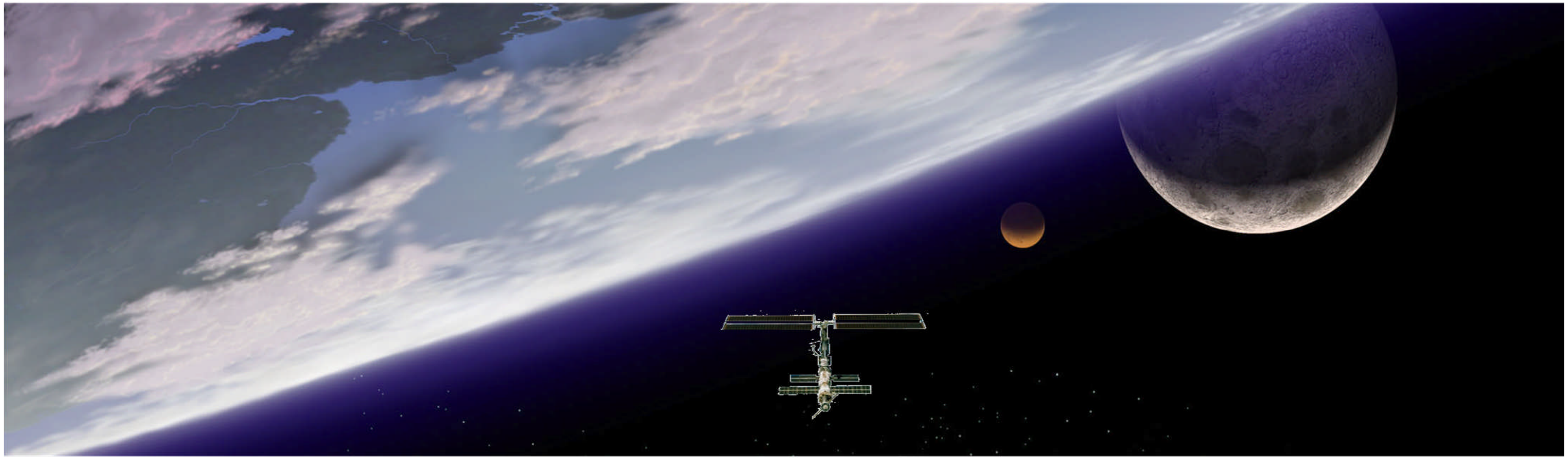
"Cool Flames" in Space, a Hot Prospect on Earth!

Anomalous combustion of alkane fuel droplets in space



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July 16-18, 2013 Denver, Colorado

Flame Extinguishment Experiment (FLEX) Science Team

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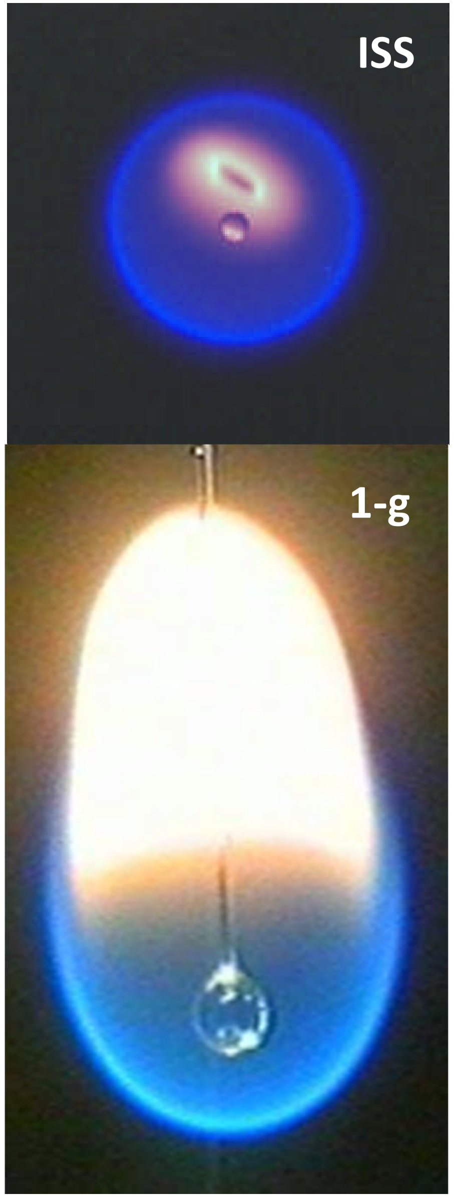
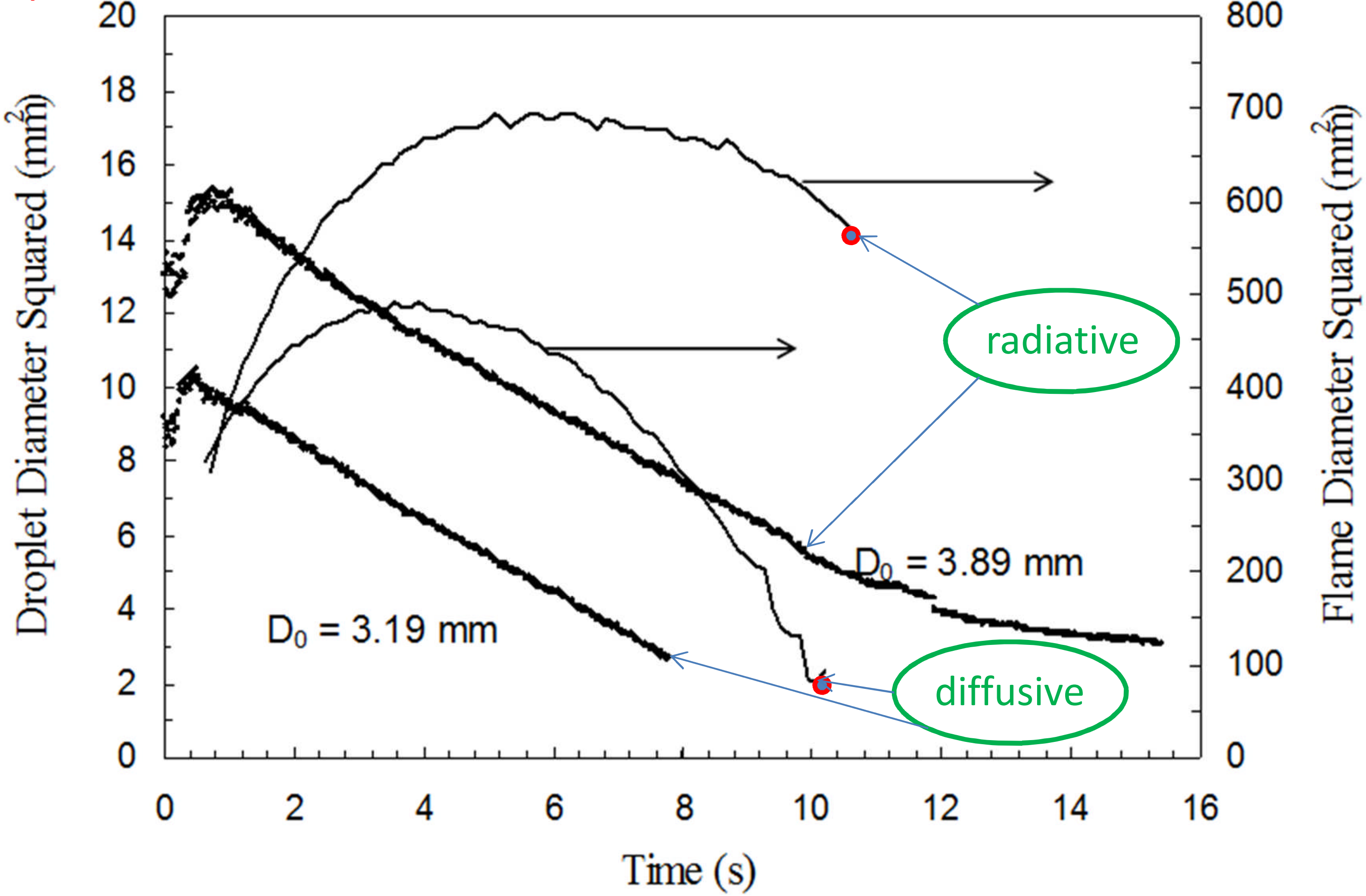
ISS FLEX Experiments - Background



- Microgravity droplet combustion experiments aimed at understanding the flammability boundaries of liquid fuels in a variety of ambient conditions – spacecraft fire safety
- Sooting and non-sooting fuels are burned in nitrogen, helium, carbon dioxide, and xenon environment at various oxygen concentrations at different pressures (effectiveness of fire suppressants in spacecraft environments – CO_2 is used in ISS)
- Conventional understanding has been that the droplet flame can extinguish via two modes:
  - Diffusive extinction (high Oxygen, small droplet) or
  - Radiative extinction (low oxygen, large droplet)
  - Pure evaporation following extinction
- Existing theories and numerical simulations supported this view

ISS FLEX Experiments

- Example of two modes of extinction: Droplet combustion experiment (DCE) Space Lab Mission MSL-1

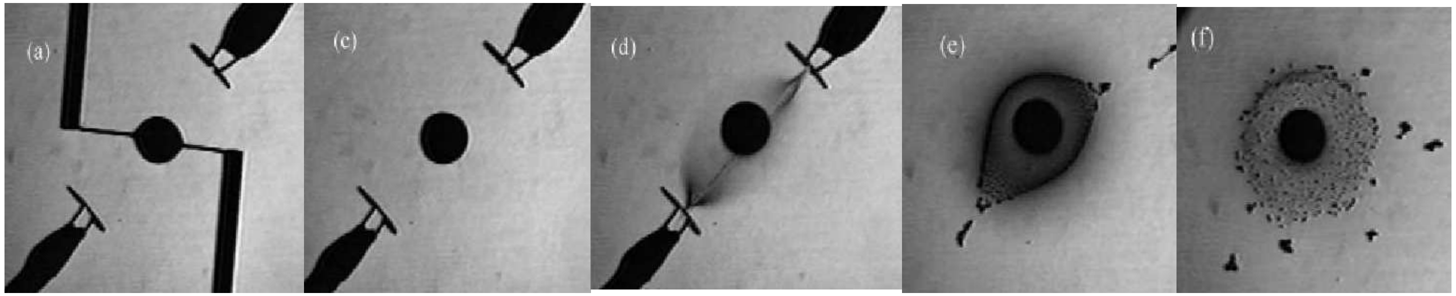


n-heptane in 30-70% oxygen-helium environment at 1 atm

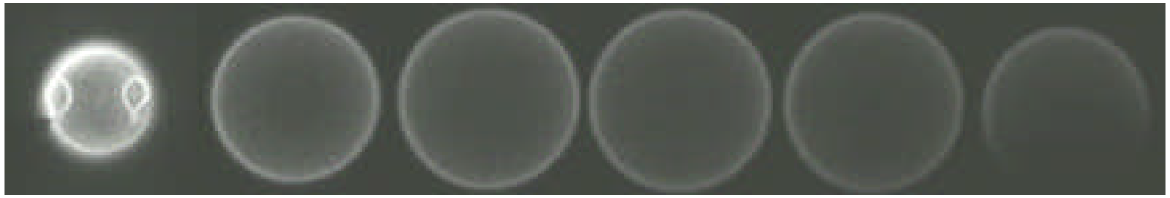
ISS FLEX Experiments

- Droplet combustion experiment (DCE) Space Lab Mission (MSL-1)

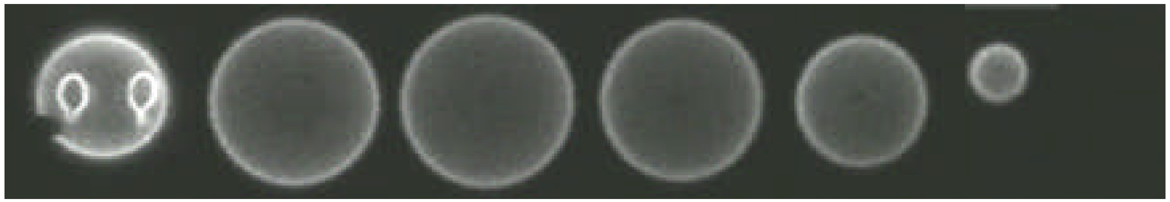
Backlit images of the droplet



Radiative extinction **UV images of the flame**



Diffusive extinction **UV images of the flame**

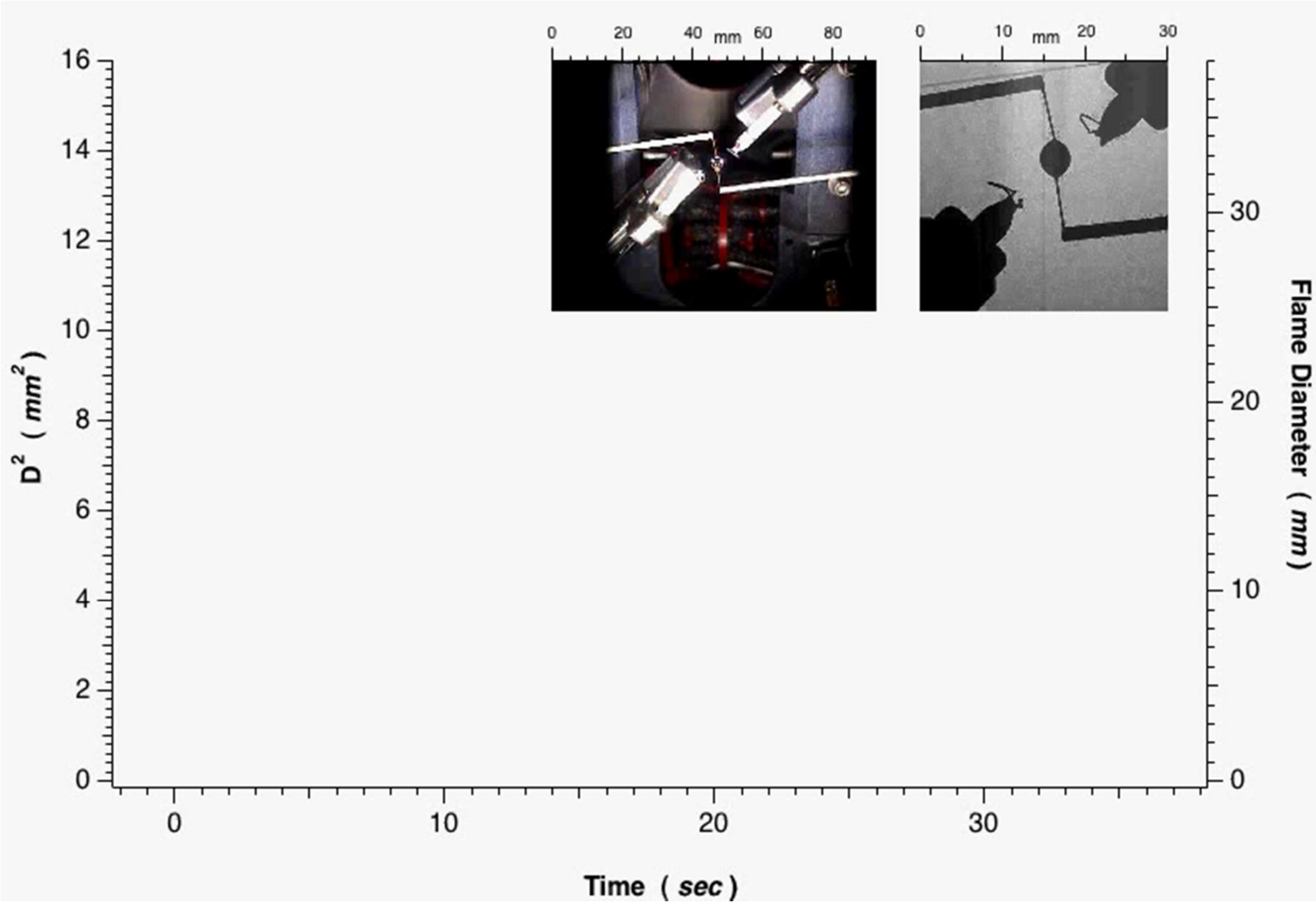


n-heptane in 30-70% oxygen-helium environment at 1 atm

ISS FLEX Experiments

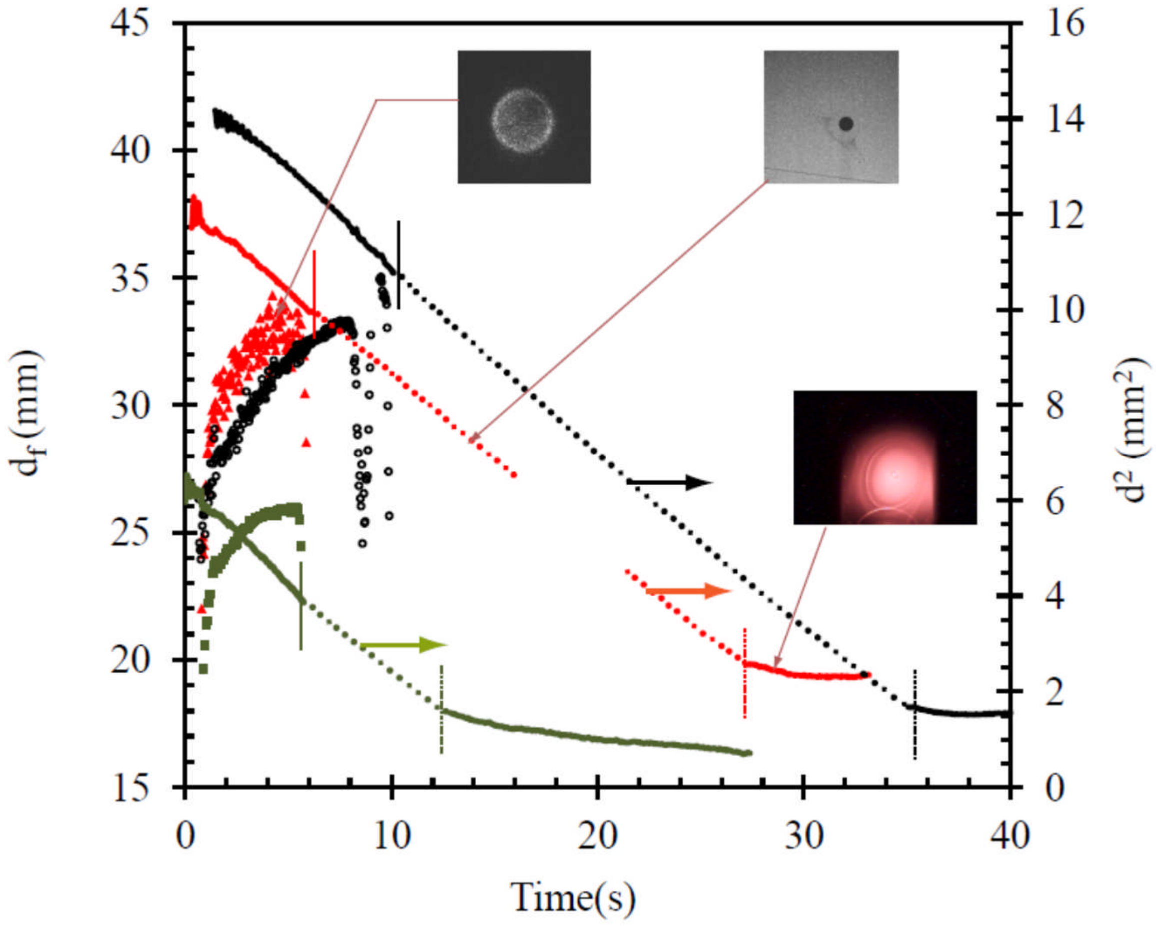
- Anomalous Combustion

ISS FLEX “Anomalous” Combustion



heptane droplet burning in air at 1 atm pressure

ISS FLEX “Anomalous” Combustion

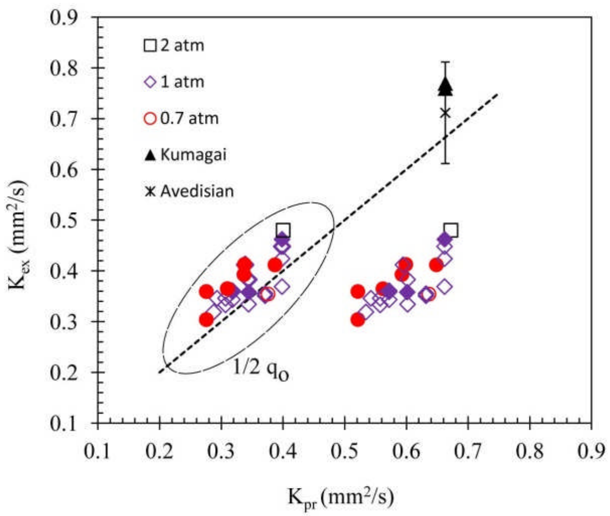


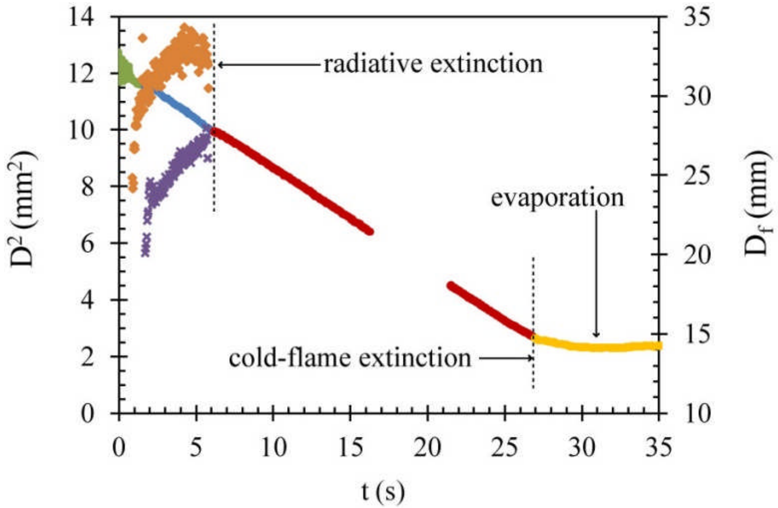
Three examples of 2nd stage combustion: heptane in air, 18-82%O2-N2, 18-67-15% O2-N2-CO2

More recent test show similar behavior in n-octane, and n-decane fuels

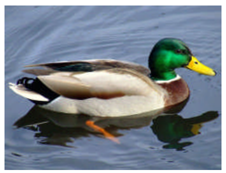
ISS FLEX “Cool Flame” Combustion

- Over 50 years of microgravity droplet combustion experiments (drop-towers, parabolic-flights, and space shuttle) and the 2nd stage low-temperature combustion has never been observed
- Initial attempts at explaining this behavior using pure vaporization could not agree with quasi-steady d-square law behavior. Diffusion controlled surface catalytic reaction models required unacceptably high diffusion coefficients for oxygen





- low heat release rate
- quasi-steady burning
- 2nd extinction
- lower activation energy



Passes “the duck test” – it must be cool-flame supported combustion!

ISS FLEX “Cool Flame” Combustion

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Can cool flames support quasi-steady alkane droplet burning?

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ABSTRACT

Experimental observations of anomalous combustion of n-heptane droplets burning in microgravity are reported. Following ignition, a relatively large n-heptane droplet first undergoes radiative extinction, that is, the visible flame ceases to exist because of radiant energy loss. But the droplet continues to experience vigorous vaporization for an extended period according to a quasi-steady droplet-burning law, ending in a secondary extinction at a finite droplet diameter, after which a vapor cloud rapidly appears surrounding the droplet. We hypothesize that the second-stage vaporization is sustained by low-temperature, soot-free, “cool-flame” chemical heat release. Measured droplet burning rates and extinction diameters are used to extract an effective heat release, overall activation energy, and pre-exponential factor for this low-temperature chemistry, and the values of the resulting parameters are found to be closer to those of “cool-flame” overall reaction-rate parameters, found in the literature, than to corresponding hot-flame parameters.

Published after critical reviews from skeptical reviewers!

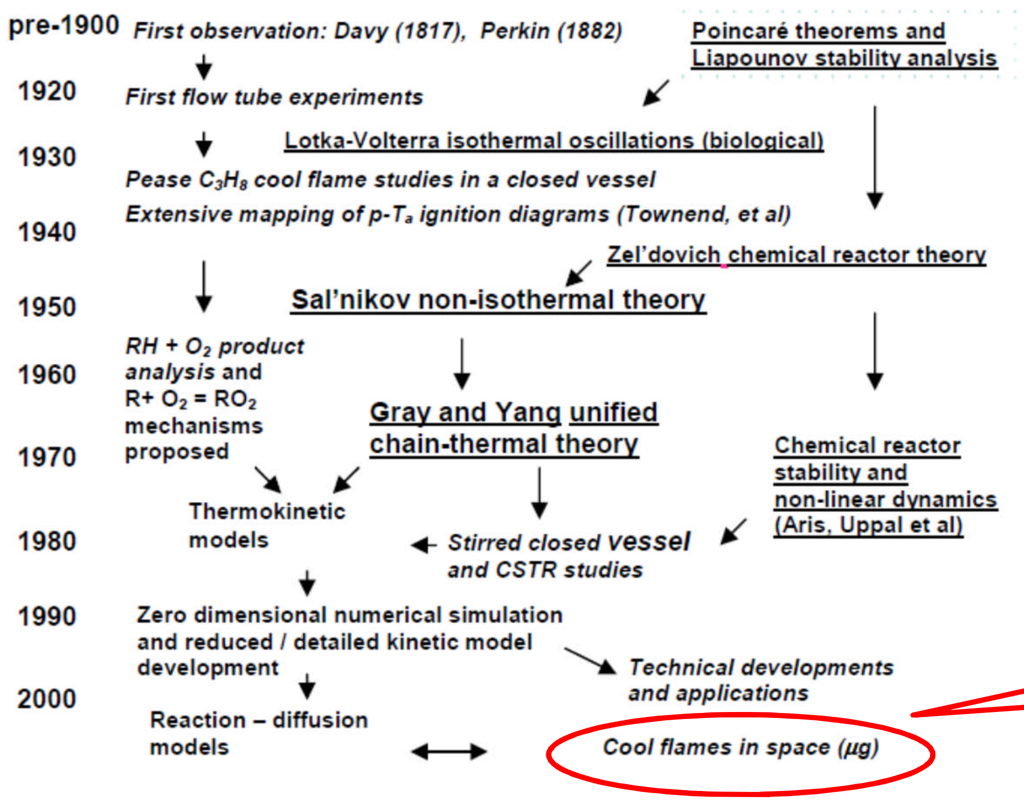
Cool Flames

Traditional view of cool flames (reason for skepticism)

- Historically cool flames are associated with premixed combustion leading to ignition of hot fuel/air mixtures. (commonly encountered in car-engine knock)

  cool flames -> ignition

  hot flames -> cool flame combustion! (**Never – until now!**)



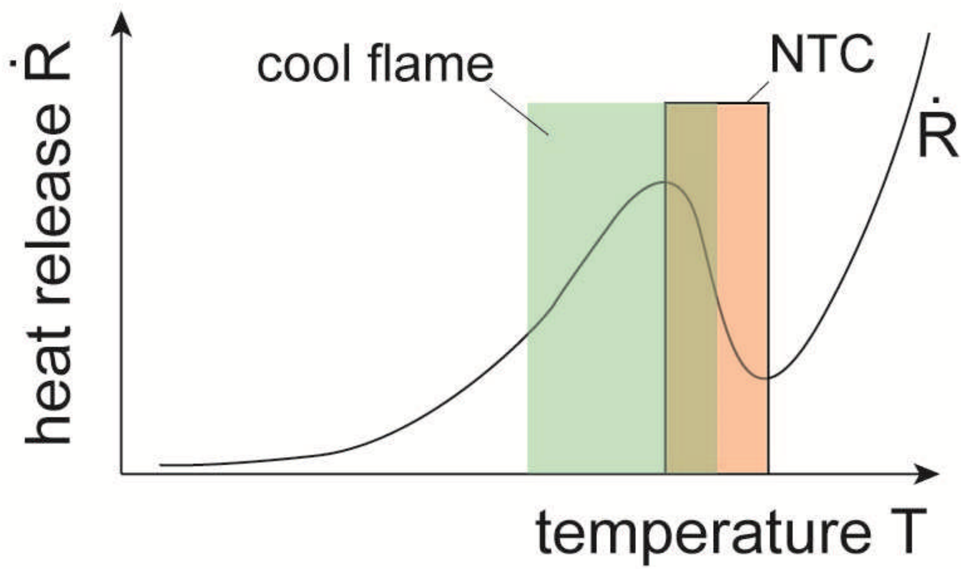
A history of cool flame research by Prof. Griffiths* (~2002)
"cool flames – a hot prospect"

Visionary?

Cool Flames

- Combustion of hydrocarbons is a complex process and involves multiple reactions involving free radicals
- The exact nature of the chemical pathways depend on molecular structure of the fuel, pressure, and temperature among others

A simple model:



ISS FLEX “Cool Flame” Numerical Validation

- Numerical simulations and confirmation of “cool-flame” combustion

ISS FLEX “Cool Flame” Numerical Validation

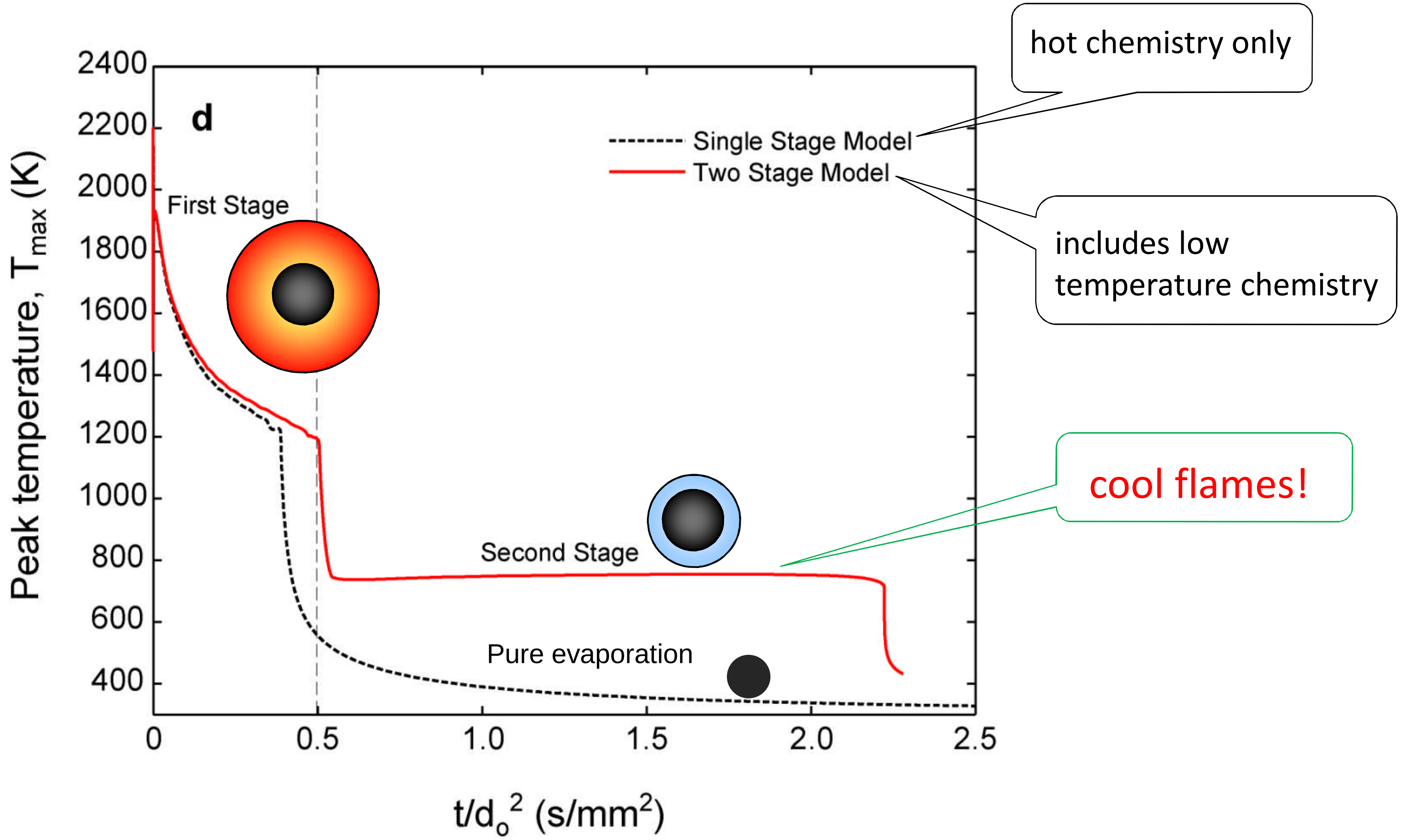
- **Numerical simulations by the Princeton Group (Farouk & Dryer)**
  - Full detailed chemical kinetics (Curran et al., 2002: Lawrence Livermore)
  - Involves 1038 species and 2739 reactions
  - Reduce mechanism with 128 species and 565 reactions using path flux analysis

TABLE A1

***n*-Heptane Mechanism for Diffusion Flames**

	ELEMENTARY REACTION	A m^3, Kmol, sec^{-1}	n	E_a J/mol	REF
1	H + O2 = OH + O	0.2000E+12	o	0.7030E+05	20-24
2	O + H2 = OH + H	0.5120E+02	2.67	0.2630E+05	20-24
3	OH + H2 = H2O + H	0.1000E+06	1.6	0.1380E+05	20-24
4	OH + OH = H2O + O	0.1500E+07	1.14	0.4200E+03	20-24
5	O2 + H + M = HO2 + M	0.6165E+14	1.42	0.0000E+00	20-24
6	HO2 + H = OH + OH	0.1680E+12	0	0.3660E+04	20-24
7	HO2 + H = H2 + O2	0.4270E+11	0	0.5900E+04	20-24
8	HO2 + OH = H2O + O2	0.2890E+11	0	0.2080E+04	20-24
9	HO2 + H = H2O + O	0.3000E+11	0	0.7200E+04	20-24
10	HO2 + O = OH + O2	0.3190E+11	0	0.0000E+00	20-24
11	HO2 + HO2 = H2O2 + O2	0.1860E+10	0	0.6440E+04	20-24
12	H2O2 + H = H2O + OH	0.1000E+11	0	0.1500E+05	20-24
13	H2O2 + H = HO2 + H2	0.1700E+10	0	0.1570E+05	20-24
14	H2O2 + O = HO2 + OH	0.6600E+09	0	0.1660E+05	20-24
15	H2O2 + OH = H2O + HO2	0.7830E+10	0	0.5570E+04	20-24
16	H2O2 + M = OH + OH + M	0.1200E+15	0	0.1900E+06	20-24
17	H + H + M = H2 + M	0.1000E+13	1	0.0000E+00	20-24
18	H + H + M = H2 + M	0.9200E+11	0.60	0.0000E+00	20-24
19	H + H + M = H2 + M	0.6000E+14	1.25	0.0000E+00	20-24
20	H + H + M = H2 + M	0.5490E+15	2	0.0000E+00	20-24
21	H + OH + M = H2O + M	0.2200E+17	2	0.0000E+00	20-24
22	O + O + M = O2 + M	0.6170E+10	0.5	0.0000E+00	20-24
23	CO + OH = CO2 + H	0.4400E+04	1.5	0.3100E+04	20-24
24	CO + HO2 = CO2 + OH	0.1500E+12	0	0.9893E+05	20-24
25	CO + O + M = CO2 + M	0.2510E+08	0	0.1901E+05	20-24
26	CO + O2 = CO2 + O	0.2500E+10	0	0.2000E+06	20-24
27	CH + O2 = CHO + O	0.3300E+11	0	0.0000E+00	20-24
28	CH + CO2 = CHO + CO	0.3400E+10	0	0.2900E+04	20-24

Numerical simulations

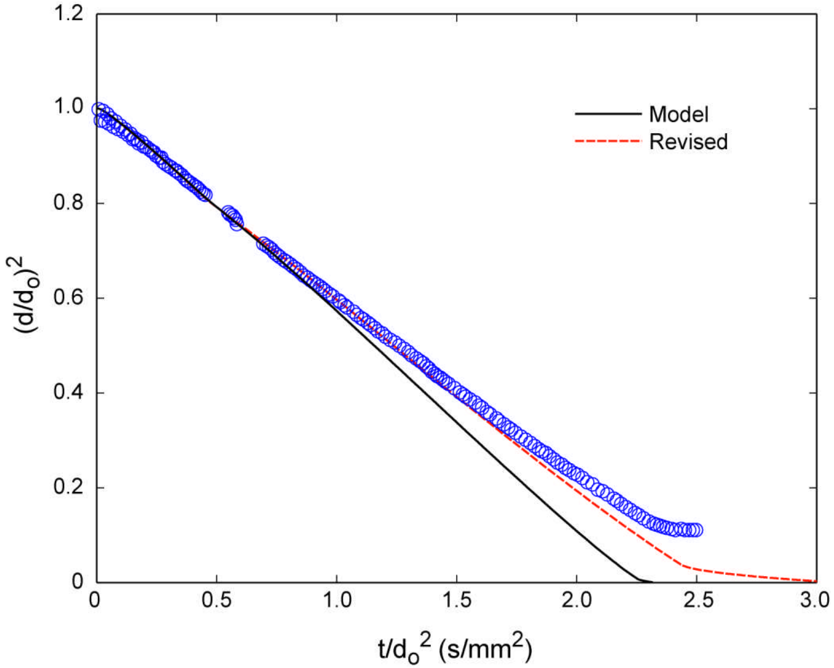


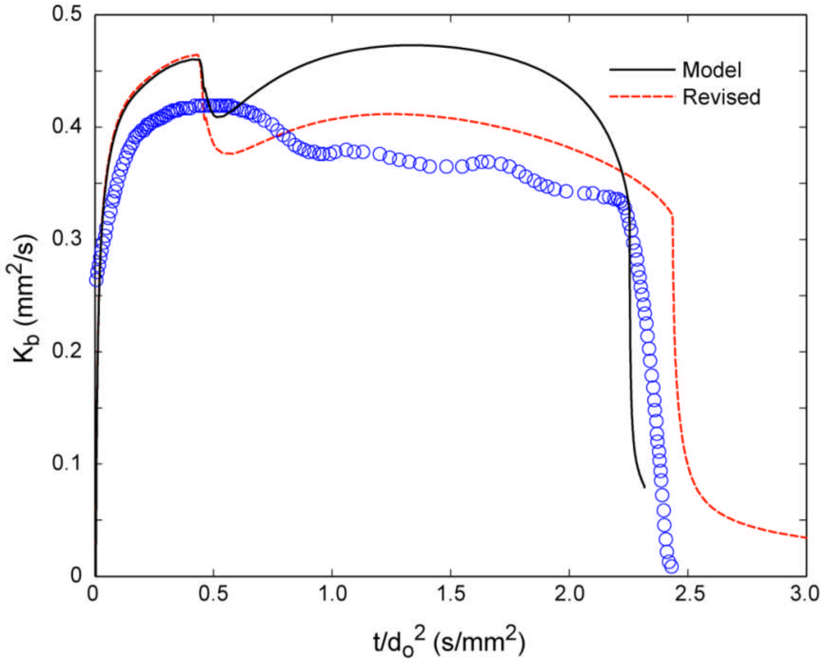
Evolution of, flame temperature (n-heptane, d_o = 3.91 mm, air, atmospheric pressure)

Captures the low-temperature combustion – but how good is it?

Numerical simulations

- Predicted droplet diameter and burning rate evolution compared experiments





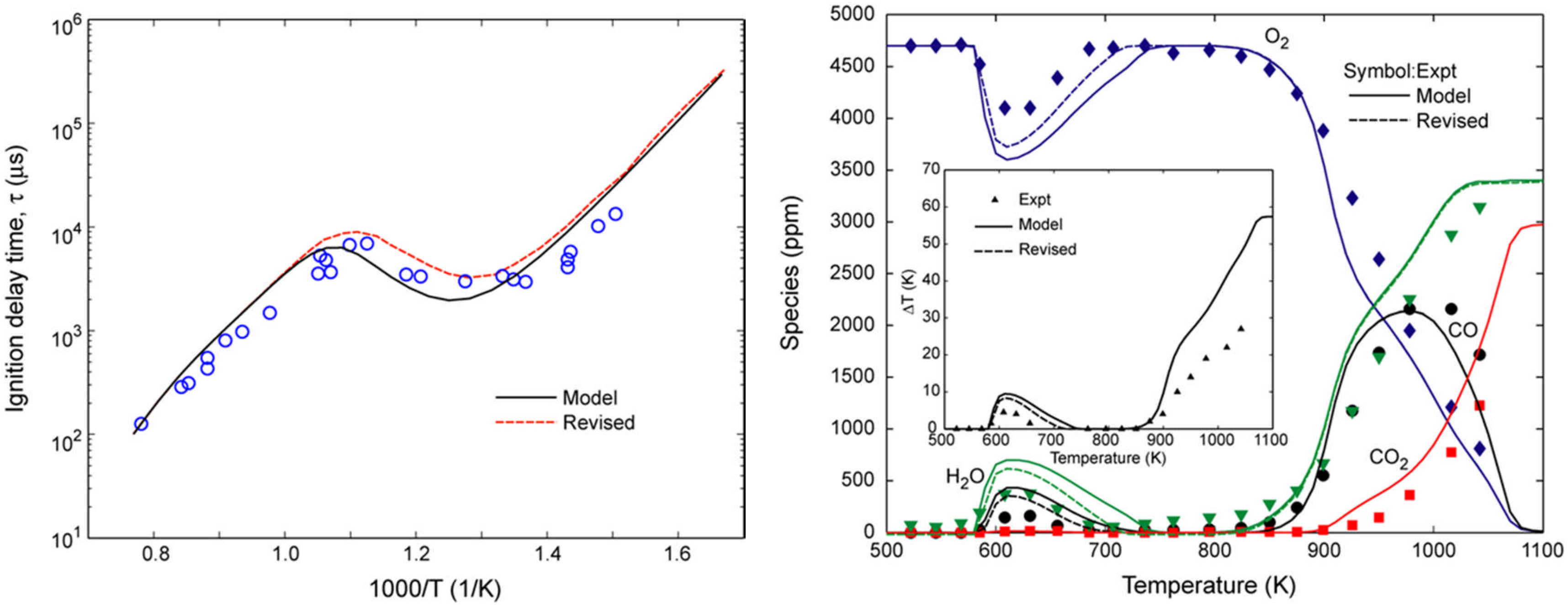
Model => Curran chemistry with PFA reduction

Revised model => The reaction rates for the most sensitive reactions are modified

- $QOOHO_2$ -> QOOH + O_2 (was increased: A factor increased by 2)
- $QOOHO_2$-> Ketohydroperoxide + OH (was decreased: A factor decreased by 2).

Numerical simulations

- Revised kinetics improves ignition delay and reactivity predictions in the low-temperature region



Predicted shock tube ignition delay and flow reactor reactivity with revised chemical kinetics model.

Droplet combustion improves predictions of results from other universally used experimental techniques

Numerical simulations

- Further confirmation of “cool-flame” 2nd stage burning by Italian researchers

XXXVI Meeting of the Italian Section of the Combustion Institute

COOL FLAMES IN DROPLET COMBUSTION

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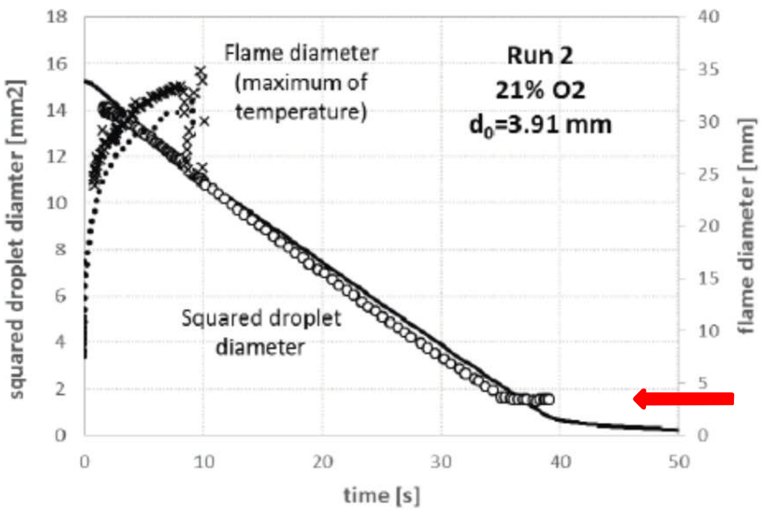
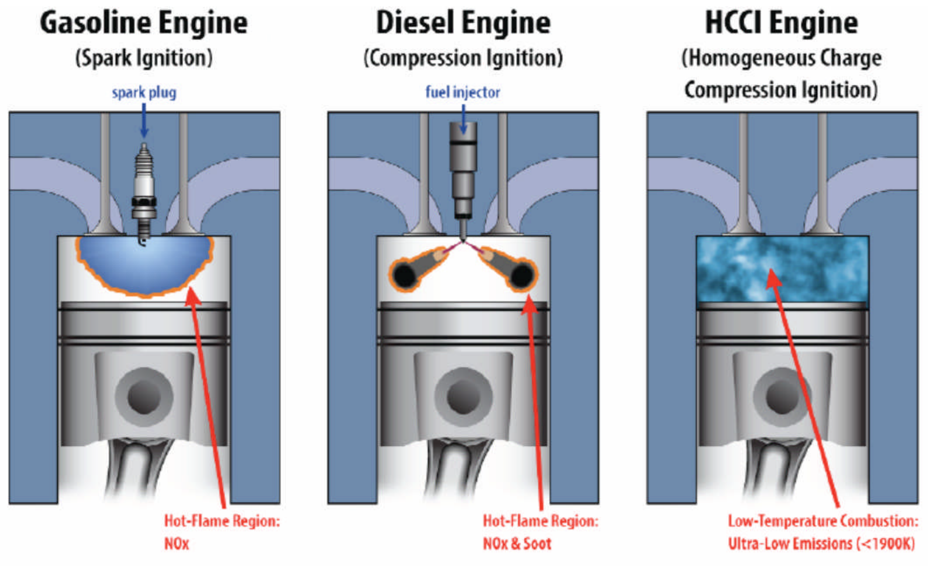


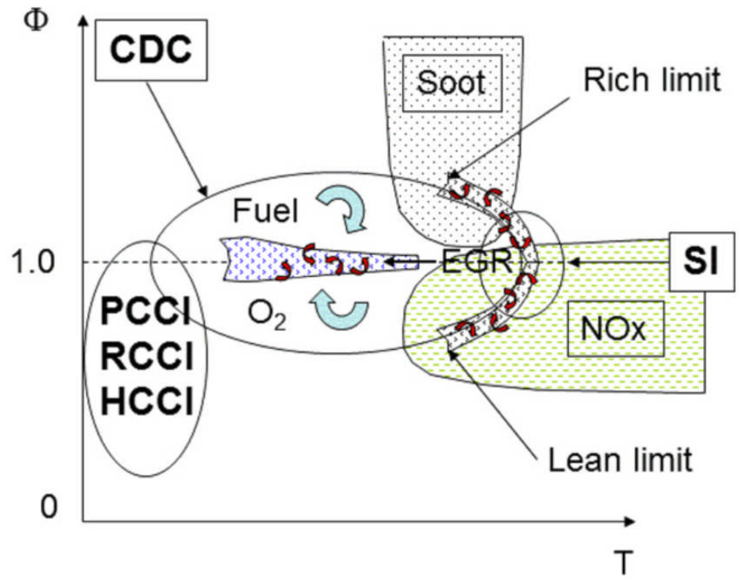
ISS FLEX Experiments

- Potential applications of “cool-flame” combustion

Potential applications

- Advanced low temperature combustion engines*
  - Homogeneous charge compression ignition engine (HCCI)
  - Provides low emissions and improved efficiency (~15% fuel savings)
  - Major technical challenge is control of ignition timing

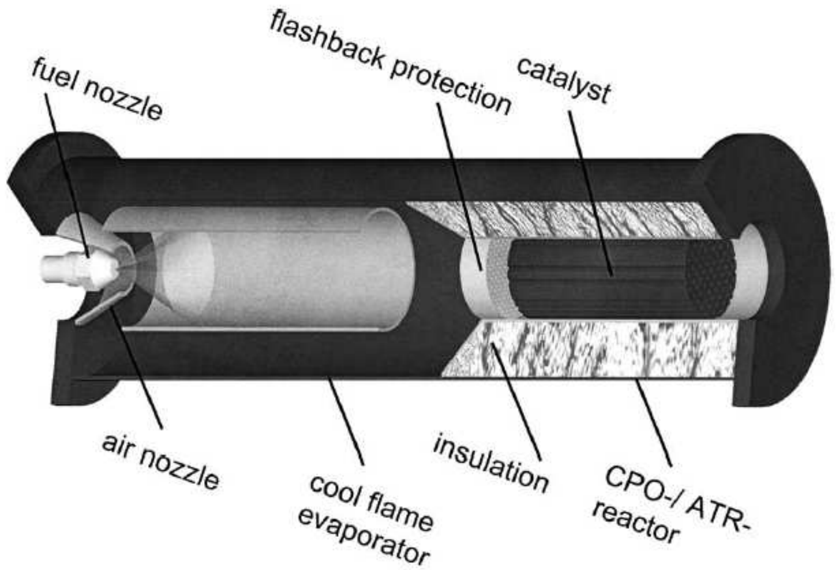




*Reitz, R.D., Combustion and Flame, 2013

Potential applications

- Fuel reforming technologies*
  - Heavy fuels are partially oxidized (using “cool flame”) and used in gaseous burners with reduced emission and good power modulation and hydrogen for fuel cells



Catalytic diesel reformer

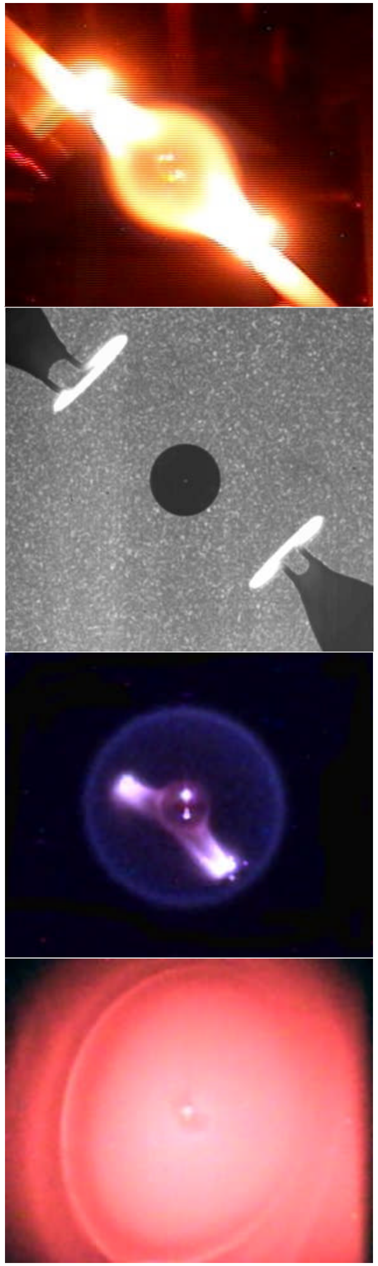
- New burner technologies
  - The possibility to use cool-mode combustion of individual droplets may lead to entirely different design concepts of spray burners (A. Cuoci, et al., 2013)

*Hartman et al., J. of Power Sources, 2003

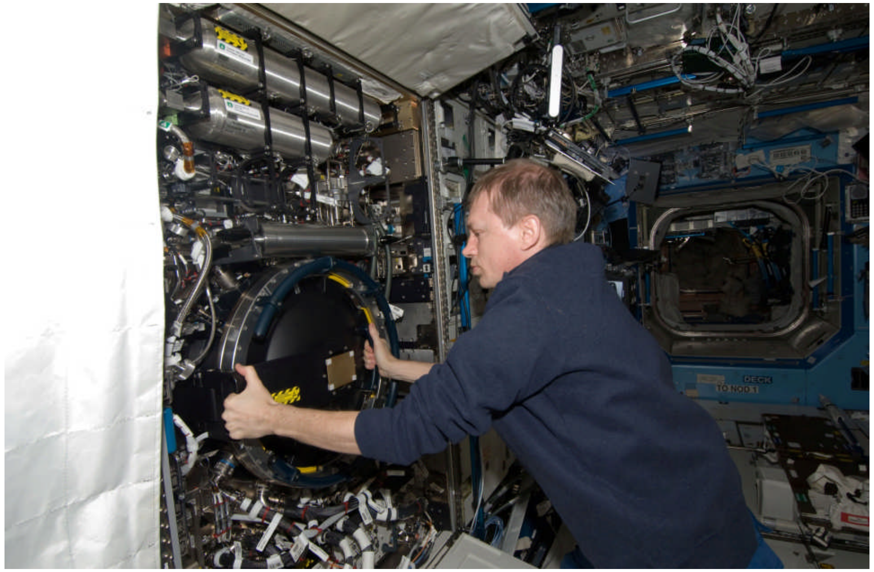
Potential applications

- Fire safety
  - On Earth spontaneous combustion and explosion of liquid fuel vapors in chemical industry is a major concern
  - In space “cool flame” can persist after hot flame extinction and generate combustible vapor that can reignite (similar to smoldering combustion in solid fuels)
  - Recent results show re-ignition with decane

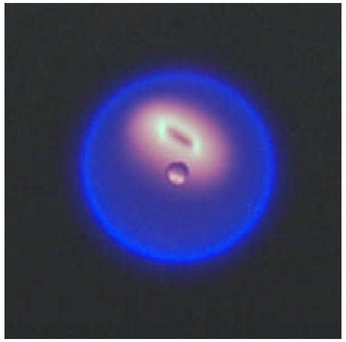
Concluding Remarks

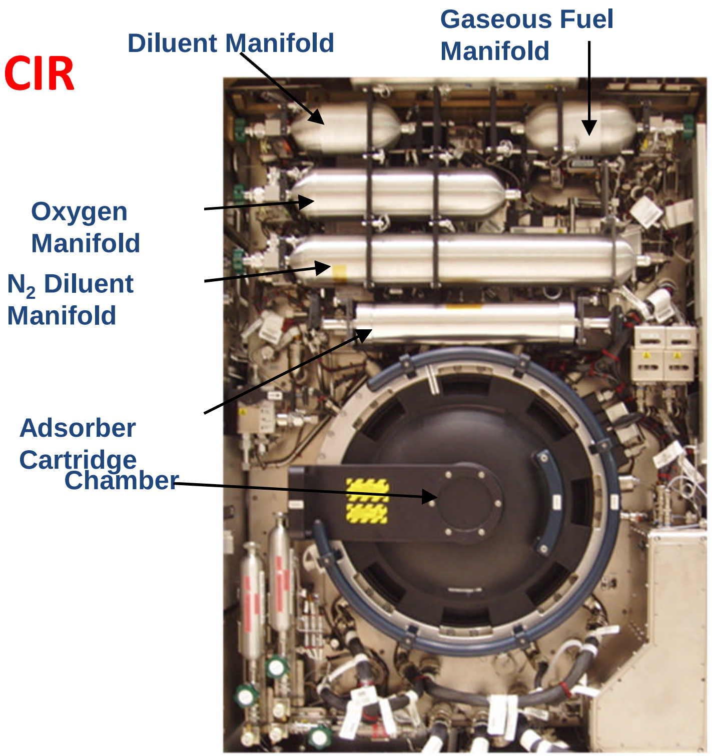


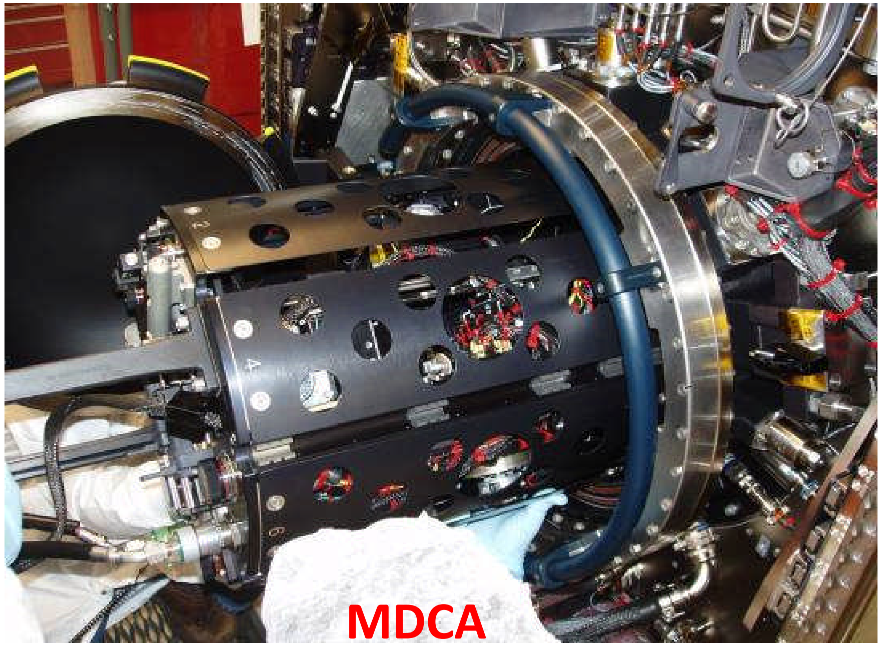
- A new phenomenon where a hot flame extinction leads to a low-temperature, "cool-flame" burning in microgravity has been observed for the first time
- These cool flames produce partially oxidized fuel and potentially re-ignite to hot flames posing fire safety concerns in spacecraft environments
- Existing, widely-used detailed chemical kinetic models do not accurately predict the 2nd stage cool flame extinction and need further improvement
- Improved low temperature chemistry will have wide ranging applications including advanced internal combustion engine design and development
- The new phenomena may lead to new innovative burner designs and fuel reforming technologies



Questions?




CIR
Diluent Manifold
Gaseous Fuel Manifold
Oxygen Manifold
N_2 Diluent Manifold
Adsorber Cartridge
Chamber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