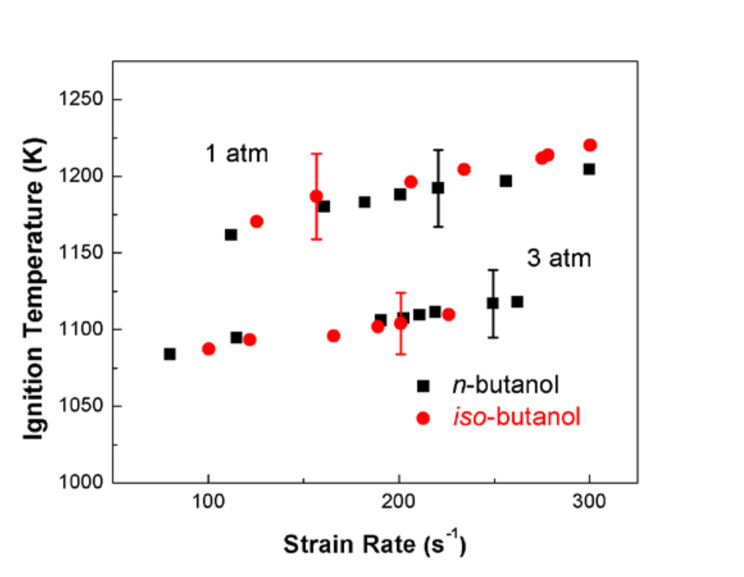
Specification of Fuels and Mechanisms

- Fuels studied: n-butanol, iso-butanol, methyl butanoate
- Detailed mechanisms
  - n-Butanol: Dagaut 2009 (Mech. A); 117 species and 884 reactions
  - Methyl butanoate
    - Dagaut 2008 (Mech. B); 275 species and 1549 reactions
    - Curran 2009 (Mech. C);301 species and 1516 reactions
- Algorithms for mechanism reduction
  - Skeletal reduction: DRG and DRGAGA
  - Time-scale analysis: CSP
- Reduced mechanisms
  - Mech. A: 91-species skeletal and 66-species reduced mechanisms
  - Mech. B: 102-species skeletal and 68-species reduced mechanisms
  - Mech. C: 87-species skeletal and 60-species reduced mechanisms

Results and Comparisons: Ignition Temperatures

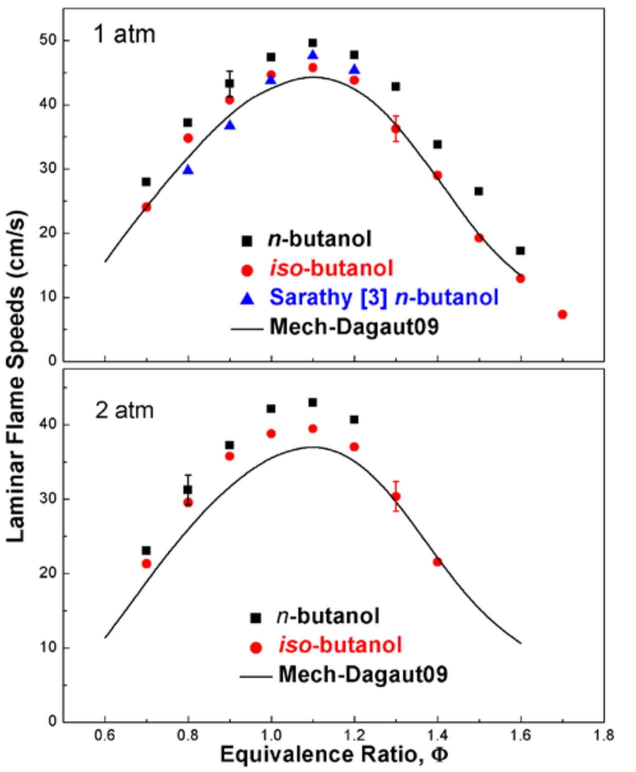
- n-Butanol
- n-Butanol vs. iso-Butanol



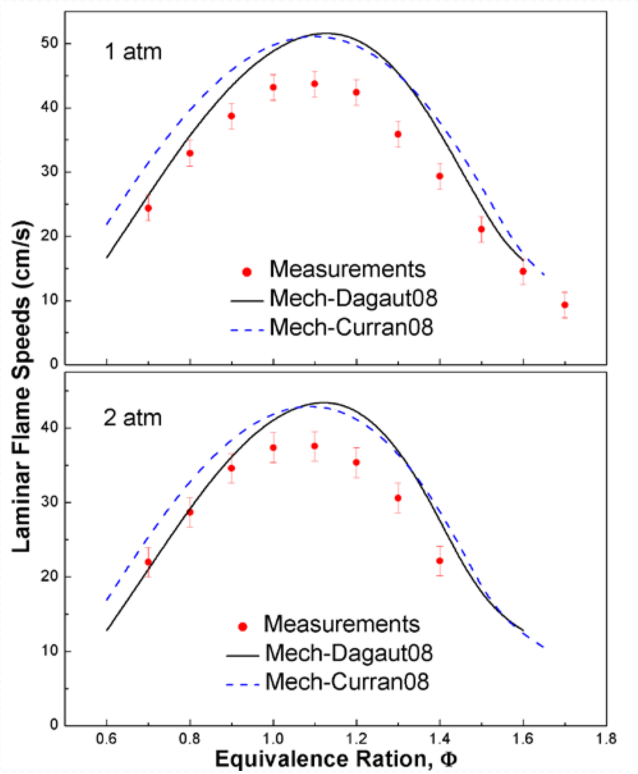


Results and Comparisons: Laminar Flame Speeds

- N-Butanol & iso-Butanol



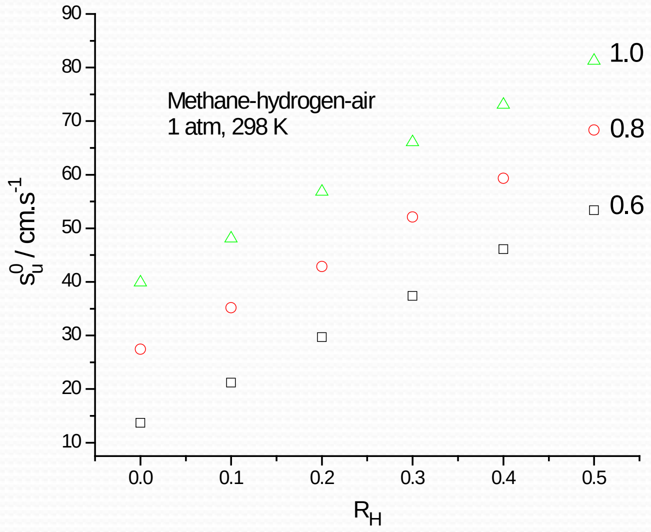
- Methyl butanoate



Effects of Hydrogen Addition on Laminar Flame Speeds of Hydrocarbon/Air Flames

Possibility of Near-linear Correlation

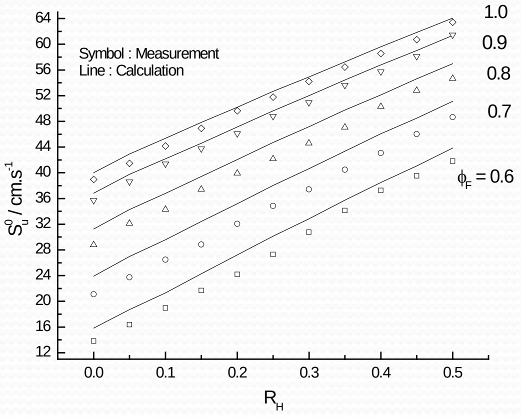
- Previous experimental study on methane and propane showed an almost linear correlation between laminar flame speed and an addition parameter R_H.

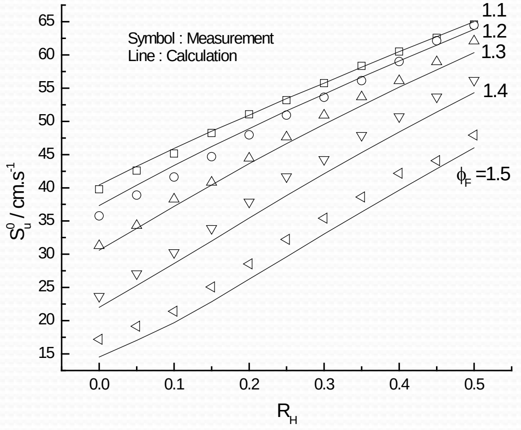


$$R_H = \frac{C_H + C_H/(C_H/C_A)_{stoic}}{C_F + [C_A - C_H/(C_H/C_A)_{stoic}]}$$

Current Study

- Linearity further confirmed
  - Independent investigation using two different expanding spherical flame burners
    - Single chamber at Xi’an Jiaotong University in China
    - Double chamber at Princeton
  - Ethane, ethylene, acetylene, butane
  - Lean and rich
  - Experimentally and computationally





Dominant Cause of Near-linearity

- Influence due to hydrogen addition
  - Flame temperature (T_{ad})
  - Kinetic augmentation (E_a)
  - Enhance diffusion (Le)
- Sensitivity analysis shows:

  $E_a > T_{ad} > Le$

$$(S_u^0)^2 \sim Le \exp(-E_a / R^0 T_{ad})$$

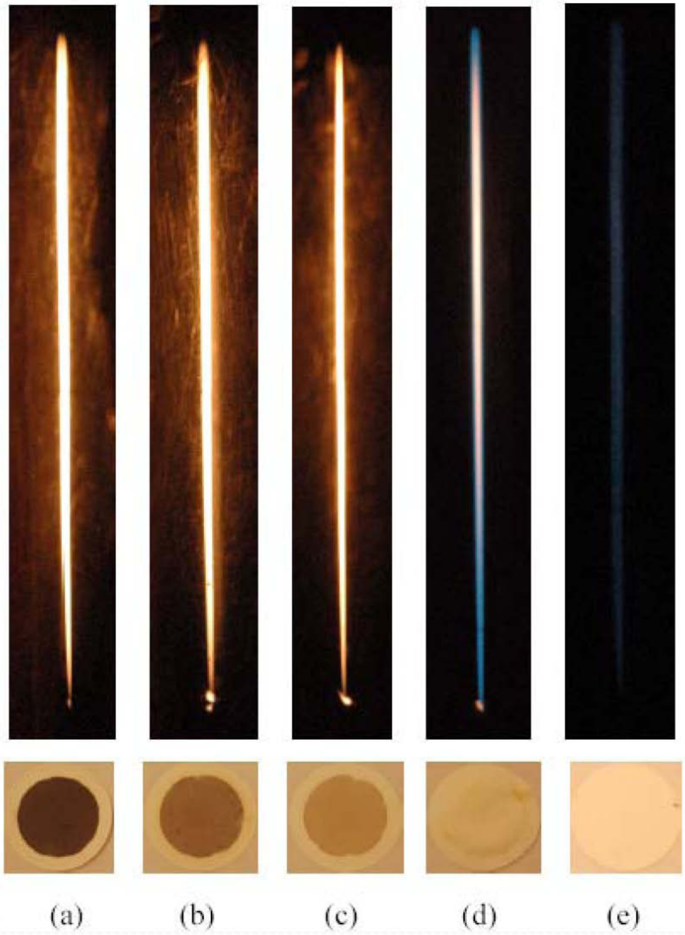
$$\frac{\partial \ln f}{\partial \ln R_H} \sim \frac{1}{2Le}\frac{dLe}{d\ln R_H} - \frac{1}{2T_{ad}}\frac{dT_a}{d\ln R_H} + \frac{T_a}{2T_{ad}^2}\frac{dT_{ad}}{d\ln R_H}$$

Soot Formation and Disruptive Burning of Droplets of Diesel, Biodiesel and Ethanol Blends

Motivation of Study

- Characteristics of diesel fuels:
  - Less volatile (than gasoline)
  - Sooty
- Candidate biofuels for diesel applications
  - (Bio)-ethanol: volatile and non-sooting
  - Biodiesel: less volatile than diesel, less sooty
- Develop strategy for blending to improve burning characteristics of diesel
  - Reduce soot
  - Manipulate volatility differential to optimize liquid fuel gasification

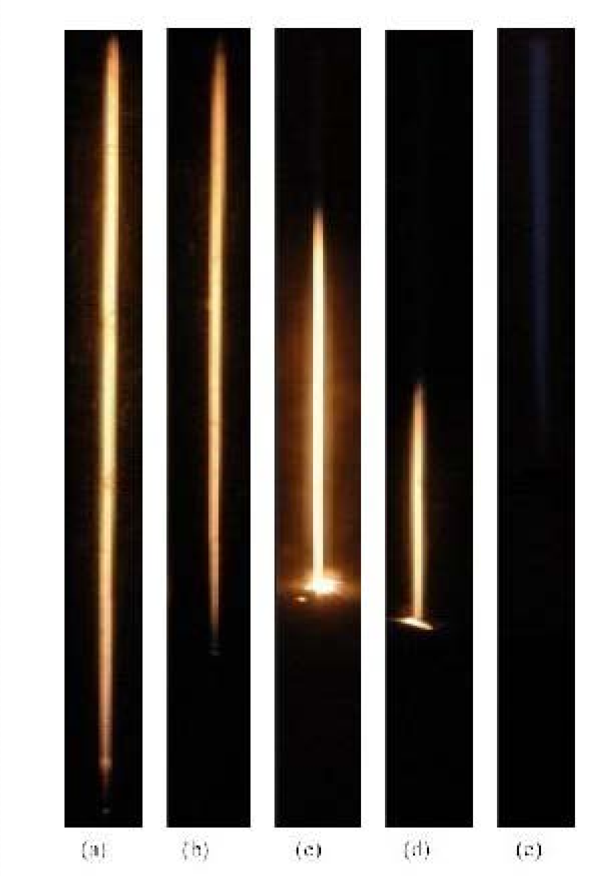
Biodiesel Blending: Soot Reduced



Blending ratio

(a) Neat diesel
(b) 10% biodiesel
(c) 20% biodiesel
(d) Neat diesel
(e) hexadecane

Ethanol Blending: Soot Reduced and Droplet Exploded (Hence gasified)



Blending ratio

(a) Neat diesel
(b) 25% ethanol
(c) 50% ethanol
(d) 75% ethanol
(e) Pure ethanol

Future Work

- Flame data, modeling, and mechanism reduction for biofuels
- Soot studies of biofuels using stagnation and counterflow flames
- Experiments on high-pressure turbulent expanding flames
- Liquid-phase reactions within gasifying/burning high-boiling-point fuel droplets