Combustion & Fuels Research Laboratory

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Areas of Interest

Chemical Kinetics and Reacting Systems of Conventional & Alternate Fuels
Microscale Propulsion
Microgravity Combustion and Extinction of Isolated Droplets
Advanced Internal Combustion Engine-Related Research
Hydrogen Fuel Economy-Related Research

Chemical Kinetics and Reacting Systems

- Combustion chemistry affects:
  - Ignition
  - Rate of energy release
  - Conversion efficiency
  - Emissions
  - Fuel conversion/modification
- Applications: Design and optimization models need chemical kinetics for simulating:
  - Conventional fuels
  - Alternative fuels
  - Fuel additive effects
  - Onboard modification/conversion
  - Environmentally friendly-chemical rocket propellants

- Conventional Fuels typically contain large numbers of species
  - Detailed kinetic mechanisms too large to used for design codes
  - Minimal-sized detailed models needed

Experimental Techniques

- **Variable Pressure Flow Reactor**
  - A variable pressure flow reactor is used to determine the time evolution of reactant, intermediate, and product species as well as mixture temperature.
  - A hot-water cooled stainless steel probe continuously samples and convectively quenches a small percentage of the total flow. Gas temperature is measured with a silica-coated type R thermocouple.
  - On-line diagnostic instruments include an electrochemical oxygen analyzer, a hydrogen analyzer, and an FTIR spectrometer for H_2O and NOx measurements.
  - High flow rates and dilute mixtures (typically 1% fuel) minimize spatial gradients, thereby suppressing diffusion and creating a convective-reactive system.
  - The flow reactor approximates isobaric, plug flow operation, with negligible axial diffusion in comparison to convection. These conditions enable zero-dimensional modeling of the reacting system.
- **Laminar Pre-mixed Flames**
  - Define unstretched reference S_L for pure large hydrocarbon fuels, simple fuel mixtures and reference gasoline as a function of equivalence ratio, unburned gas temperature, exhaust gas dilution, and pressure for further validation of kinetic mechanisms.
  - Investigate the effects of composition, fuel contaminants and additives on sooting phenomena.

Kinetic Mechanisms for Design

Detailed Mechanism Reduction Example: n-Heptane

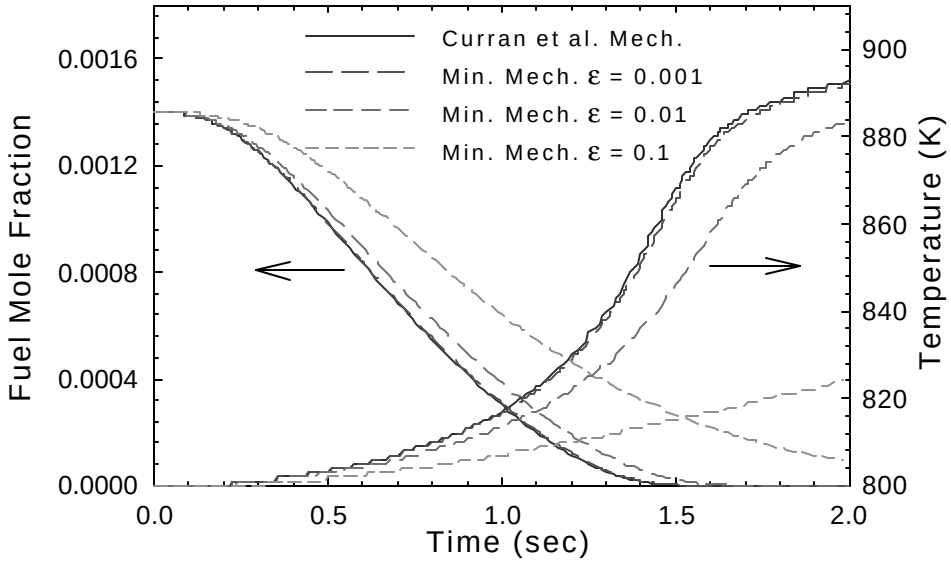
- *n*-heptane mechanisms are common
  - More developed for flame speed prediction
  - Limited number available for autoignition behavior
- Curran et al. mechanism (1998): 2540 reactions, 556 species
  - Specifically developed to include autoignition chemistry
  - Validated against flow reactor, shock tube, rapid compression machine data
  - Recently applied to counter-flow ignition (Seiser, et al.)
  - Further refinement and validation are desirable
- **BUT, mechanism is so large that it is difficult to perform mathematical analyses to improve the mechanism or to use it in multi-dimensional reactive flow computations and engineering design tools.**

Model Minimization Results

- Minimized mechanisms validated against a set of computations over the range of pressures, temperatures and equivalence ratios used in validating the original detailed mechanism.
- As the size of the minimized mechanism decreases, the disagreement between the minimized and original mechanism is increased.
- The minimized mechanism for ε=0.001 closely replicates all predictions of the original detailed mechanism.
- Minimizing the mechanism results in significantly reduced computational resource requirements to apply numerical sensitivity and path analyses to improve the model and/or for performing 1-D modeling (e.g. of laminar flames, droplet burning).
- Other methods (e.g. CSP) can be applied to produce application-specific, smaller dimensional models from an optimized-minimized mechanism.

C_7 Mechanism	Reactions	Species
Original Mechanism	2446	545
Min. Mech. ε =0.0001	1111	385
Min. Mech. ε =0.001	778	308
Min. Mech. ε =0.01	443	216
Min. Mech. ε =0.1	196	131

Size difference between the original mechanism from Curran et al. and minimized versions for varying threshold parameter, ε.



0.14% n-heptane oxidation time history at 12.5 atm, phi=1. Minimized n-heptane mechanisms compared to predictions by the Curran et al. model.

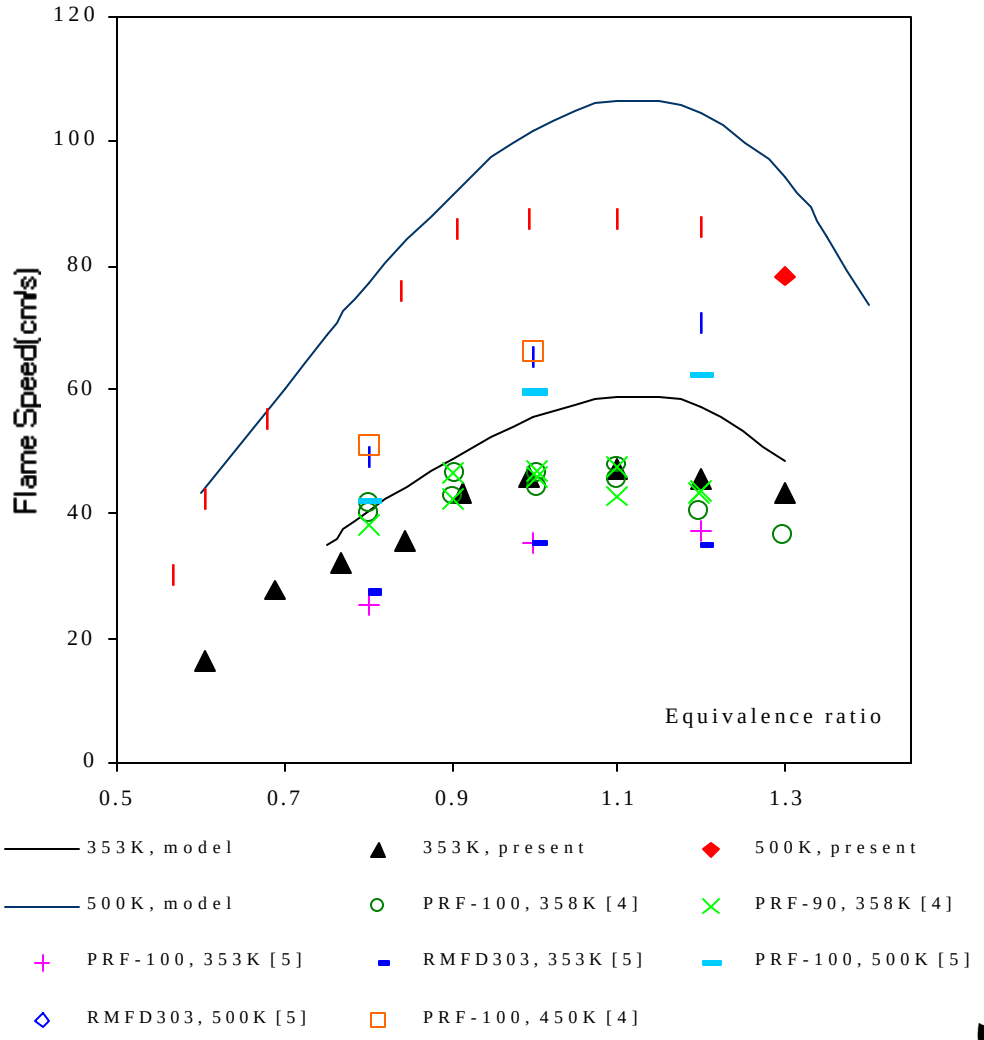
(Presented at the Joint Sectional Mtg of the Combustion Institute, Spring 2003)

Surrogate Fuel and Gasoline Premixed Laminar Flame Properties

Can simple mixtures of n-heptane and iso-octane be used to emulate the combustion properties of full blend gasolines in existing and new engine cycles?

Similar model minimizations of large detailed mechanisms allow comparisons of experimental results with detailed flame speed predictions that cannot be performed with the original mechanism dimensional size.

Laminar Flame Speeds are affected by unburned gas temperature and dilution (exhaust gas re-circulation). We are performing both experiments and model investigations.

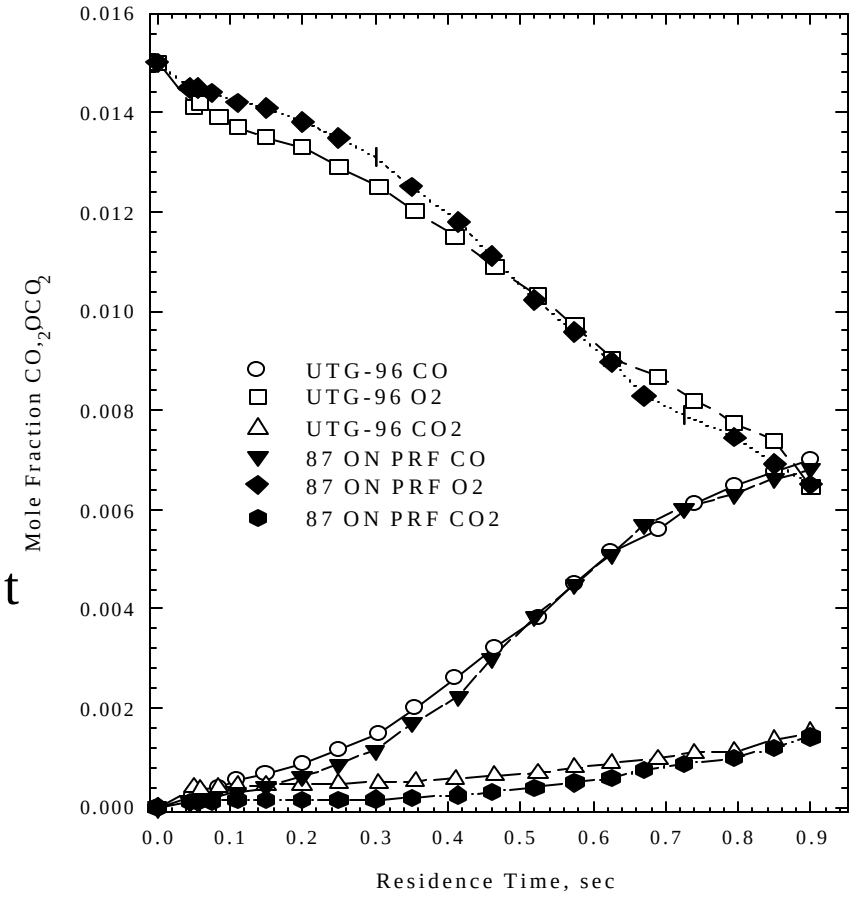


(published in SAE No 2003-013265, SAE Transactions, 2004)

Conventional Fuel Comparisons with Gasoline Surrogates

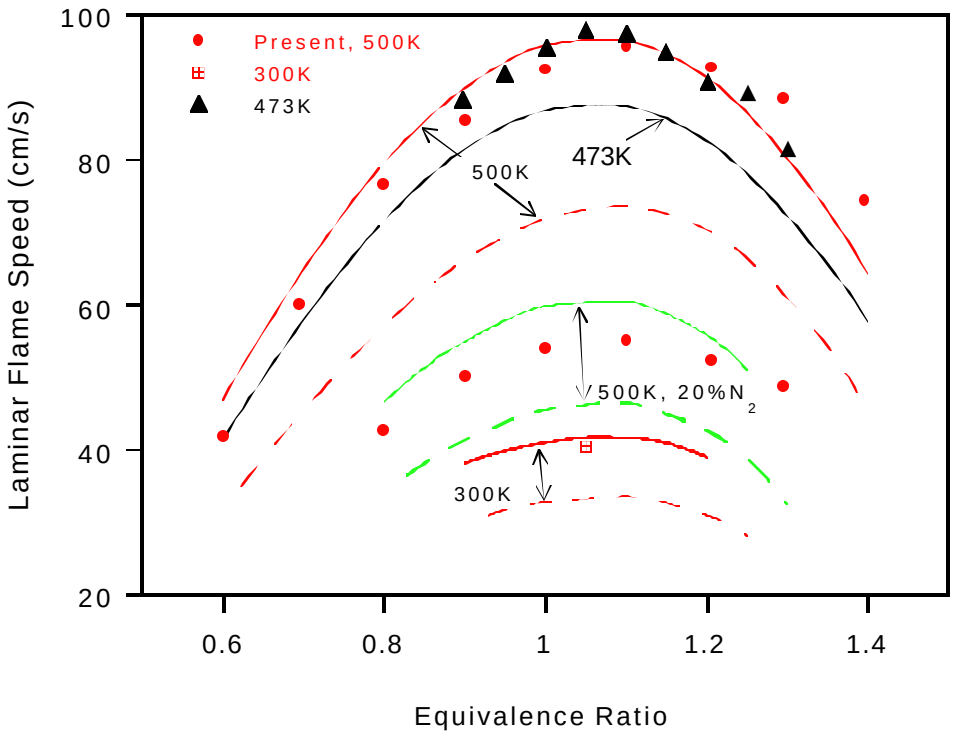
Comparison of species time histories for a Reference Gasoline (MON=89) and an ON 87 Primary Reference Fuel under β-scission dominated conditions. P = 6 atm, T ≈ 923K, ϕ=1.0, 1% Carbon.

These type of data and comparisons with results using simple component mixtures can be used to develop simple mixtures of components that behave as full blend fuels.
Ternary blends of components are presently under investigation



Experimental Laminar Flame Speed Data and Model for n-Decane

- Robust kinetic models are needed to predict the combustion process in engines that use distillate fuels such as Direct Injection Diesel, HCCI or gas turbine engines.
- *n*-Decane has some chemical characteristics similar to distillate materials.
- In recent work, we have extended our prior partially reduced mechanism validation by generating new laminar flame speed data on n-decane anad validating a revised mechanism against these results as well as burner-stabilized flame, jet-stirred reactor, shock tube, atmospheric flow reactor data



line: model predictions (dashed line- Zeppieri et al. (2000), solid line - present *n*-decane model)

473K: Skjøth-Rasmussen et al. (2003)

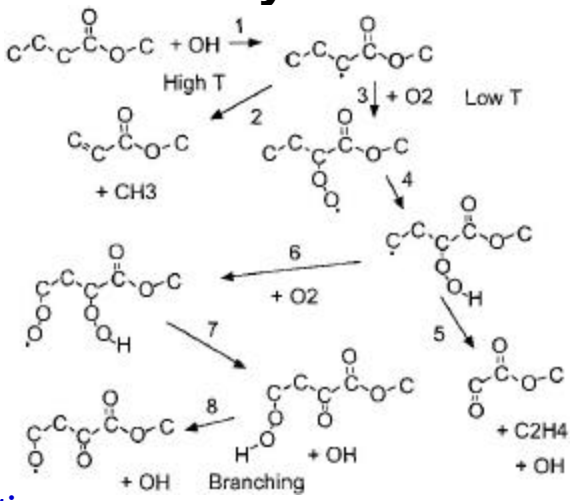
300K: Wagner & Dugger(1955)

Published in Zhao et al., Combust. Sci. and Tech, 176, 1705 (2004)

Characterization of Bio Fuel and Surrogates for Diesels

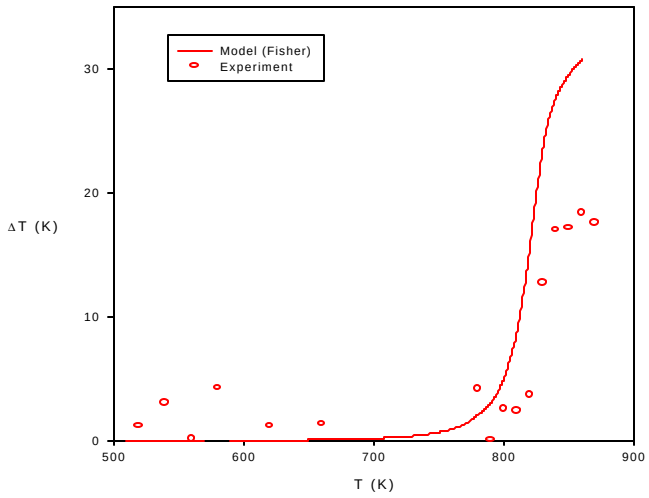
Fisher and coworkers have developed a detailed chemical kinetic mechanism of methyl butyrate oxidation shown schematically as:

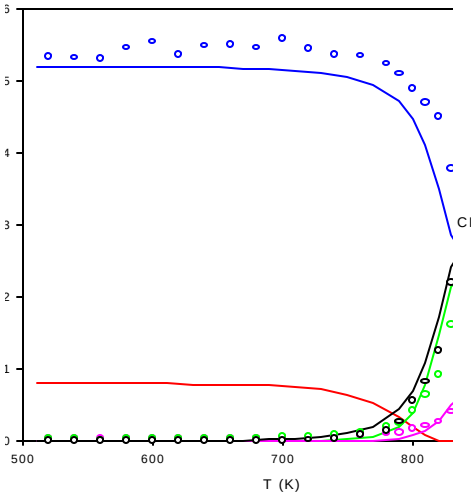
A detailed mechanism was developed for methyl butyrate, but no data exist for validating the result. We are studying experimentally and numerically this chemistry under flow reactor conditions

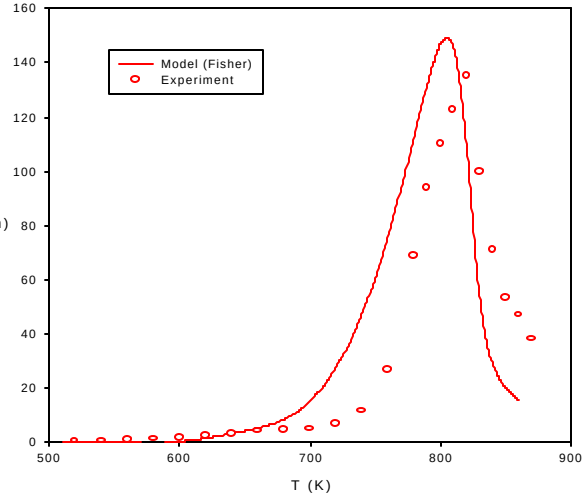


Below are some initial VPFR reactivity results and model predictions (f = 1.0, P = 12.5 Atm, x_f = 800 ppm, t_{res} = 1.8 s).

Work in Progress Poster at the 30th Int Sym on Combustion





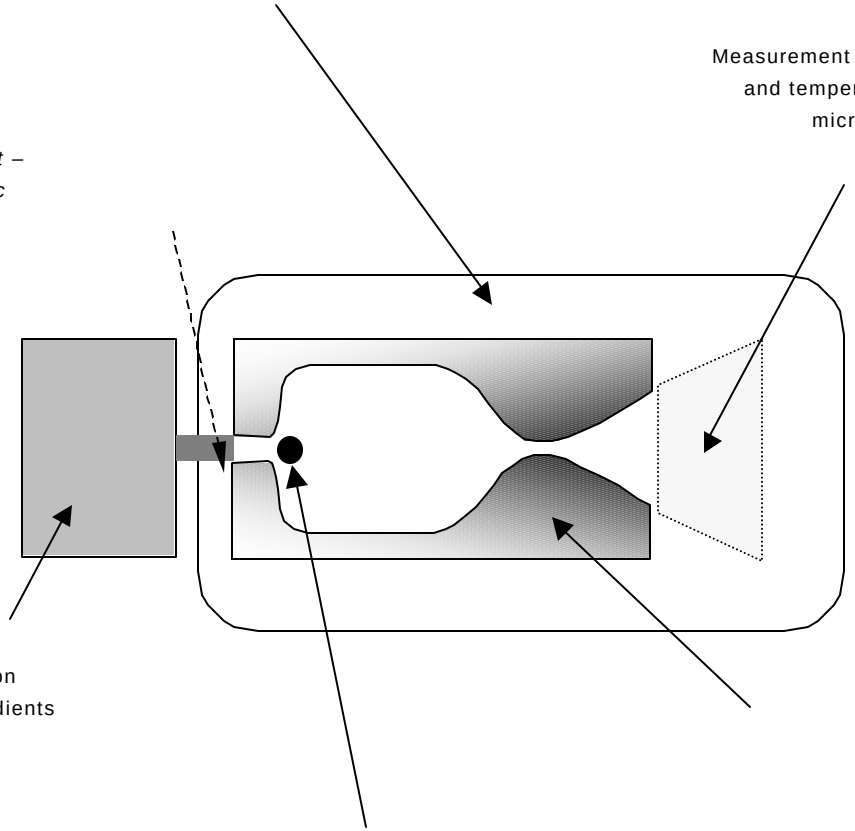


Chemically-Based Micro Propulsion

Detailed modeling of 3-D flow and chemistry
for design and analysis

Measurement of velocity, composition,
and temperature with micro PIV,
micro PLIF, and GC

Interface-module not part of the current proposed proof-of-concept *effort – flows will be controlled by macroscopic devices for* proof-of concept



Design and characterization
of novel liquid propellants based on
alcohol, water, ADN, and HNF ingredients

Design and fabrication of uni-body
alumina combustor / nozzle
with ceramic stereo-lithography

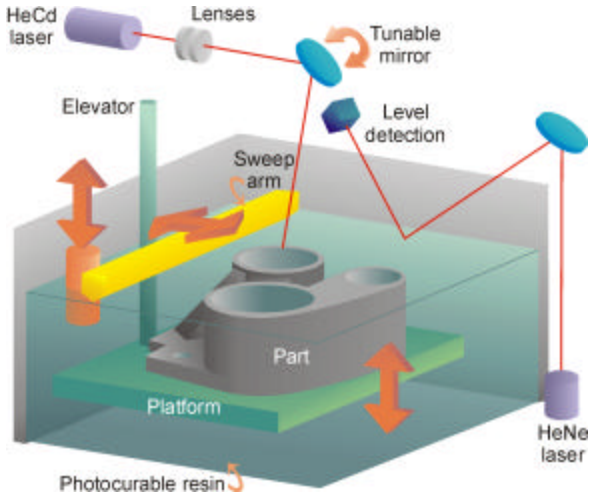
Design and characterization
of ignition and combustion systems
using palladium coated surfaces, electrodes, etc.

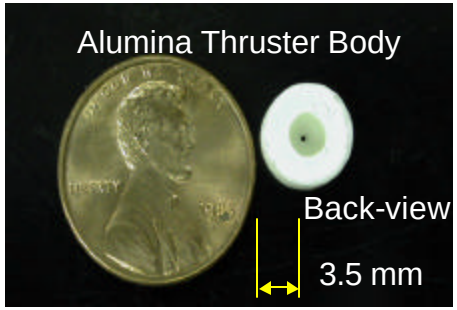
Thruster Prototype Design and Fabrication

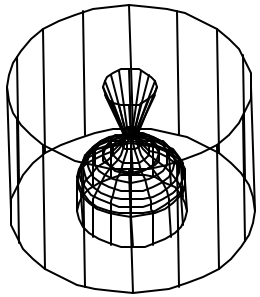
Fabrication: Ceramic Stereolithography

Materials: Mullite ($3Al_2O_3{\cdot}2SiO_2$) and alumina

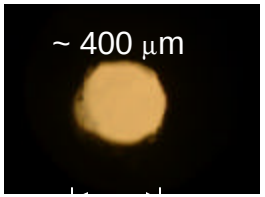
Unique Features:
- 3-dimensional uni-body structures
- high temperature capability
- materials compatibility







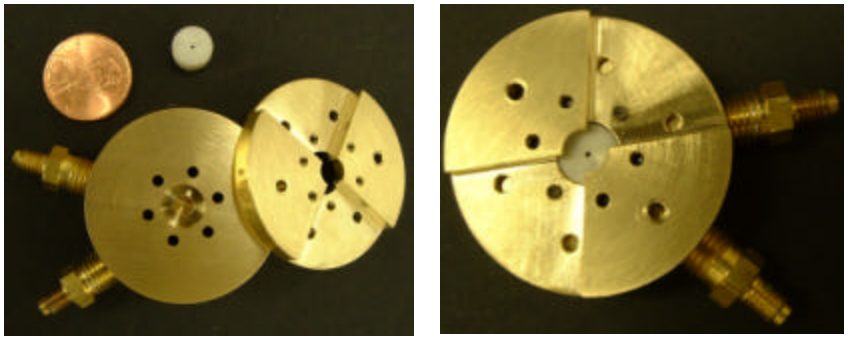
Wireframe of thruster body



Microscope backlit image of throat x-section

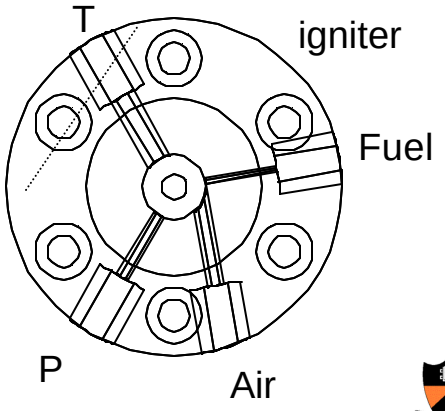
Thruster Design: Gas-phase combustion based on asymmetric whirl combustion

Features: high flame stability, minimal heat loss, increased particle flow time, film cooling by liquid fuel vaporization and endothermic decomposition along combustor wall



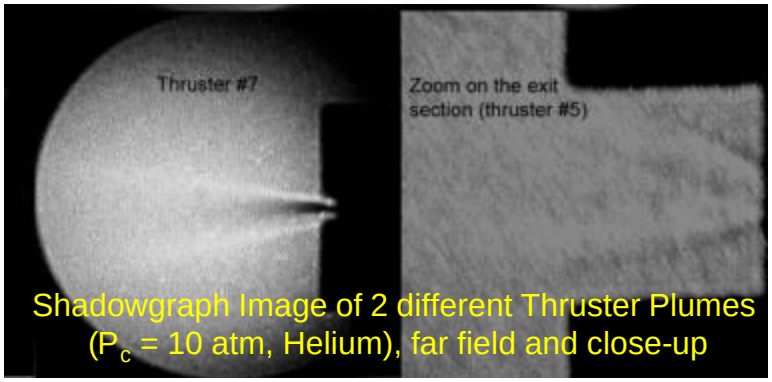
Thruster body (Front-view) and Cold Flow Manifold

Hot Flow Manifold Illustrating Combustor Vortex Flow with Gaseous Fuel. For Liquid Propellant, Air Port is replaced with Liquid Port

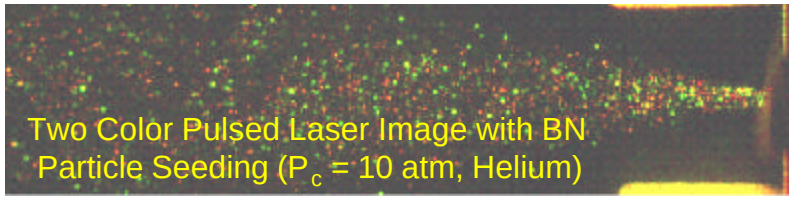


Thruster Operation and Characterization

Cold Flow with Helium and Air



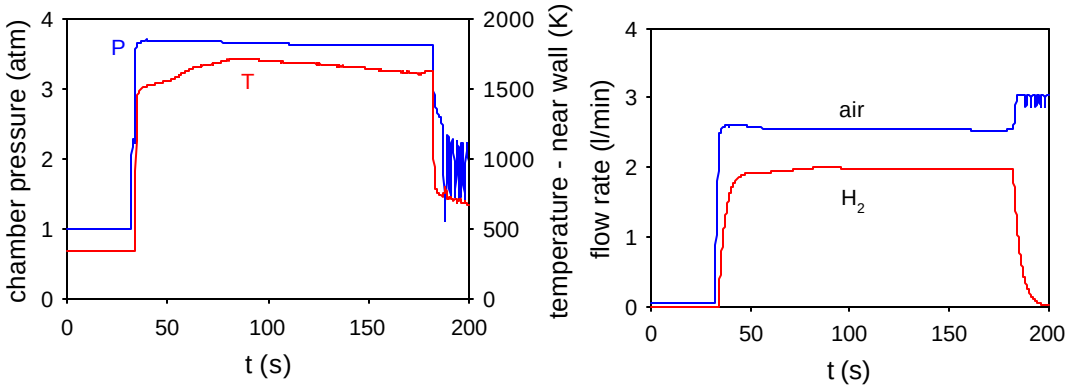
Shadowgraph Image of 2 different Thruster Plumes (P_c = 10 atm, Helium), far field and close-up



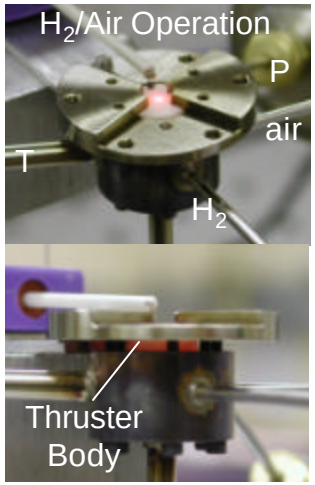
Two Color Pulsed Laser Image with BN Particle Seeding (P_c = 10 atm, Helium)

- Some thruster to thruster plume trajectory variation
- Cold flow PIV measurements underway
- C* efficiency affected by viscous effects, under expanded flow, and A* uncertainty

Hot Fire Flow with H_2/Air Mixtures

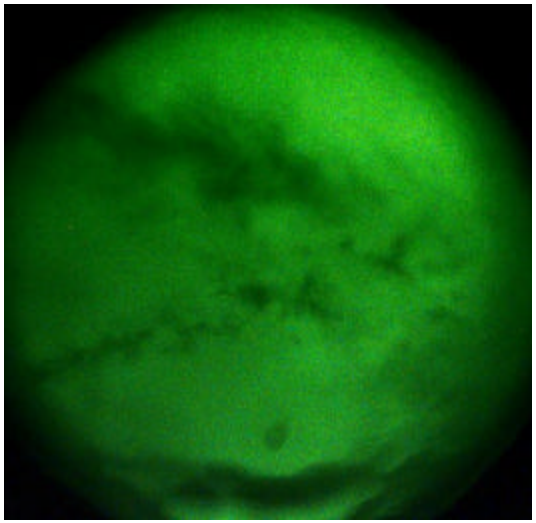


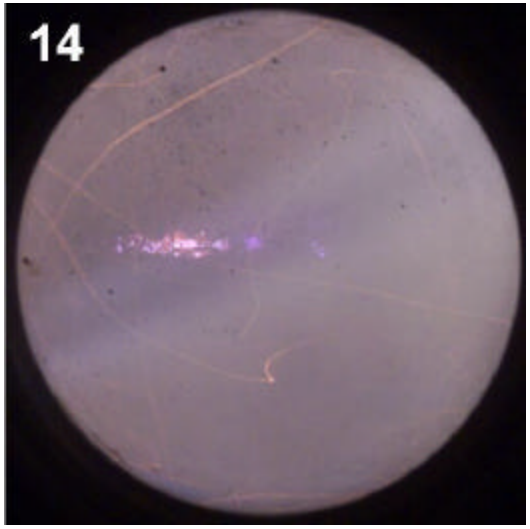
Start-up & Shut-down of Thruster, V_c = 57 mm^3, d_c= 3.5mm, d*=463μm



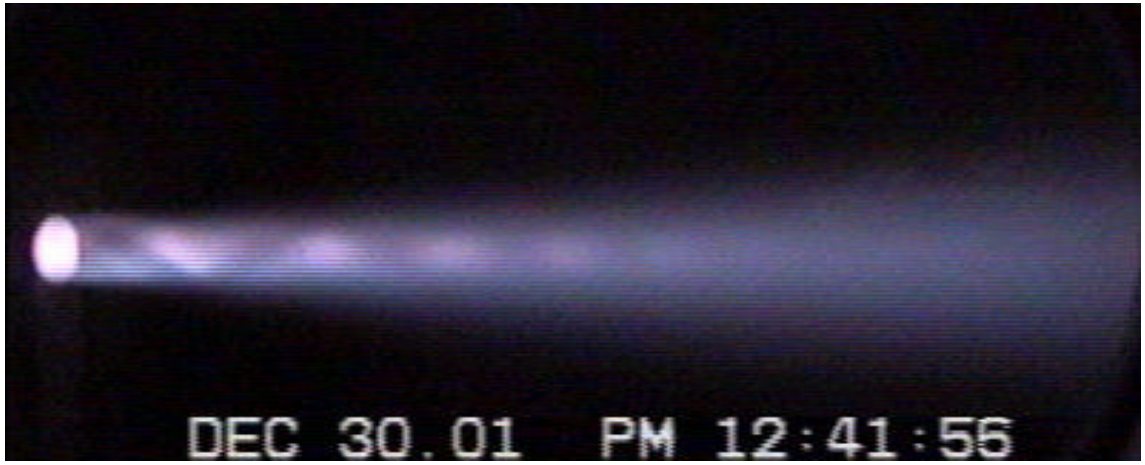
- Hot fire operation with H_2/air
- High combustion efficiency
- Minimal heat loss

Laser Ignition of Ethanol/Oxygen Sprays under Simulated Space Conditions

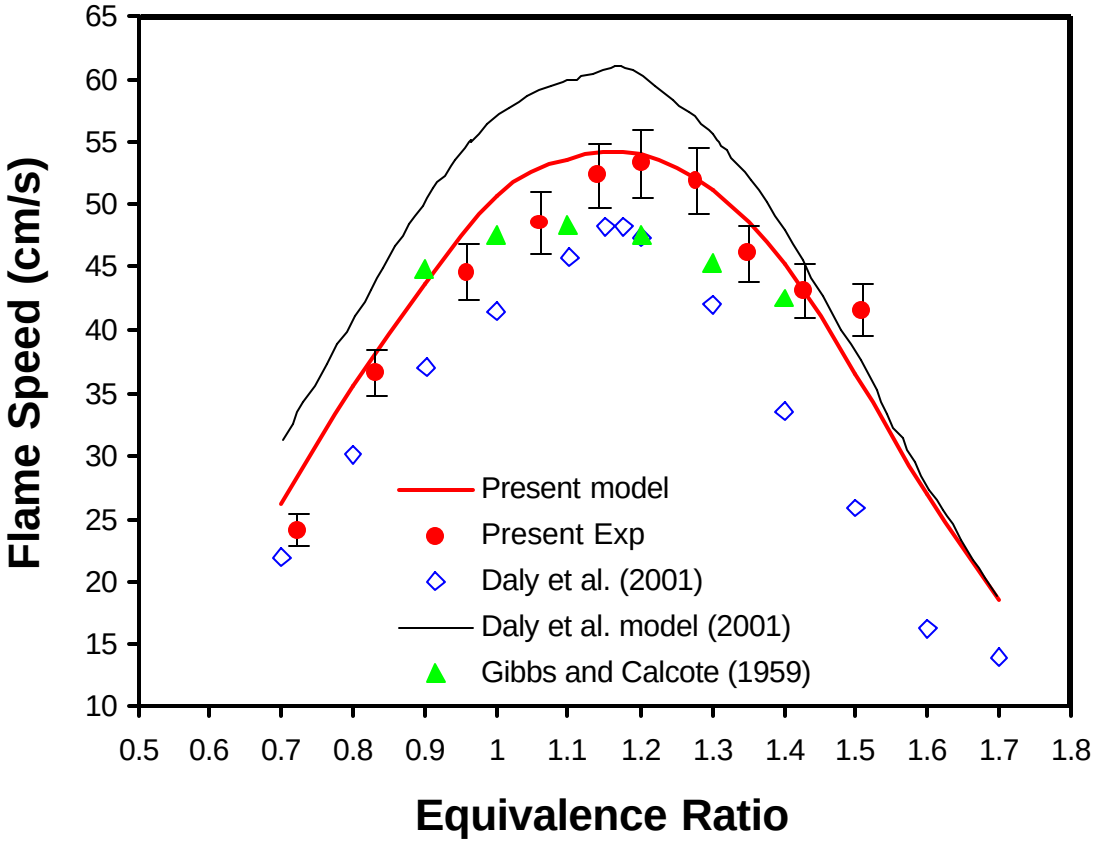




•Ethanol is a viable alternative to extremely environmentally unfriendly hypergolic fuels, presently used for Orbital Maneuvering Systems (OMS) of NASA spacecraft. A prototype laser ignition system was developed to ignite impinging sprays of ethanol and liquid oxygen (top left). Laser–induced plasma (bottom left) is used as an ignition spark. Conventional electric spark plugs wear extremely fast in such a heavily oxidizing environment. To simulate the space conditions, experiments were conducted in a vacuum chamber, as indicated by the checkered pattern of the pilot flame (below).



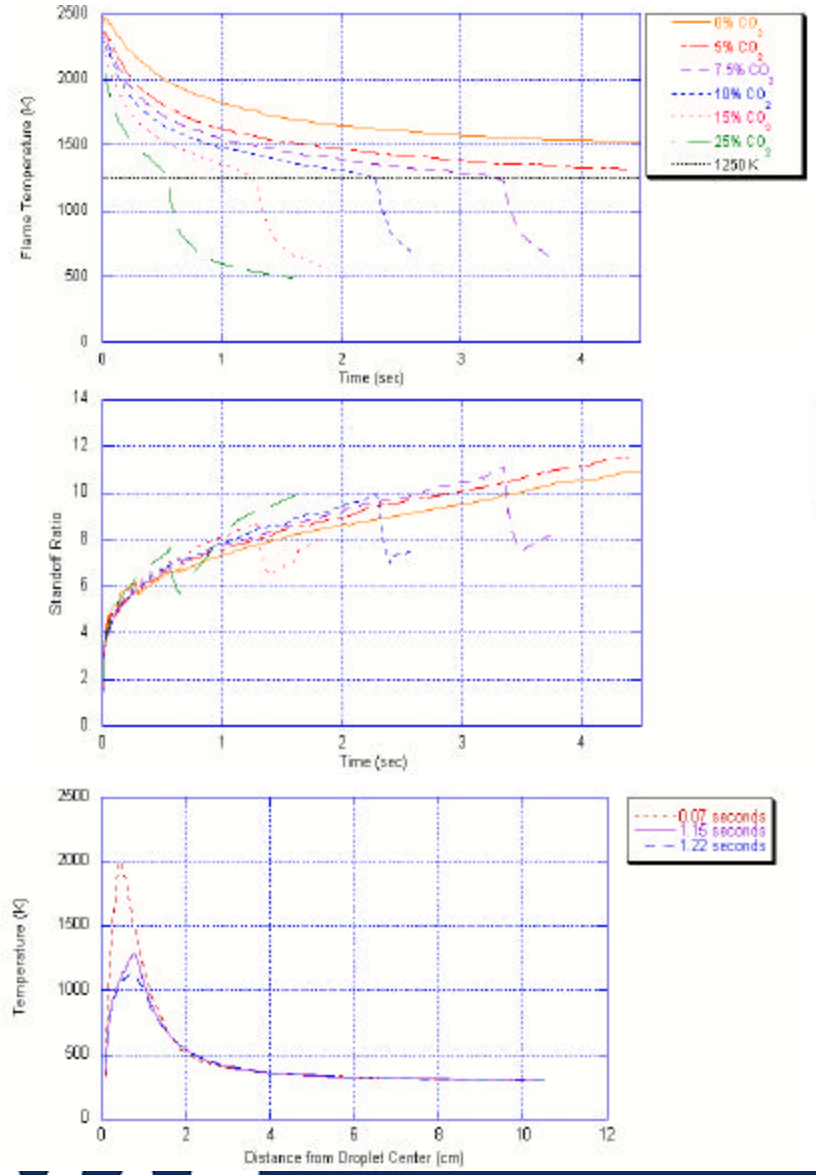
DME/Air Flame Speed Results



- Our experimental data show good agreement with the model predictions based upon the detailed kinetics developed by our group (Fischer et al., 2000)

Published in Zhao et al., Combust Flame 139, 52 (2004)

Physical v Kinetically-Limited Droplet Burning Extinction



- Simulations of 2 mm *n*-heptane droplets in the listed mole fraction of CO_2 mixed with air (21% O_2/79% N_2).
- As CO_2 mole fraction is increased, extinction, as characterized by a region of high negative curvature, begins at higher temperatures. This time corresponds exactly with a rapid decrease in burning rate.
- The rapid decrease in standoff ratio which occurs near extinction corresponds exactly with 1250 K. It therefore decorrelates from extinction time as the mole fraction of CO_2 increases.
- As visible in the temperature profiles at differing times within a characteristic burning history, we see the fundamental difference between the temperature profile before the decrease in standoff and thereafter is the loss of a sharp peak. This peak is associated with local heat generation, and thus chemical reaction.
- We therefore have a simple technique for differentiating kinetically-limited extinction from extinction resulting from other effects.
- The suppressant effect of carbon dioxide is therefore not only because of an increase in local heat capacity, but also due to some more active source of heat loss. These losses could most easily be attributed to an increase in spectral radiative heat transfer from the flame zone.