Isolated Single Droplet Combustion:
FLEX Experiments onboard the International Space Station

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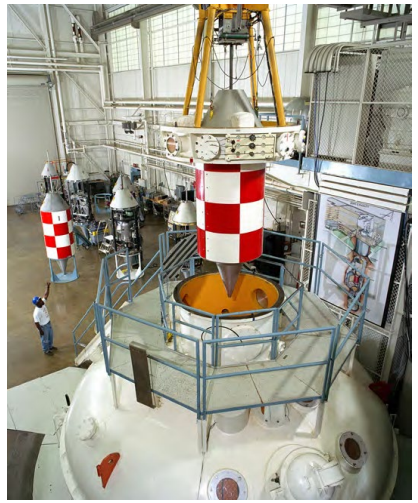
Daniel L. Dietrich
NASA Glenn Research Center

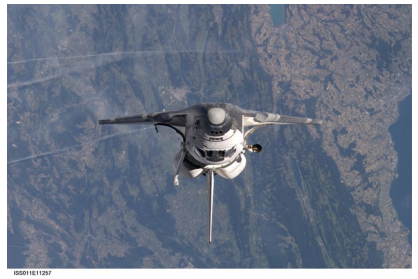
Forman A. Williams
University of California San Diego

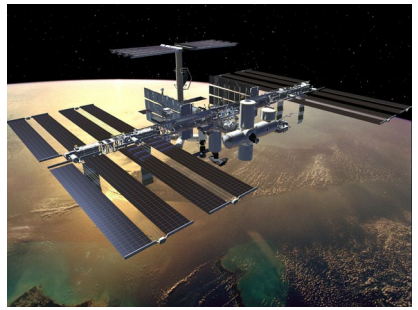
JASMAC
Conference of the Japan Society of Microgravity Appllication

October 15, 2021

History Leading to ISS FLEX Experiments







- The first publication in the field:
  S. Kumagai, "Combustion of fuel droplets in falling chambers with special reference to the effect of natural convection", *Jet Propulsion*, Vol. 26, 1956, p. 786.
- NASA drop-tower experiments: 1974-present
  2.2 second tower, Zero gravity facility (5 seconds)
  Lear Jet, KC-135, DC-9 parabolic flights
- Fiber-supported droplet combustion (FSDC):
  STS73-USML-2,1995
- Droplet combustion experiment (DCE):
  STS94-MSL-1,1997
  FSDC-2 during the 2nd flight
- Flame Extinguishment experiments (FLEX): ISS 2008-2016
  - FLEX
  - FLEX-2
  - FLEX-ICEGA
  - FLEXJ
- Cool Flame Investigation (CFI): ISS 2017

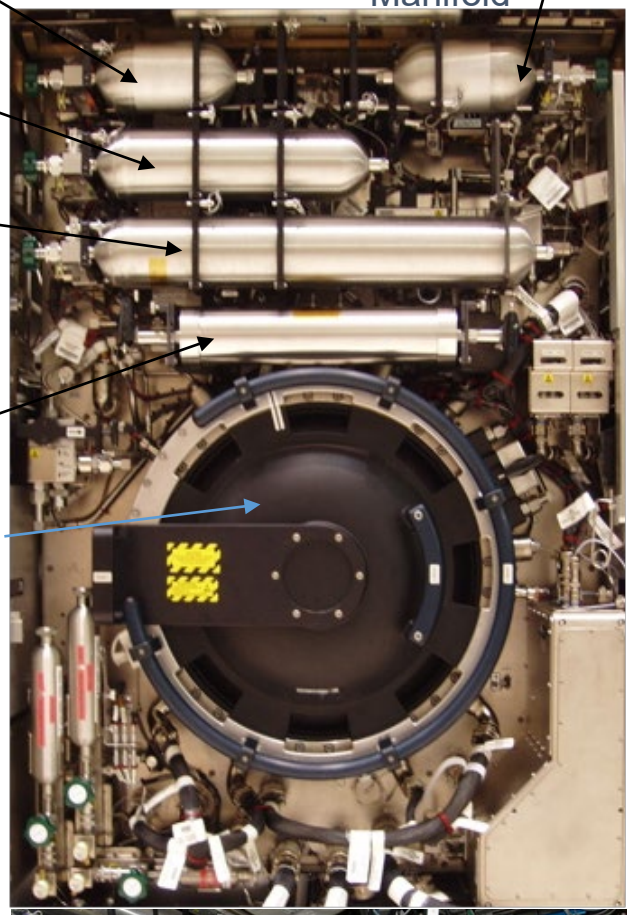




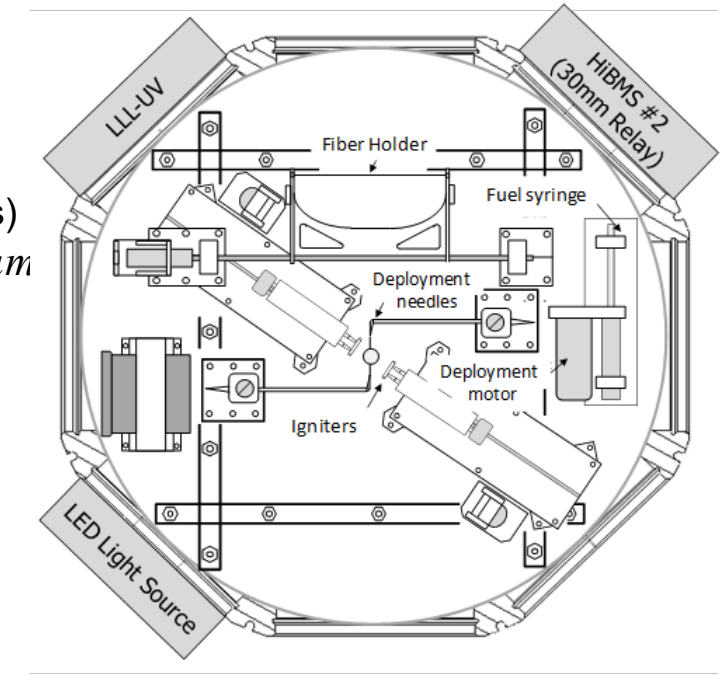
FLEX Hardware: CIR & MDCA

Combustion Integrated Rack (CIR)

- Chamber
  - 100 Liters capacity
  - Operating pressure: 0.02 to 5 atmospheres and contains pressures up to 9 atmospheres
  - 8 Sapphire windows
- Supplies gaseous fuel, oxidizers and diluents to the combustion chamber



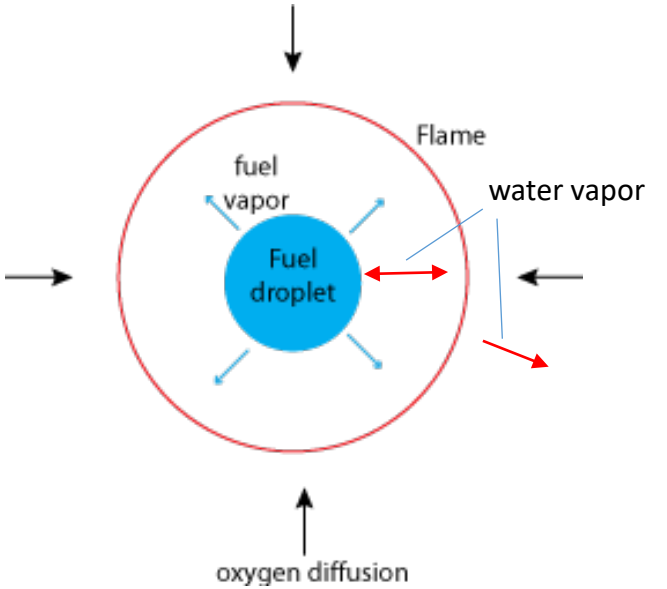
- **Multi-user Droplet Combustion Apparatus(MDCA)**
- Diagnostics
  - Backlit, black and white high speed camera (droplet view)
  - LLUV flame view camera (OH*,CH*)
  - Color camera (downlinked, operations)
  - Radiometers (Wide band $0.6 - 10.0\ \mu m$ and narrow band $5.0 - 6.5\ \mu m$)

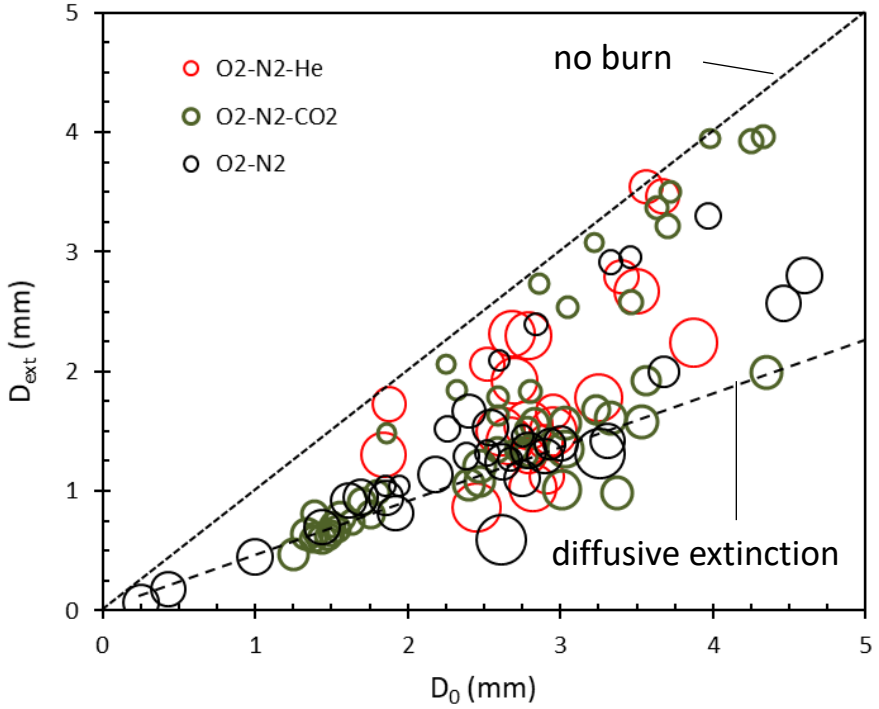




Methanol Droplet Combustion

- A wide range of conditions were investigated:
  - $13\% < O_2 < 30\%$
  - $5\% < CO_2 < 75\%$
  - $5\% < He < 45\%$
  - $1 < D_0 < 4.5$ mm
- Diffusive extinction due to water absorption, and radiative extinction were observed. The limiting oxygen index (LOI) ~ 12-13% oxygen at atmospheric pressure.
- Simplified theoretical models (Nayagam, 2013), and numerical simulations (Farouk & Dryer,2012) explain experimental observations reasonably well.

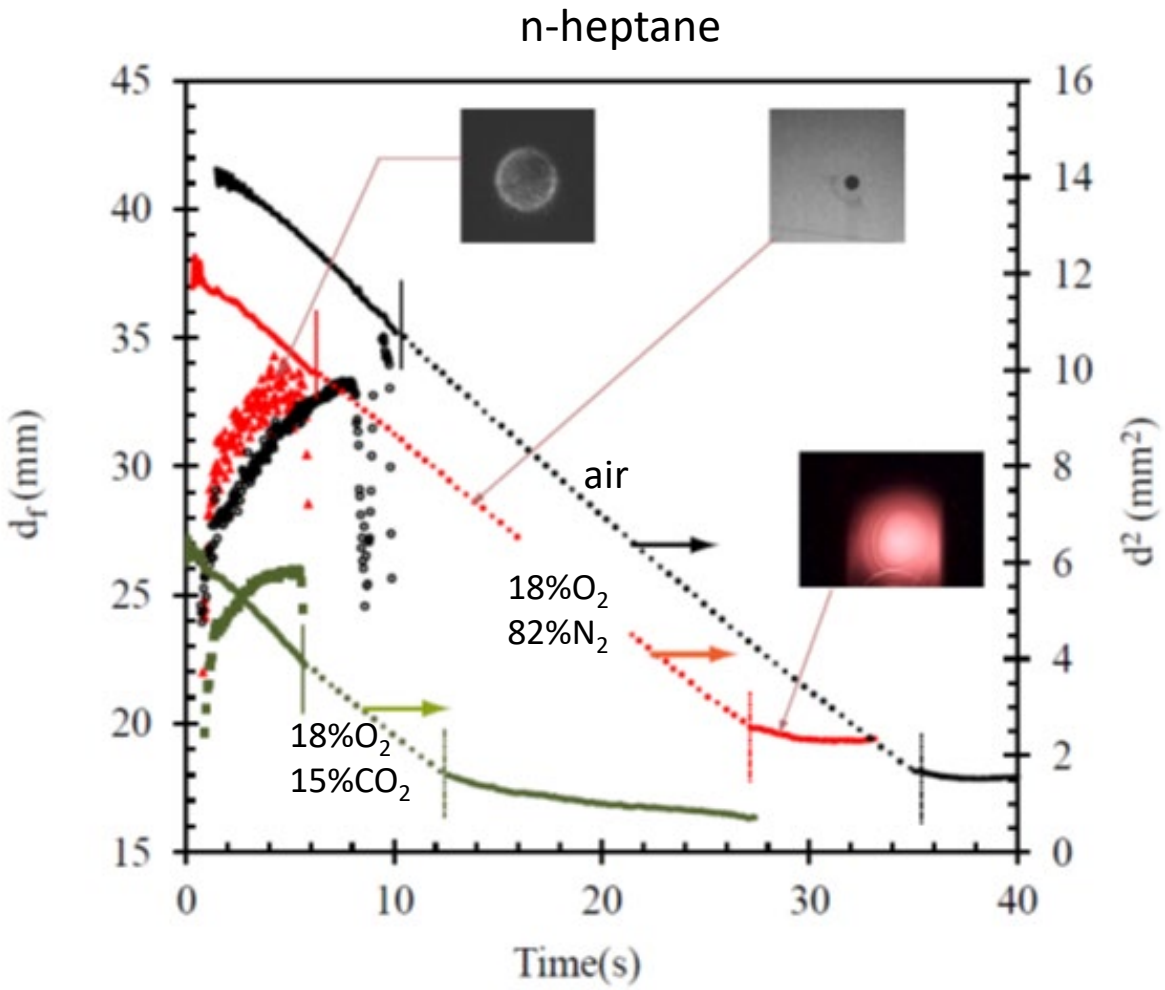




Bubble size proportional to oxygen concentration

Quasi-steady Cool Flames

- One of the major findings during FLEX experiments is the observation of low-temperature chemistry controlled, quasi-steady burning and extinction of n-alkane fuel droplets.

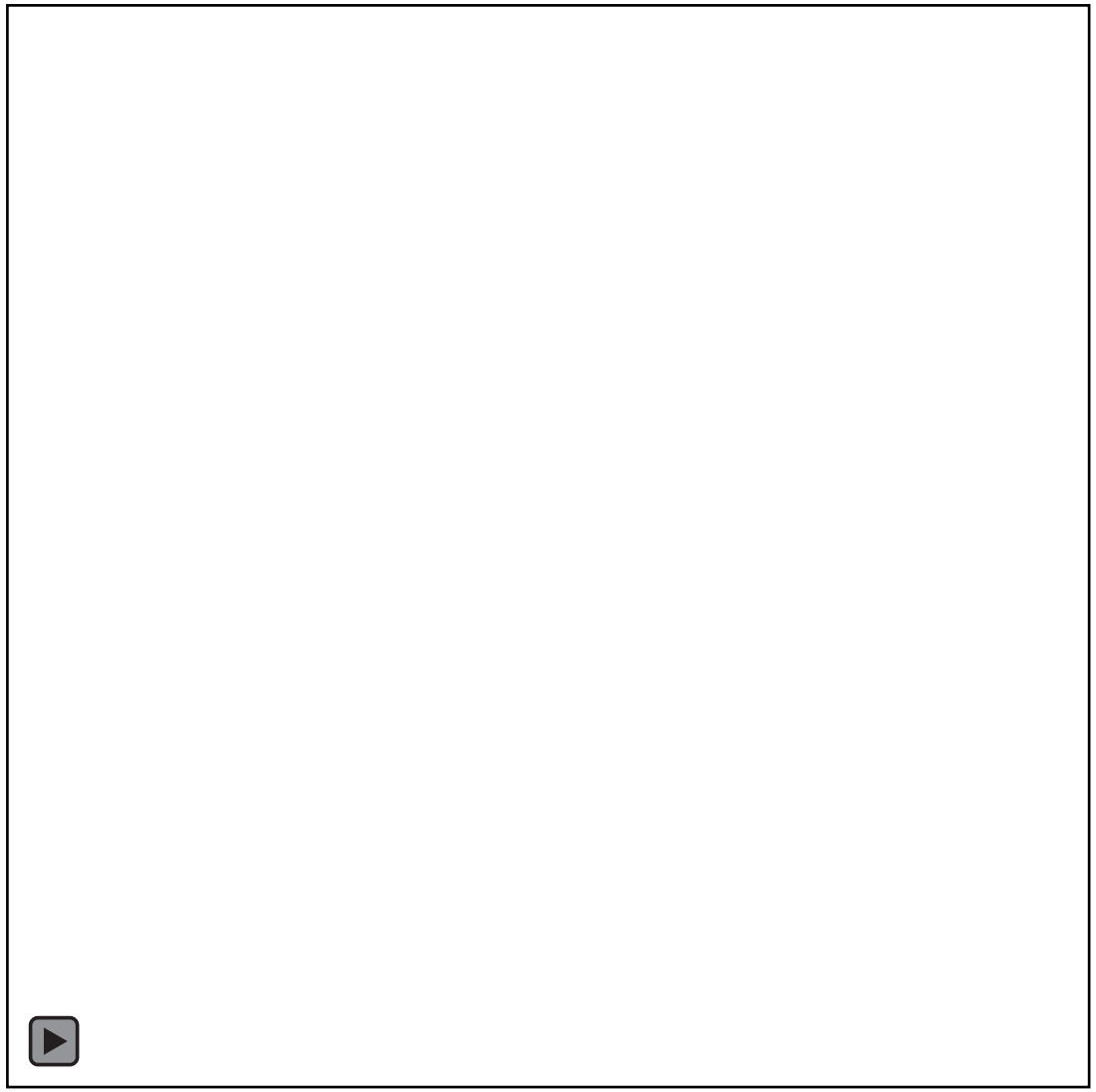


- Large droplets => Radiative extinction
- Second-stage cool-flame combustion
- Cool flame extinction
- Vapor cloud formation

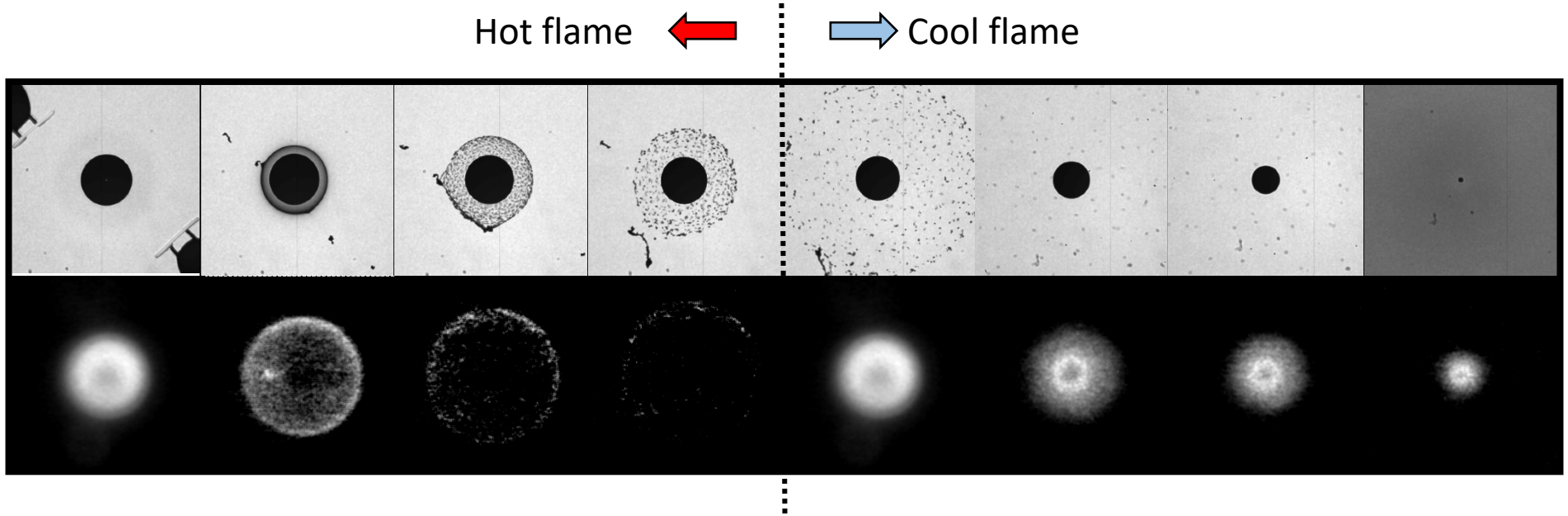
- Similar observations for other n-alkanes:
  - n-octane
  - n-decane
  - n-dodecane fuels

Quasi-steady Cool Flames

N-decane - ½ atm pressure - 21% O_2 and 79% N_2



Quasi-steady Cool Flames (with cool flame imaging)

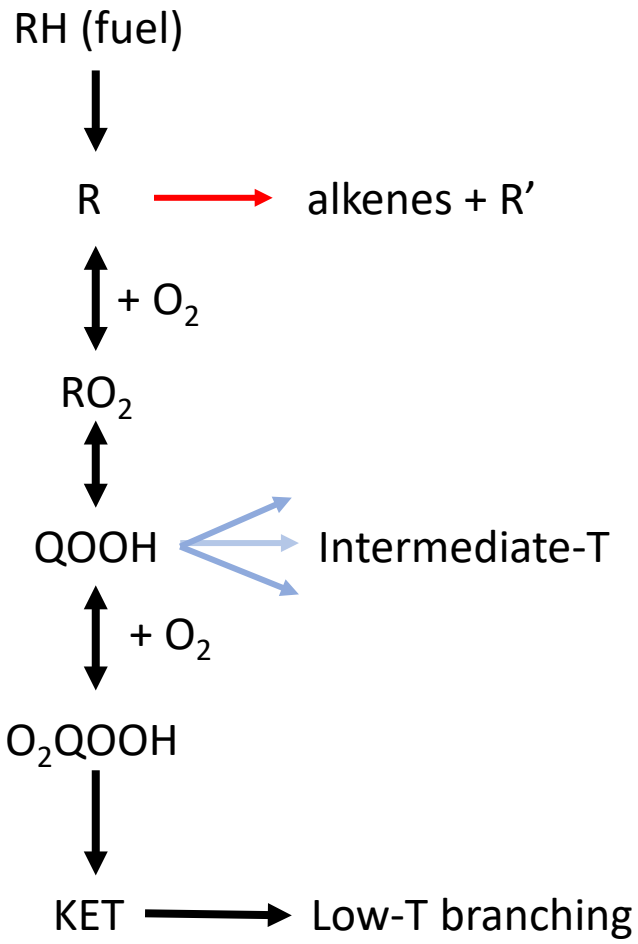


- FLEX-377
  - N-decane
  - ½ atm
  - air
  - D_0 =4.0 mm

- Cool flames are very weak (frame averaged here)
- They are broad (unlike hot flames)
- They are located closer to the droplet surface compared to the hot flames

Quasi-steady Cool Flames

- Fuel is oxidized using chemical kinetic pathways
- The chemical kinetic pathways change from LTC chemistry to HTC chemistry in the NTC zone
- Cool flames arise in the Negative Temperature Coefficient (NTC) region
- Cool flames are fundamentally different compared to hot-flames (chemical kinetics controlled)!



Simplified Theoretical Model: Cool Flames

6-step simplified chemical kinetics (based on San Diego Mechanism)*

Rate parameters				
No.	Reaction	A C7H16 and C8H18	A C10H22 and C12H26	T_a (K)
1	$F + OH \rightarrow R + H_2O$	1×10^{12}	1.5×10^{12}	0
2	$R + O_2 \rightarrow I$	2×10^{12}	3.67×10^{12}	0
3	$I + O_2 \rightarrow K + OH$	3.5×10^{7}	6.42×10^{12}	-8360
4	$K \rightarrow P's + OH$	4×10^{13}	6×10^{7}	19,840
5	$I \rightarrow Q's$	2×10^{12}	3×10^{13}	12,090
6	$R \rightarrow S's$	3.2×10^{13}	4.8×10^{13}	15,110

A – (cm^3/mol.s) (for bimolecular reactions) & 1/s (for unimolecular reactions)
T_a – (K)

rr ~ A Exp[-Ta/T]

Heat release can be associated with this step 4

Step 1: H-atom abstraction
RH + OH → R + H2O

Step 2: First oxygen addition
R + O_2 → ROO

Step 2a: Internal Isomerization
ROO → QOOH

Step 3: 2nd oxygen addition
QOOH + O_2 → KET + OH

Step 4: KET decomposition
KET → P's + OH

Step 5: Intermediate – T path
QOOH → S's

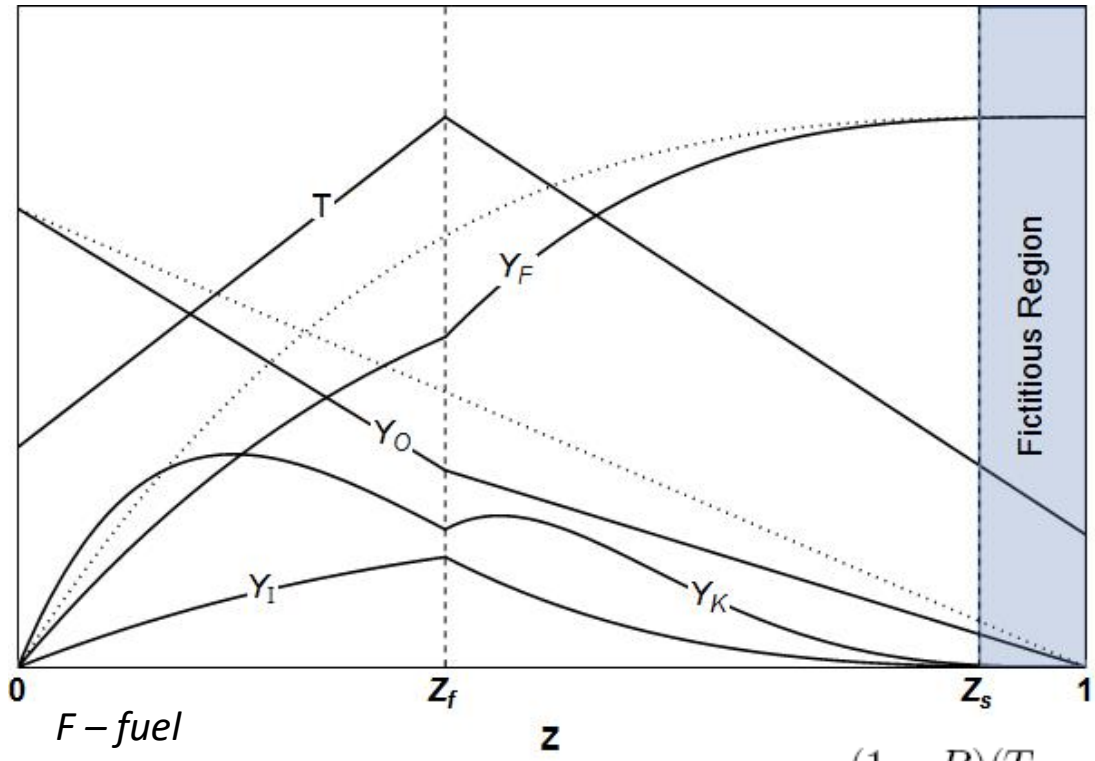
Step 6: High-T path
R → S's

Williams and Nayagam (Combustion Theory and Modelling (2019)

Williams and Nayagam (Combustion and Flame (2020)

Simplified Theoretical Model

6-step simplified chemical kinetics – cool diffusion flame structure – Activation Energy Asymptotic Theory*



- Simplified theory provides useful insights
  - KET is produced over a large region
  - Fuel and Oxygen leaks through the flame
  - Flame temperatures are low ~ 800K
  - Leaked fuel can condense forming vapor cloud

$$K_c = \frac{8\rho_\infty \alpha_{T\infty}}{\rho_l} \ln\left(\frac{2T_f - T_0 - T_\infty}{T_L}\right)$$

$$D_{ce}^2 = \frac{(\rho_l/\rho_\infty)^2 (K_c^2/\alpha_{T\infty})(T_{fe}/T_\infty)(T_{fe} - T_0)^2}{8(D_{fe}/D)^4 (2T_{fe} - T_0 + T_\infty)^2 \chi_{fe}}$$

F – fuel
R – alkyl radical
I – intermediate
K – ketohydroperoxide
P, Q, S – products

$$\chi_f = \frac{(1-R)(T_f - T_0)T_f^2 (Ae^{-T_a/T_f} + Qe^{-T_q/T_f} + He^{-T_h/T_f})}{T_a (2T_f - T_0 - T_\infty)^2} [(1+E)^{1/2} - 1]$$

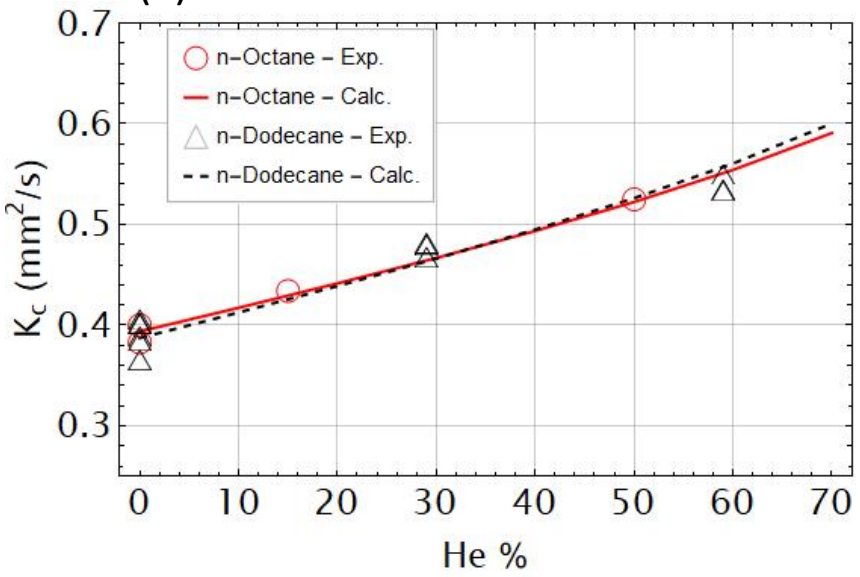
$$R = \left(1 - \frac{T_f - T_\infty}{2T_f - T_0 - T_\infty}\right)^L$$

**Williams and Nayagam (Combustion Theory and Modelling (2019)*

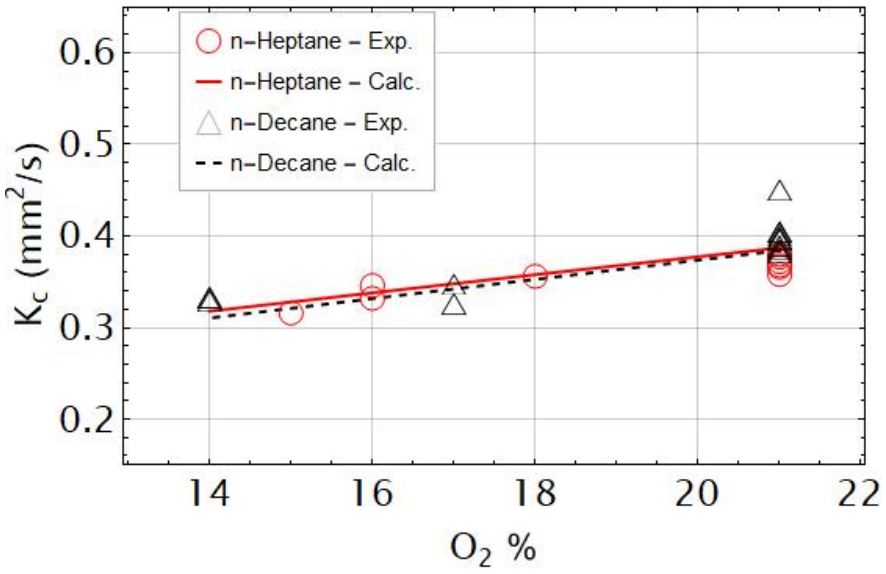
**Williams and Nayagam (Combustion and Flame (2020)*

Simplified Theoretical Model: Cool flame burning rate

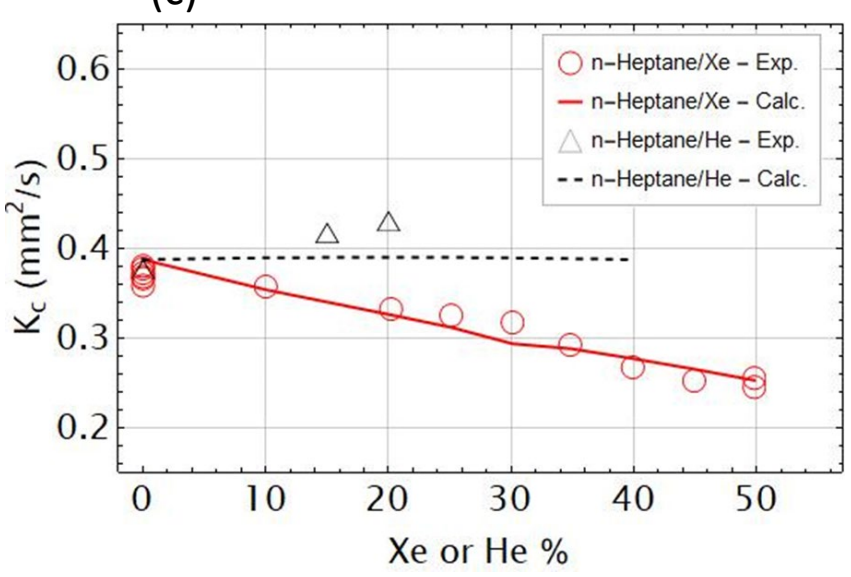
(a)



(b)



(c)



(a) 21% O_2 – He varies –displaces N_2

(b) O_2 varies –rest N_2

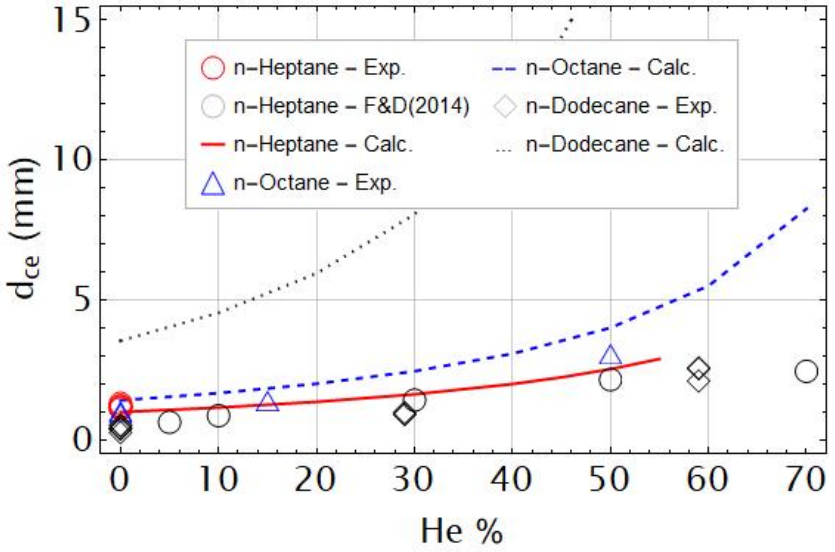
(c) Xe or He displaces air

For case (c) with He, the burning becomes highly transient – QS not valid

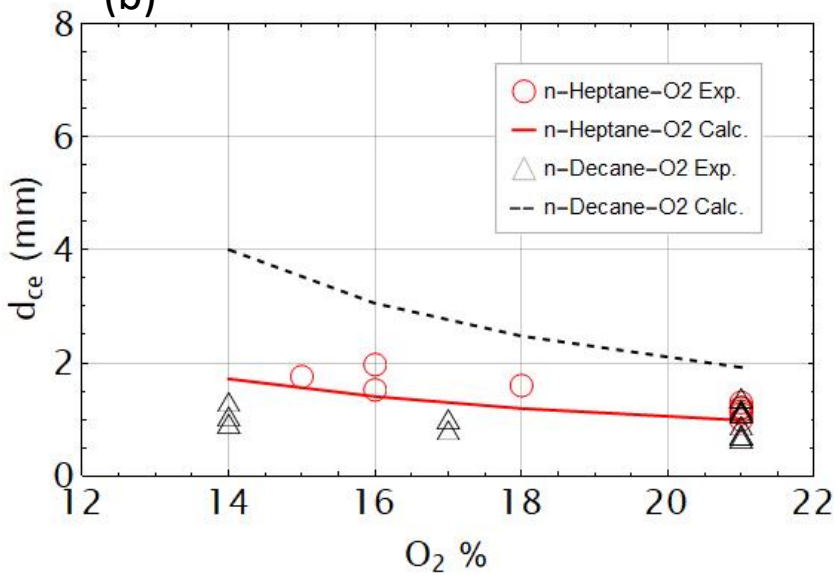
Nayagam, V., Dietrich, D. L., and Williams, F. A., Combustion and Flame (2021).

Simplified Theoretical Model: Cool flame extinction

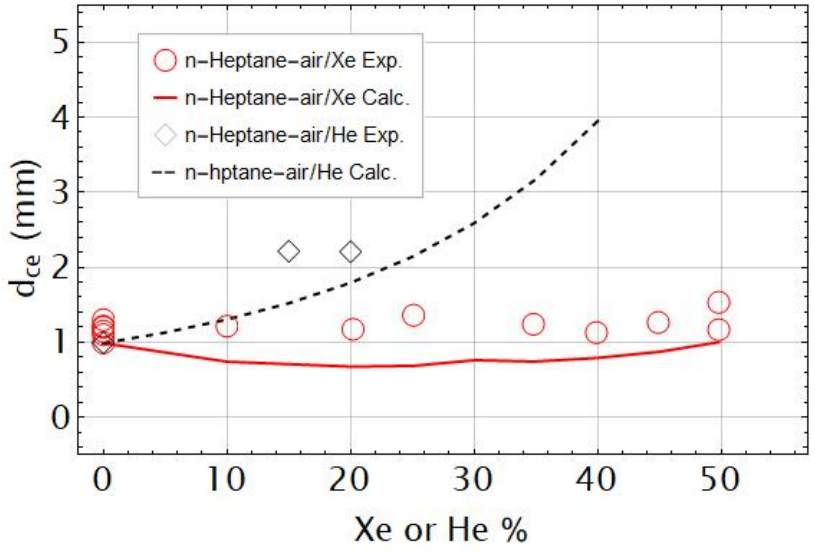
(a)



(b)



(c)



(a) 21% O_2 – He varies –displaces N_2

(b) O_2 varies –rest N_2

(c) Xe or He displaces air

Agreements for heptane and octane seem reasonable, but dodecane extinction diameters are over predicted appreciably.

Nayagam, V., Dietrich, D. L., and Williams, F. A., Combustion and Flame (2021).

Warm Flames at Elevated Pressures (CFI)

- Behavior changes when ambient pressure is increased.
  - Cool flame reignition
  - Warm flames

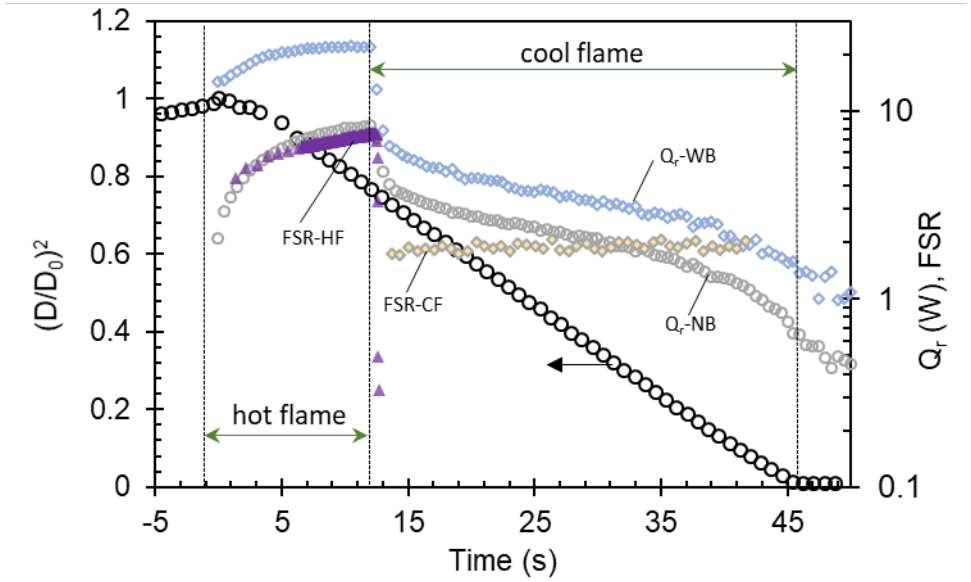
FLEX-1250:

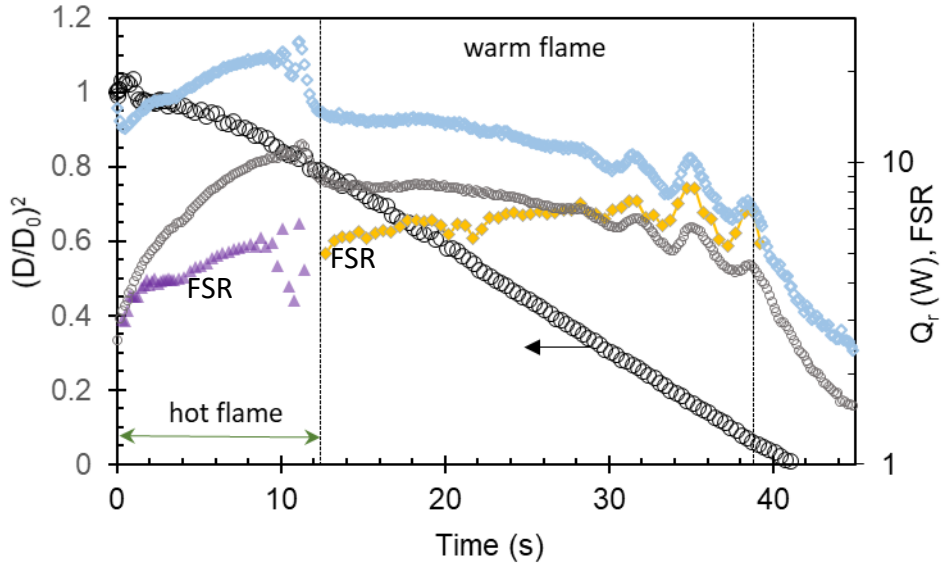
N-dodecane – Air -1 atm - D_0 = 4 mm
K_{HF} = 0.383 mm²/s
$D_{e,HF}$ = 3.55 mm
K_{CF} = 0.387 mm²/s
$D_{e,CF}$ = 0.40 mm

FLEX-1256:

N-dodecane – Air -3 atm - D_0 = 4.2 mm
K_{HF} = 0.350 mm²/s
$D_{e,HF}$ = 3.73 mm
K_{wF} = 0.491 mm²/s
$D_{e,wF}$ = 0 mm

- Warm flames are still not visible
- Flame temperature is higher than cool flame (radiation)
- Flame standoff ratio is higher (close to that of HF)
- Oscillatory extinction observed for the first time

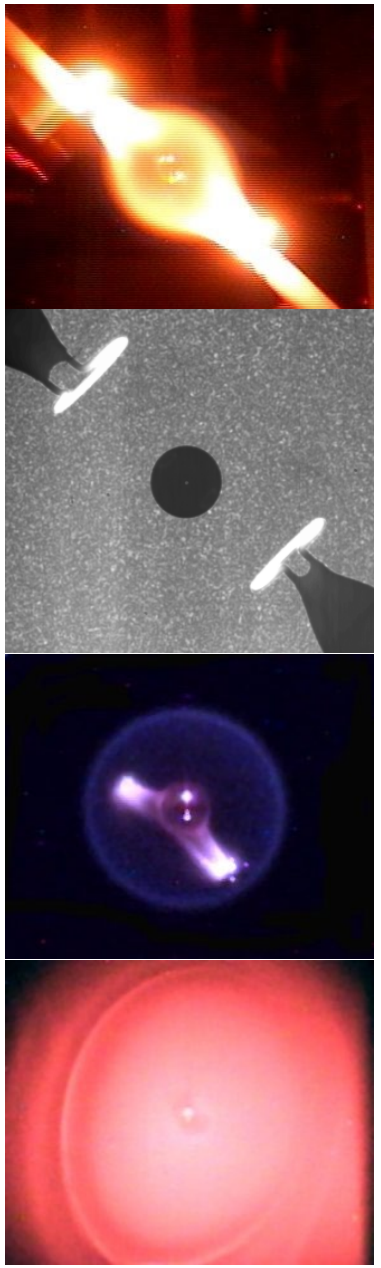




Farouk, T. I., Dietrich, D., & Dryer, F. L. (2019). Proceedings of the Combustion Institute.

Conclusions

- A wealth of experimental data with a variety of fuels, fuel mixtures, and ambient conditions (over 1500 tests)
- 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 warm flame) 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



Flame Extinguishment Experiment (FLEX) Science Team

Principal Investigator

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Project Manager

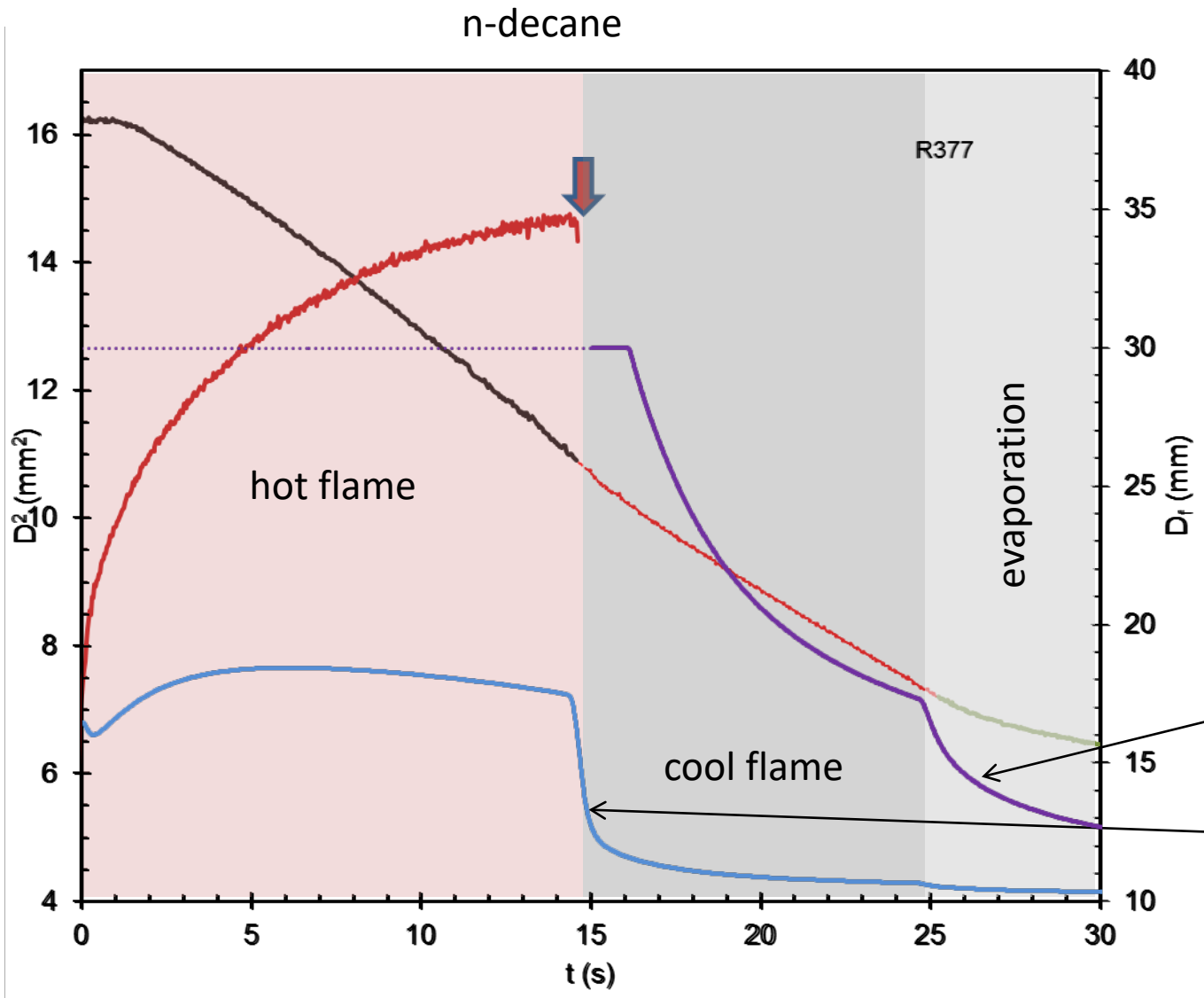
Mr. J. Mark Hickman, NASA GRC





Questions?

Quasi-steady Cool Flames (with radiometers)



- FLEX-377
  - N-decane
  - ½ atm
  - air
  - D_0 =4.0 mm
  - D_{hfe}=3.3 mm
  - D_{cfe}=2.7 mm

narrow-band radiation

wide-band radiation