Kinetic and Transport Processes in Flames

C. K. Law
Princeton University

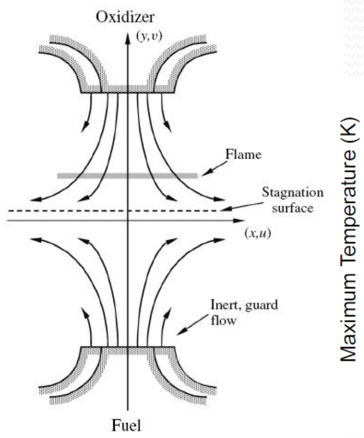
Outline of Presentation

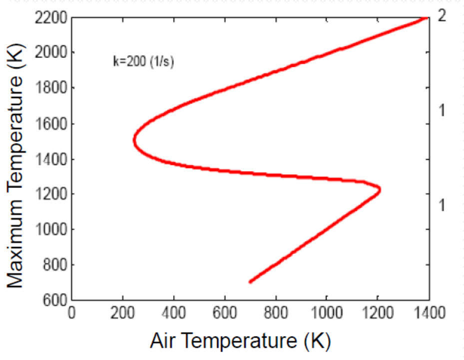
1. NTC-affected ignition in nonpremixed counterflow
2. Theory on turbulent flame propagation
3. Synergistic combustion of fuel droplets of ethanol, diesel and biodiesel blends

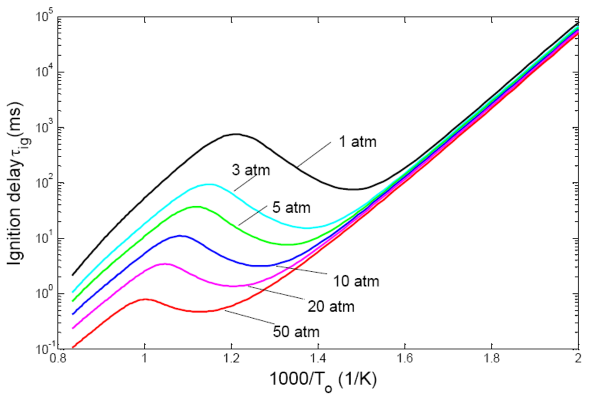
NTC-Affected Ignition in Nonpremixed Counterflow

Motivation

- NTC behavior:
  - Extensively observed in homogeneous systems
  - Inferred from detailed computational studies of transport-affected inhomogeneous flows
  - Need clear theoretical/experimental manifestation of global ignition & combustion behavior in response to flow straining and nonuniformity (e.g. counterflow)
- Search and identify NTC behavior for nonpremixed counterflow at:
  - low strain rates
  - high pressures



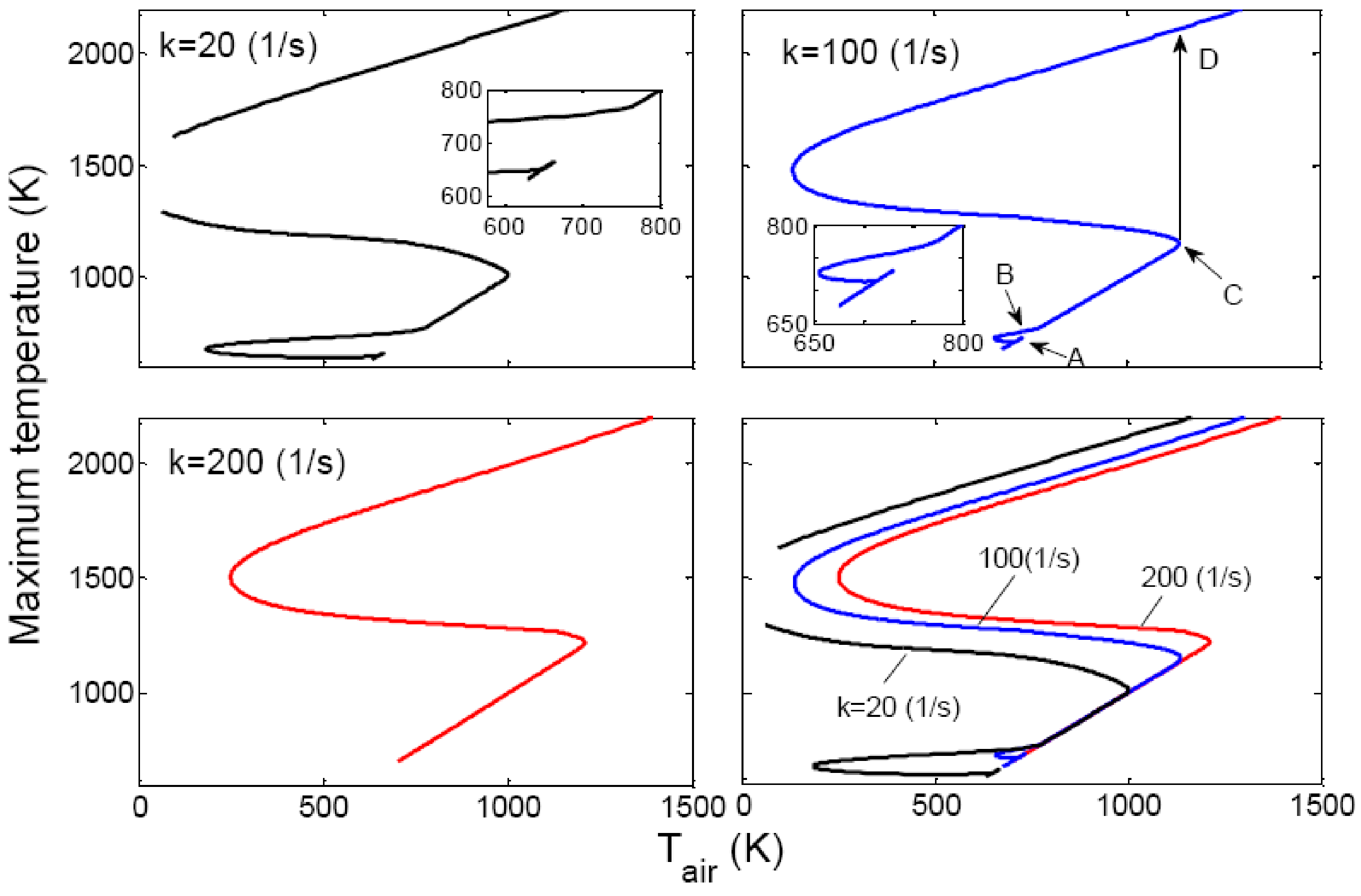




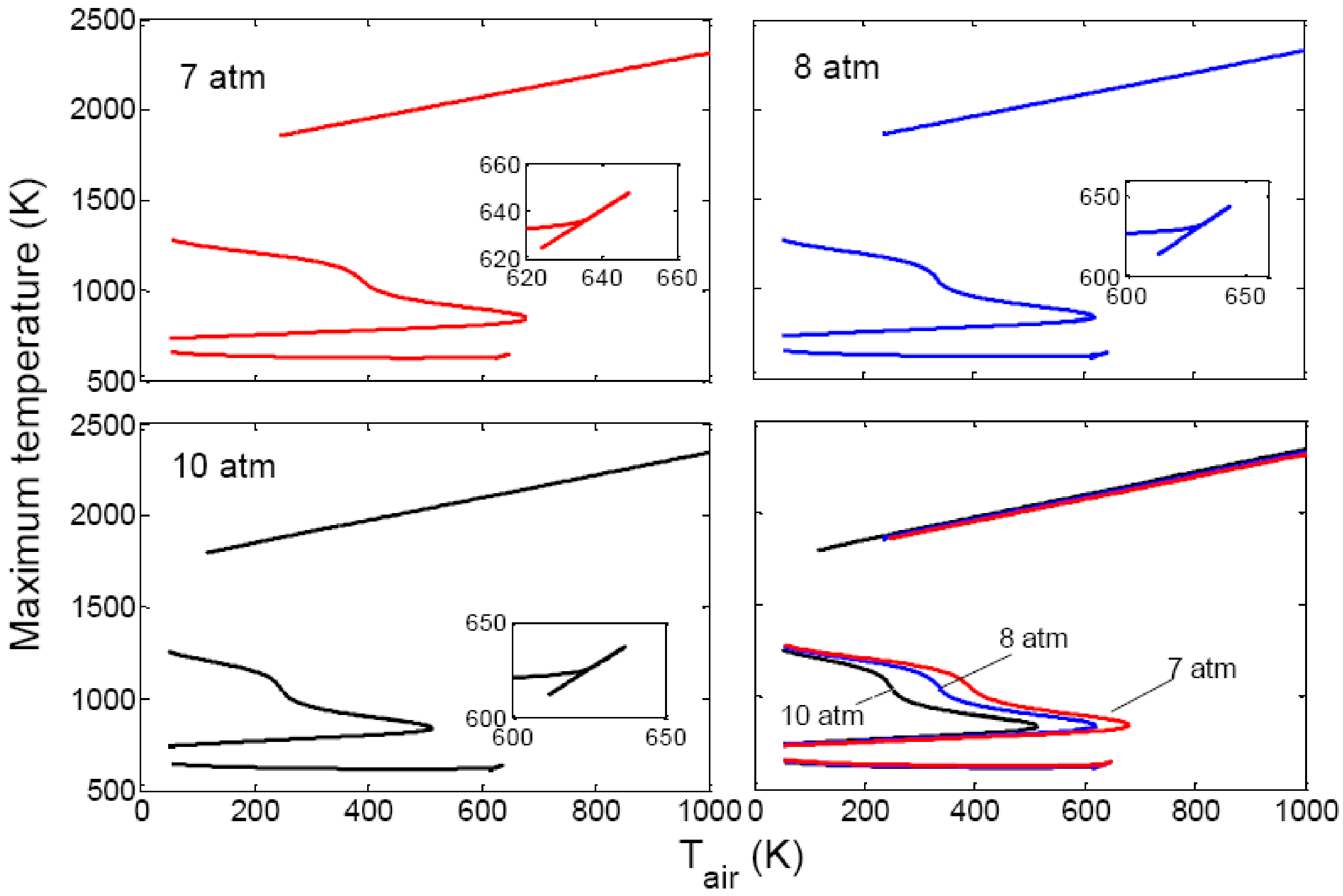
System Specifications

- Nonpremixed diluted n-heptane against heated air
- LLNL detailed mechanism of 561 species and 2539 reactions reduced to a skeletal mechanism of 88 species and 387 reactions using directed relation graph (DRG).
- Qualitatively similar results also obtained for DME

NTC Response Observed at Low Strain Rates (1 atm)

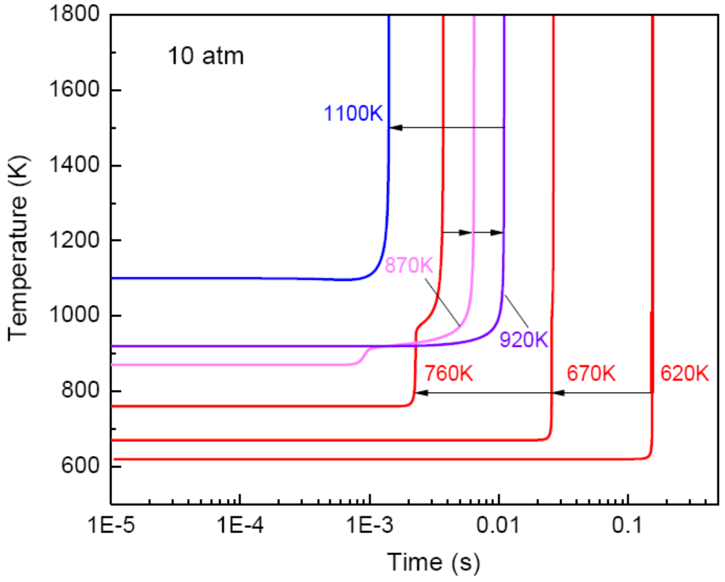


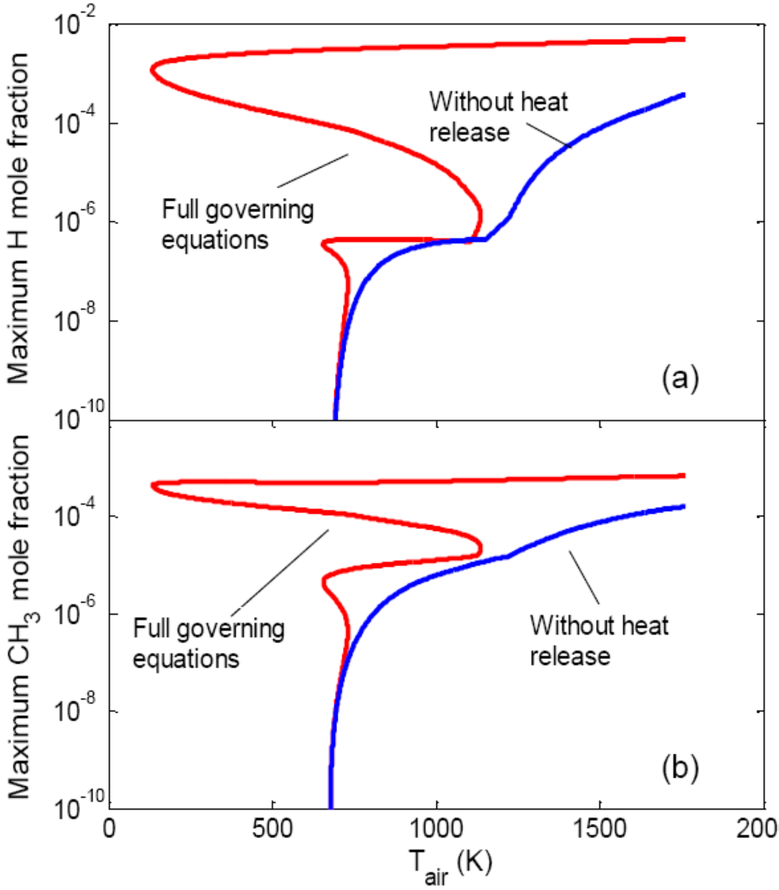
Prominent NTC Response at Elevated Pressures (100/s)



Essential Role of Heat Release

- Both primary and secondary turning points are eliminated by suppressing heat release





Summary of NTC-Affected Behavior

- NTC behavior manifested for flows at low strain rates and/or elevated pressures
- NTC response constitutes a separate (weak) flame system, with distinct (secondary) S-curve ignition-extinction states grafted onto the lower branch of the primary S-curve.
- At lower pressures ignition occurs in two stages with increasing temperature
- At sufficiently high pressures ignition occurs in a single, NTC-control stage

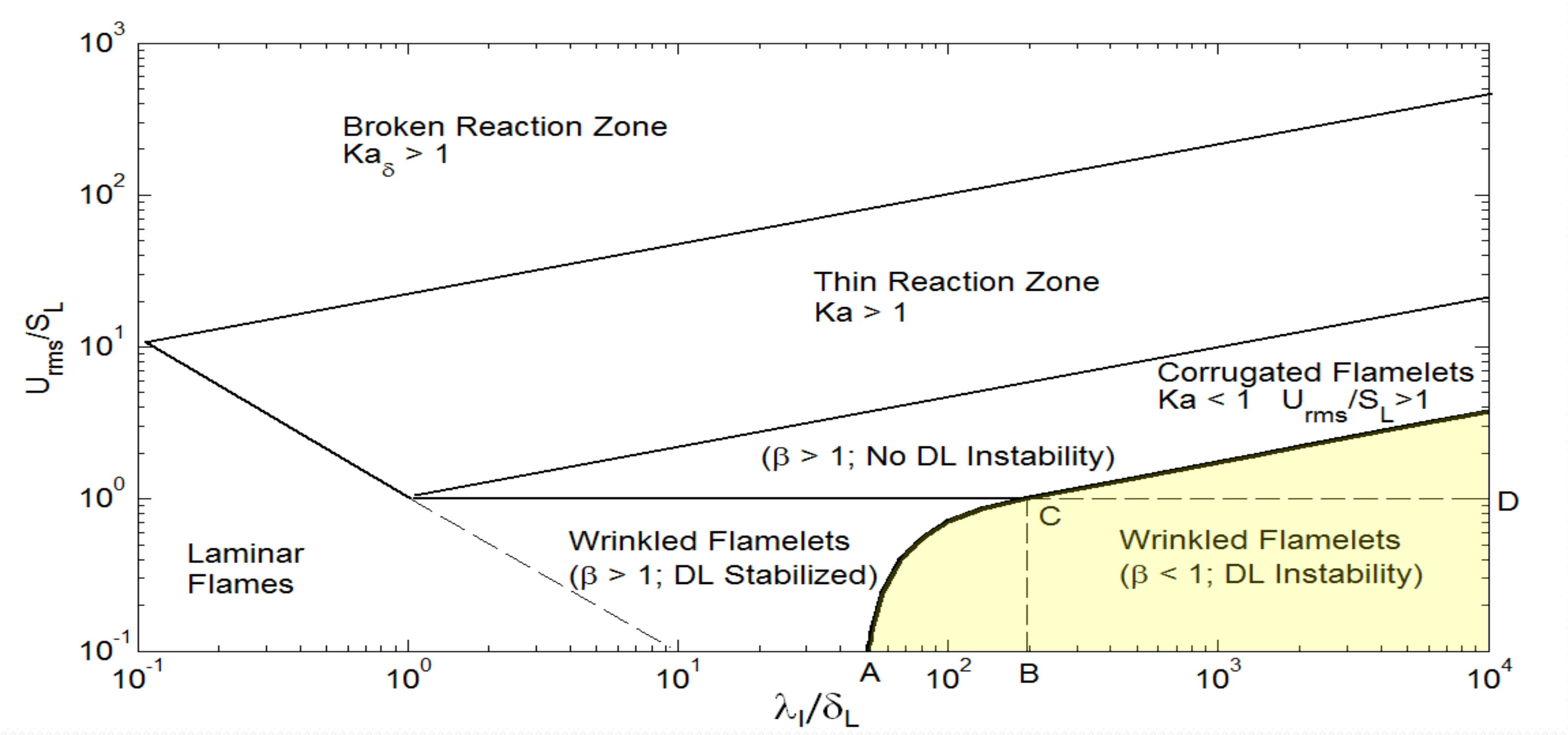
Studies on Turbulent Flame Propagation

- Modification of regime diagram
- Theory of turbulent flame speeds

Role of Darrieus-Landau Instability in Turbulent Flame Propagation

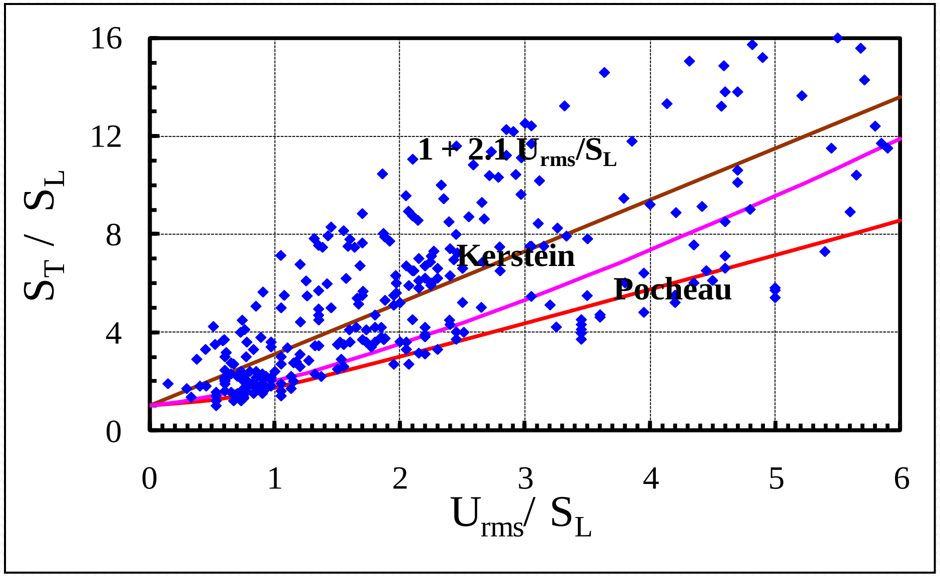
- The classical regime diagram does not account for the possible presence of the hydrodynamic (Darrieus-Landau) cells, which increase surface area and hence flame propagation speed.
- DL instability promoted with decreasing flame thickness at elevated pressures
- DL instability and flame wrinkling can be inhibited by
  - Finite flame thickness and structure
  - Finite growth rate, hence depending on turbulence intensity

Modified Regime Diagram



Modified Diagram

In Search of Relation for Turbulent Flame Speed



Experiments

{Abdel-Gayed et al., PRSL A, 1987; Aldredge et al., C&F, 1998; Kobayashi et al., PCI, 1998; 2000; 2002, Gulder C&F 2000}

Theories/models

{Clavin&Williams, JFM, 1979; Anand and Pope, PCI 1987 Yakhot, CST, 1988; Kerstein & Ashurst, PRL, 1992; Pocheau, PRE, 1994, Peters, JFM, 1999}

- It is of interest to seek a relation for the turbulent flame speed S_T in terms of turbulence and laminar flame parameters, like:

$$S_T / S_L = f\,(U_{rms}/S_L\ ;\lambda_I/\delta_L)$$

- Previous theories do not account for effects due to flame structure and instability.

Elements of Formulation

- Effective cutoff such that effective DL flame speed effect could be superimposed on turbulent flame speed ($S_{T,o}$) obtained for no instability

- $S_{T,o}/S_L$ from spectral closure of G equation

- Main contribution of $S_{T,o}/S_L$ comes from intermediate scales

- Simplifying : $$\left(\frac{S_{T,0}}{S_L}\right)^2 \sim \left(\frac{U_{rms}}{S_L}\right)\left(\frac{\lambda_I}{\delta_L}\right)$$

- Nonlinearity is inherent that causes bending

Synergistic Combustion of Droplets of Ethanol, Diesel and biodiesel Blends

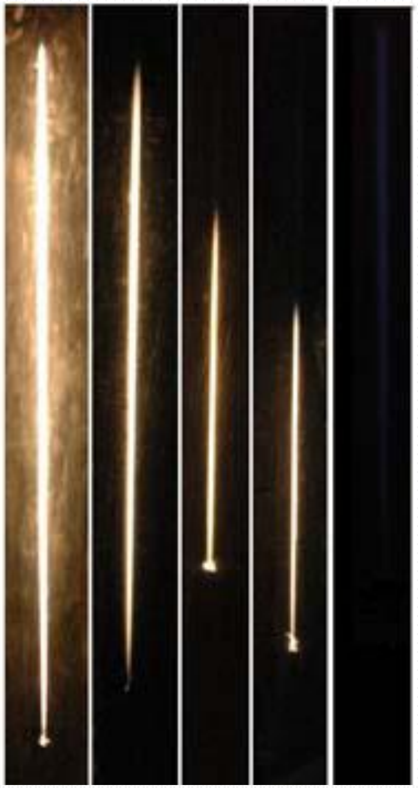
Synergy Through Blending (1/2)

- Diesel is sooty, mostly undesirable but small amount is needed for sealing
- Diesel is still economically favored
- Both ethanol and biodiesel are bio-fuels
- Both ethanol and biodiesel are minimally sooty
- Ethanol is more volatile than diesel, could affect ignition
- Biodiesel is less volatile than diesel, could affect atomization and mixture homogeneity

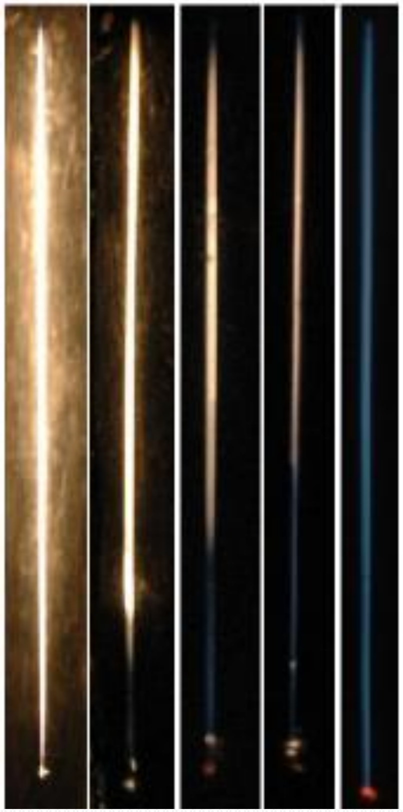
Synergy through Blending (2/2)

- Droplet gasification sequence affected by
  - Volatility differentials
  - Liquid-phase diffusional trapping
- Consequences: Gasification sequence largely controlled by volatility differentials (ethanol → diesel → biodiesel), but with some volatiles trapped by diffusional resistance
- Mixing strategy
  - Sequential gasification reduces soot formation from the early and latter parts of droplet life time from ethanol and biodiesel gasification
  - Trapping of ethanol in high-boiling-point biodiesel initiates internal homogeneous nucleation, causing instant droplet explosion and hence facilitating gasification

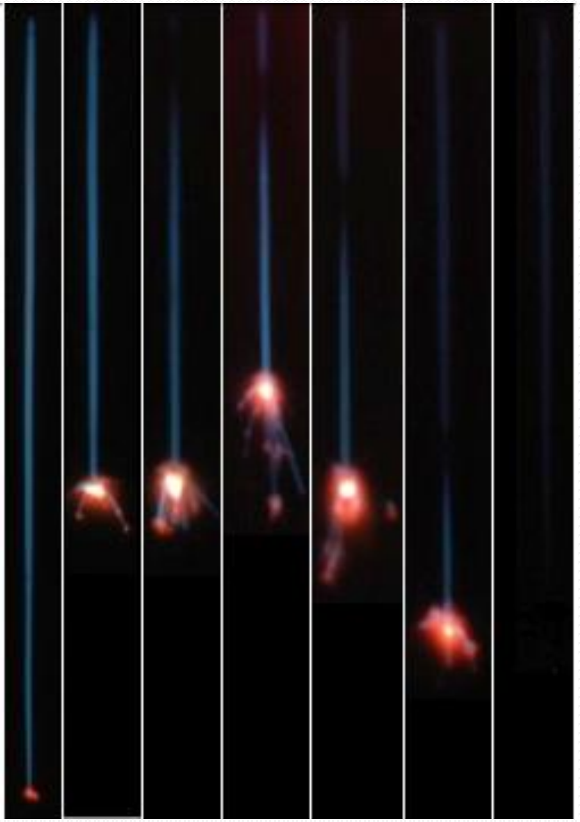
Images of Flame Streaks of Droplet Streams



Diesel → Ethanol



Diesel → Biodiesel



Biodiesel → Ethanol

Work Plan

- NTC-Affected Flame Phenomena
  - Counterflow and stagnation flow ignition experiments on DME and heptane to complement theoretical findings
  - Analyze other ignition phenomena (e.g. spark ignition, jet ignition)
  - Further study of the secondary S-curve
- Turbulent flames
  - Extend theory to spherically expanding flames with DL instability
  - Extensive experimentation with DME, at elevated pressures, up to say 20 atm.
  - Coordinate with DNS/LES simulation efforts of Chen and Pope
- Droplet combustion
  - Optimize synergy
  - Test fuels synthesized by DOE biofuels centers