Two-Stage Autoignition of Isolated n-Dodecane Droplets in Varying Ambient Oxygen Concentrations in Microgravity

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Understanding the mechanisms involved during autoignition of liquid fuels is of importance in many practical combustion devices, as well as in fire safety.
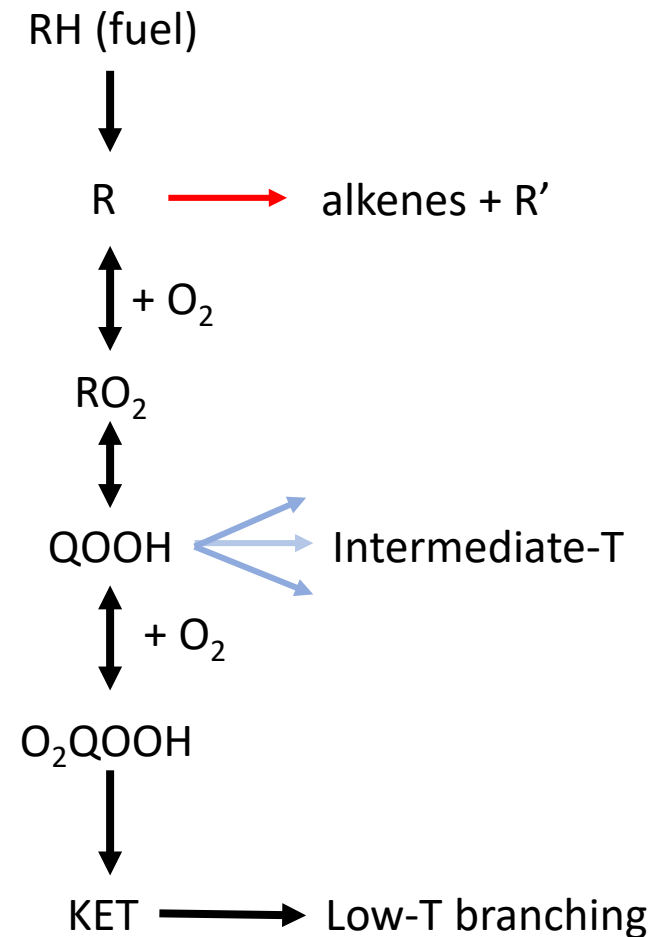
Normal alkane fuel droplets undergo two-stage ignition under certain conditions (Tanabe et. al), with the first stage controlled by low-temperature chemistry, while the second controlled by intermediate and high temperature reactions.

Our earlier study investigated droplet autoignition in air at varying ambient pressures and temperatures under normal gravity (Nayagam et. al 2020)

This study explores the variations in autoignition delay times for varying ambient oxygen levels for n-dodecane droplets in microgravity.
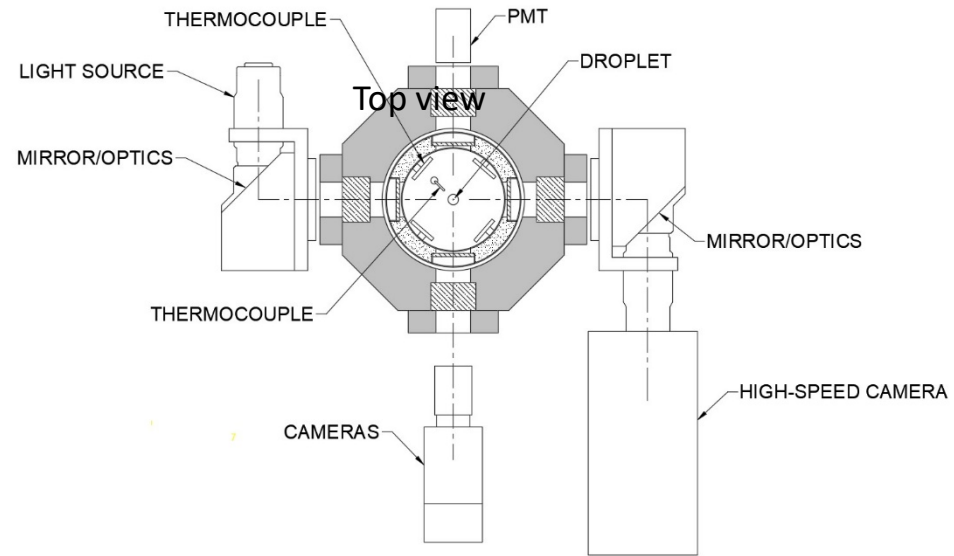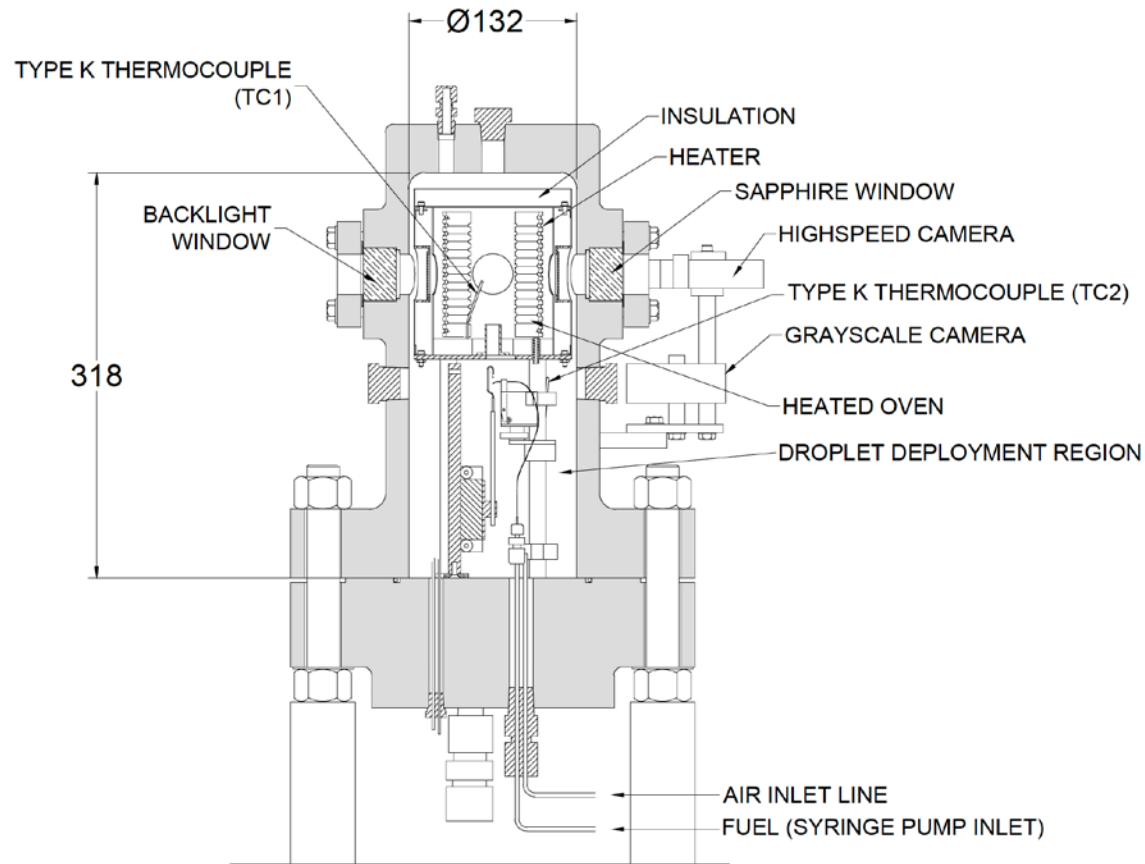
Experimental conditions (3atm, 650 K) chosen to get good separation between 1st and 2nd induction times

N-alkane oxidation
chemical kinetic pathways

RH (fuel)

R $\longrightarrow$ alkenes + R'

$+ O_2$

RO_2

QOOH $\longleftarrow$ Intermediate-T

$+ O_2$

O_2QOOH

KET $\longrightarrow$ Low-T branching

Westbrook (2009)

- Combustion chamber rated up to 100 bar and 1000 K
- Droplet view - high speed shadowgraph: 3000 fps
- Flame view - color camera: 300 fps
- Thermocouples

- Chamber is pressurized and preheated first
- Droplet is dispensed in the bottom chamber and inserted into the oven during free fall.

Fuel: N-dodecane, P= 3 atm, T_{oven} = 650 K

| Test #	X_{O2}	D_0 (mm)	τ_1 (s)	τ_t (s)	τ_2 (s)	V_{cf} (mm/s)
Z021	0.18	1.20	1.580	2.010	0.43	49
Z022	0.14	1.26	1.620	2.230	0.61	38
Z023	0.12	1.17	1.850	2.770	0.92	39
Z025	0.11	1.19	1.480	2.480	1.00	28
Z026	0.21	1.17	1.410	1.680	0.27	56
Z027	0.14	1.23	1.520	2.210	0.69	40
Z033	0.16	1.17	1.460	1.950	0.49	43
Z034	0.10	1.26	1.590	3.180	1.59	18
Z035	0.10	1.24	1.605	2.809	1.20	19
Z054	0.12	1.19	1.720	2.570	0.85	35
Z055	0.13	1.23	1.569	2.366	0.80	36
Z056	0.15	1.27	1.750	2.350	0.60	41
Z057	0.17	1.24	1.550	2.030	0.48	44
Z058	0.19	1.38	1.720	2.100	0.38	53
Z059	0.20	1.24	1.550	1.860	0.31	57

$$0.10 \leq X_{O2} \leq 0.21$$

τ_1 – first induction time (time between droplet entrance to the oven to the first observation of a cool flame)

τ_t – total induction time (entrance into oven to first observation of a hot flame)

$\tau_2 = \tau_t - \tau_1$ Second induction time

V_{cf} – Initial cool flame speed (with respect to lab coordinates)
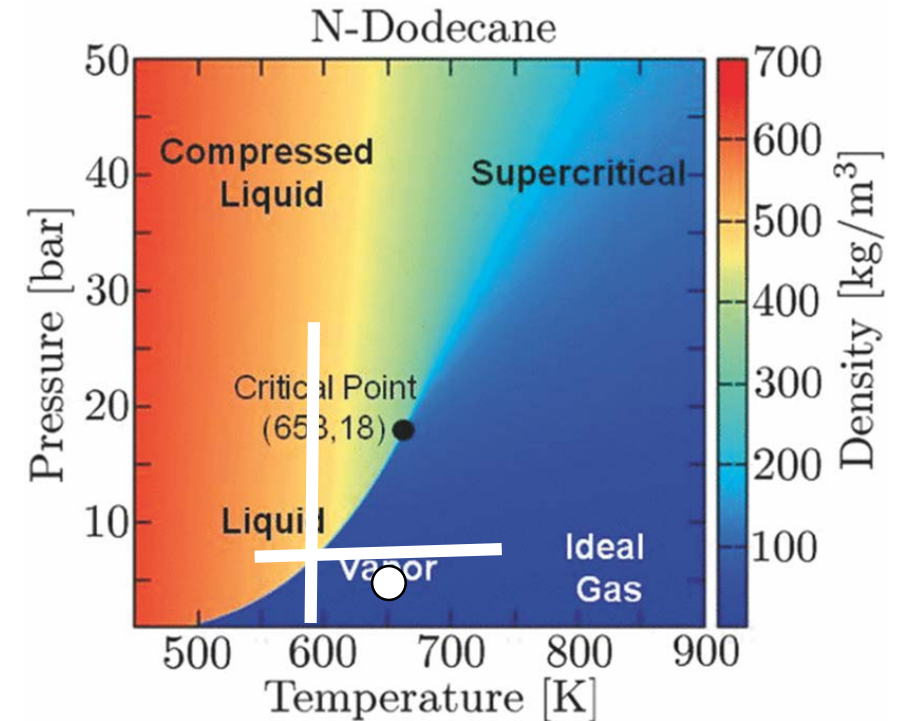
Induction Times

- Droplet autoignition involves evaporation of the fuel, followed my mixing with ambient oxygen, and then chemically controlled ignition

$$\tau_d = \tau_{phy} + \tau_{chem}$$

- Physical time remains essentially a constant for these experiments, since pressure and temperature are fixed and physical properties of O_2 and N_2 are very similar.

- Chemically controlled first induction time (e.g., in a PSR) is not sensitive to equivalence ratio. Controlled by KET decomposition reaction.

- Therefore the first induction time for the droplet, τ_{d1} remains essentially a fixed irrespective of the ambient O_2 mole fraction.

- For comparison – case where T_O varies with P at 3 atm from our earlier results at 1g (Rose et al. 2021)

N-dodecane, P= 3 atm, T_o = 650 K
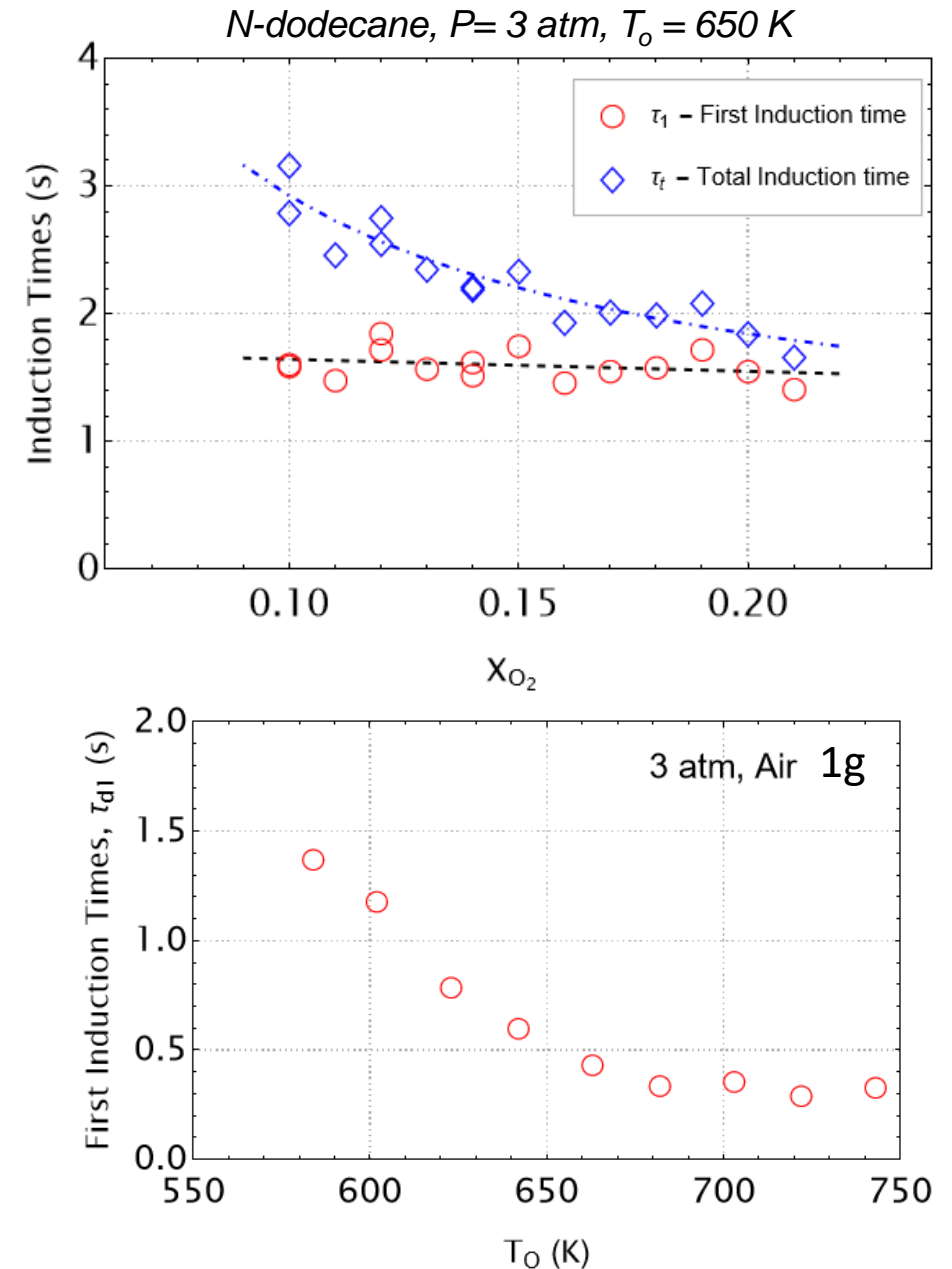
- Hot flame ignition takes place in the wake of the cool flame, where preheated, and partially oxidized products exist.
- The 2nd droplet induction time, τ_{d2}, depends entirely on the kinetics (Schnaubelt, Mastorakos, etc.)

- Fit shows: $\tau_{d2} \sim X_{O_2}^{-2.6}$

- Also, the heat release during first induction decreases as O_2 decreases (T_{cf} is lower) and that leads a longer 2nd induction time. (depends on the equivalence ratio too!)

- For comparison – case where T_O varies with P at 3 atm from our earlier results at 1g (Rose et al. 2021)

- 2nd induction time depends both on X_{O_2} and temperature

N-dodecane, P= 3 atm, T_o = 650 K

1g
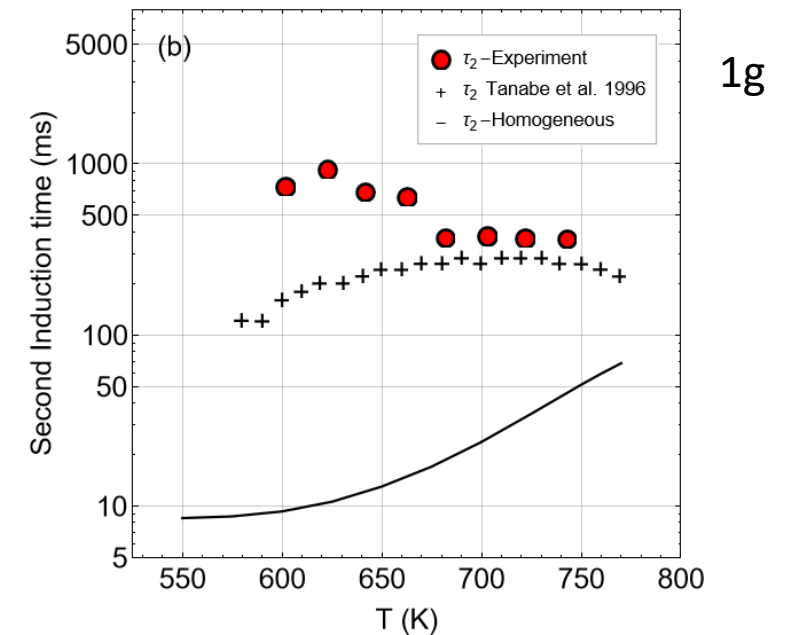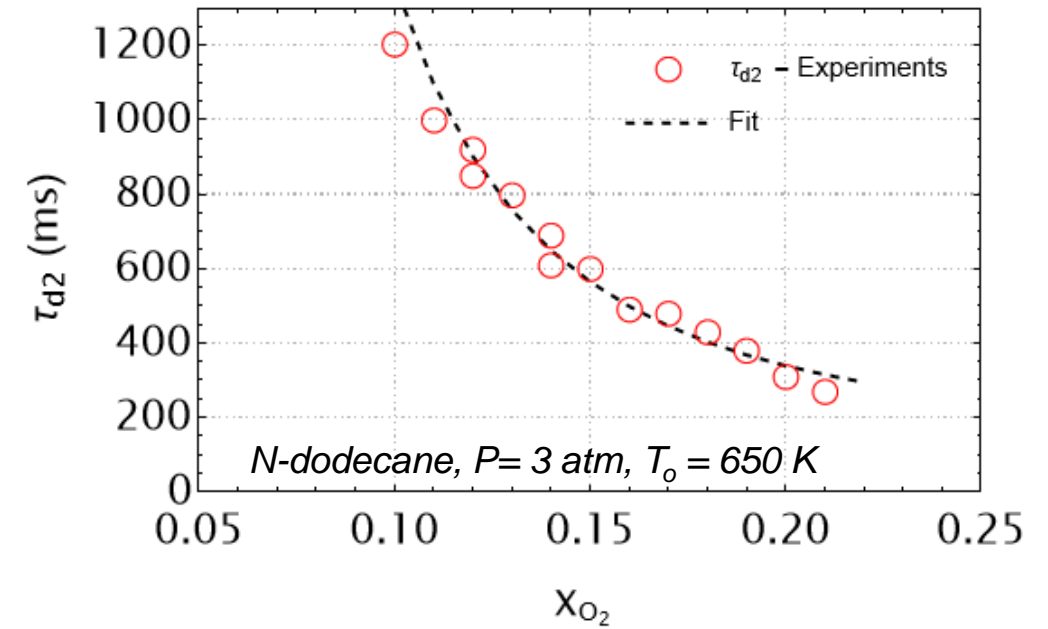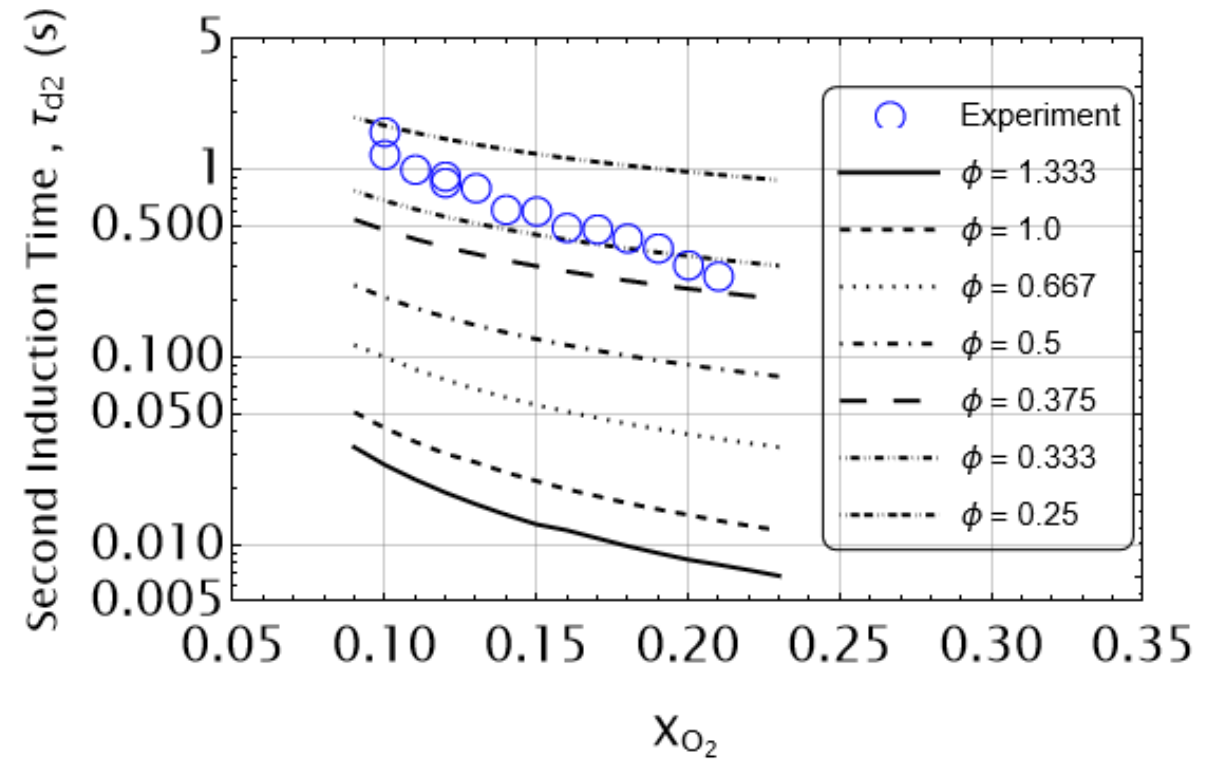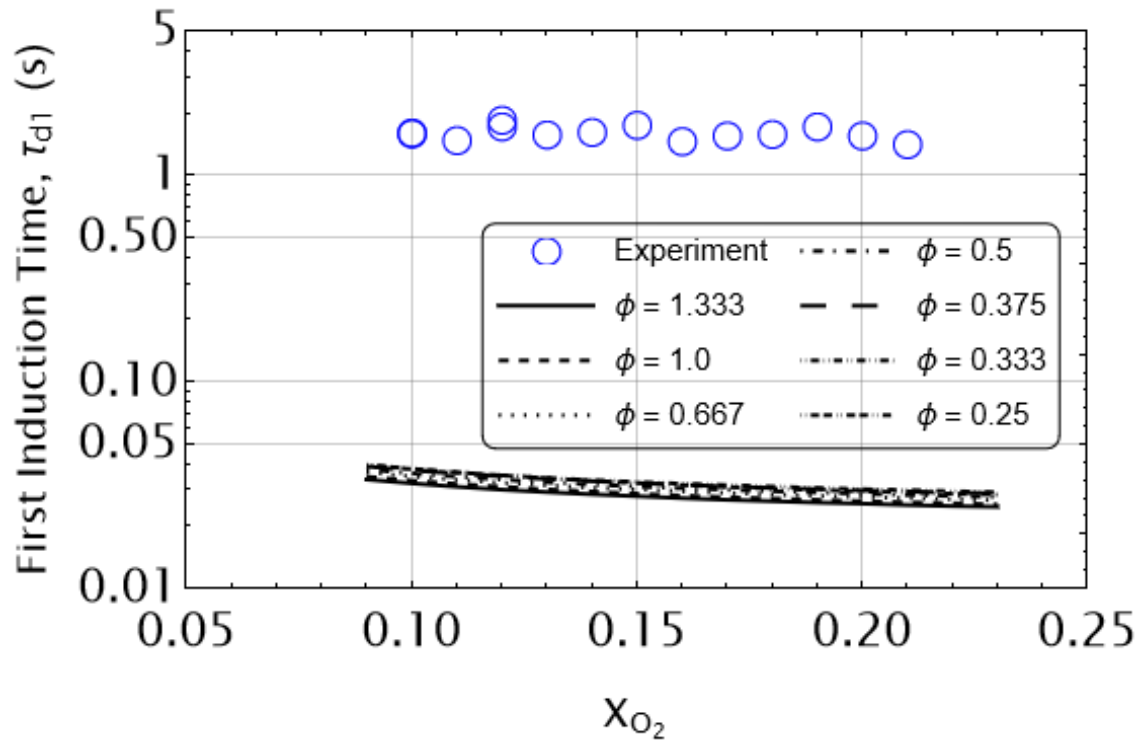
o The physical time and the chemical time effects can be distinguished by comparing against PSR induction times with detailed chemistry calculations for the corresponding conditions

o Since we don't know the equivalence ratio of the mixture surrounding the droplet, we vary it as a parameter for PSR calculations

o Agrees with the idea that cool flame ignition starts in the fuel lean conditions
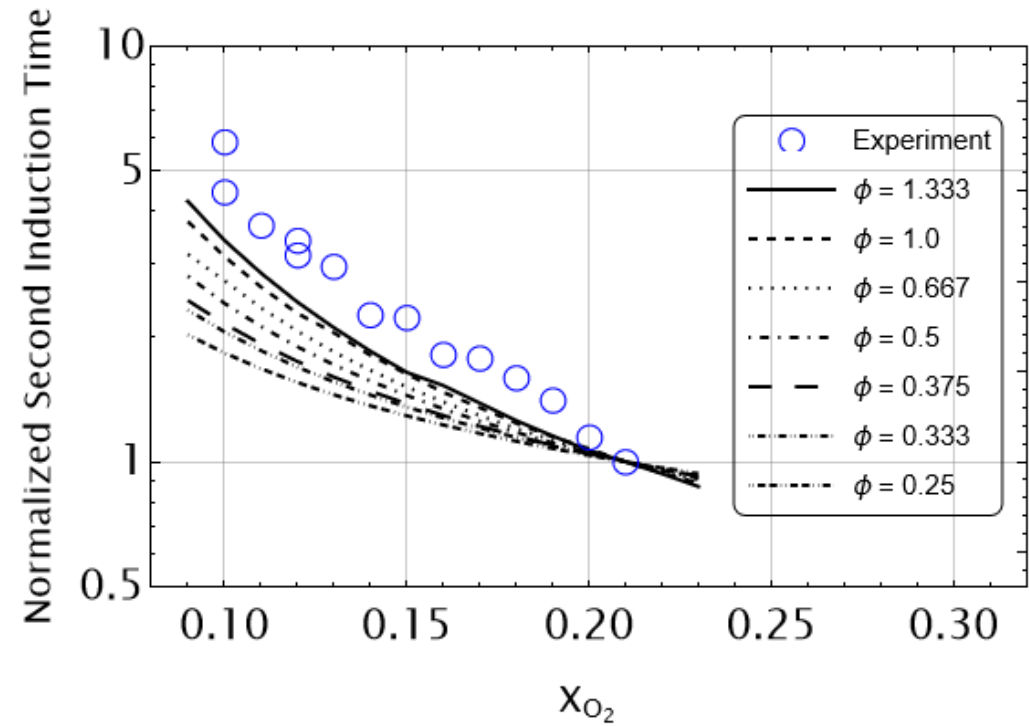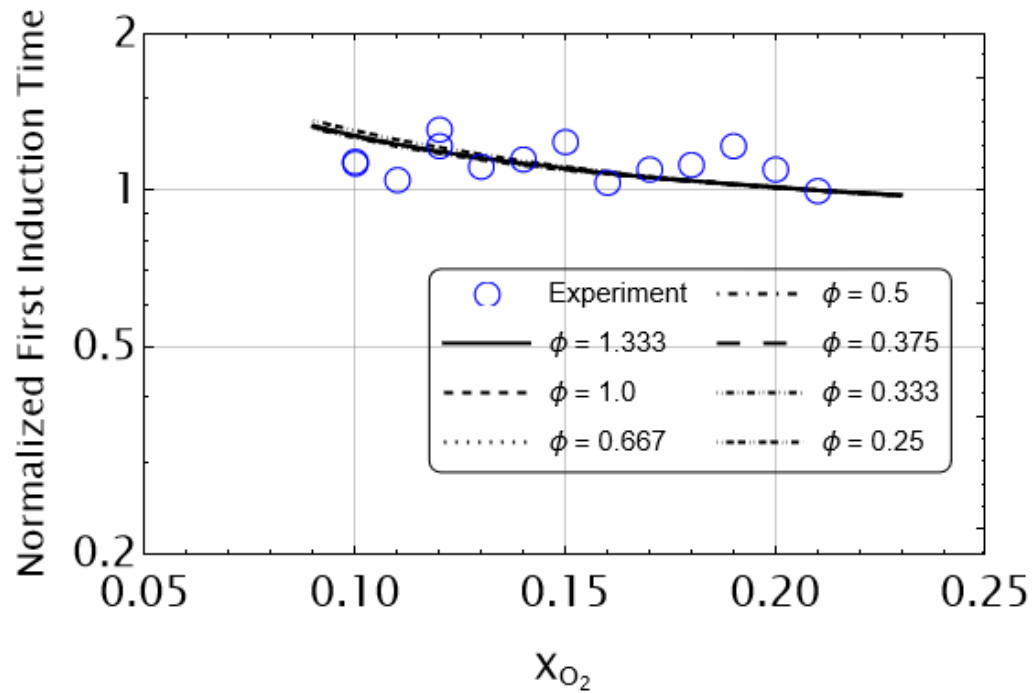
o When the physical effects are scaled out by normalizing w.r.t 21% O_2case, PSR calculations predict first induction time well.

o The second induction time seems to show the effective equivalence ratio changes with oxygen concentration
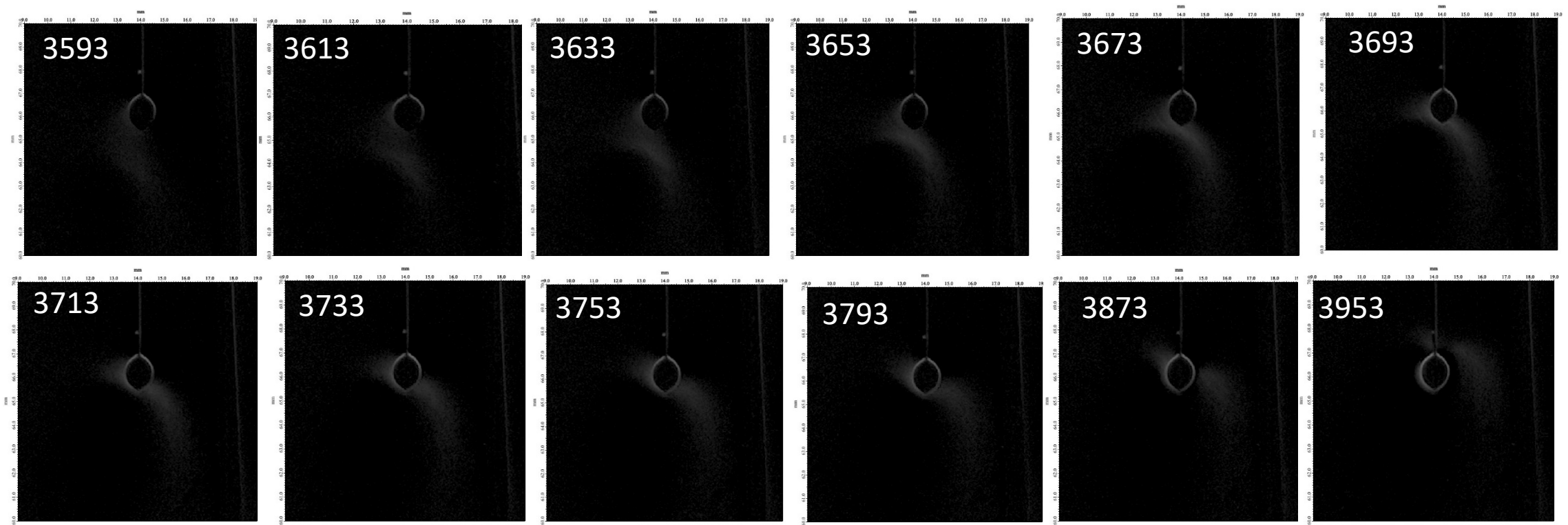
Dynamics of Two-stage Ignition

Run:Z026

Fuel: N-dodecane, P= 3 atm, T_{oven} = 650 K, Air(21% O_2)
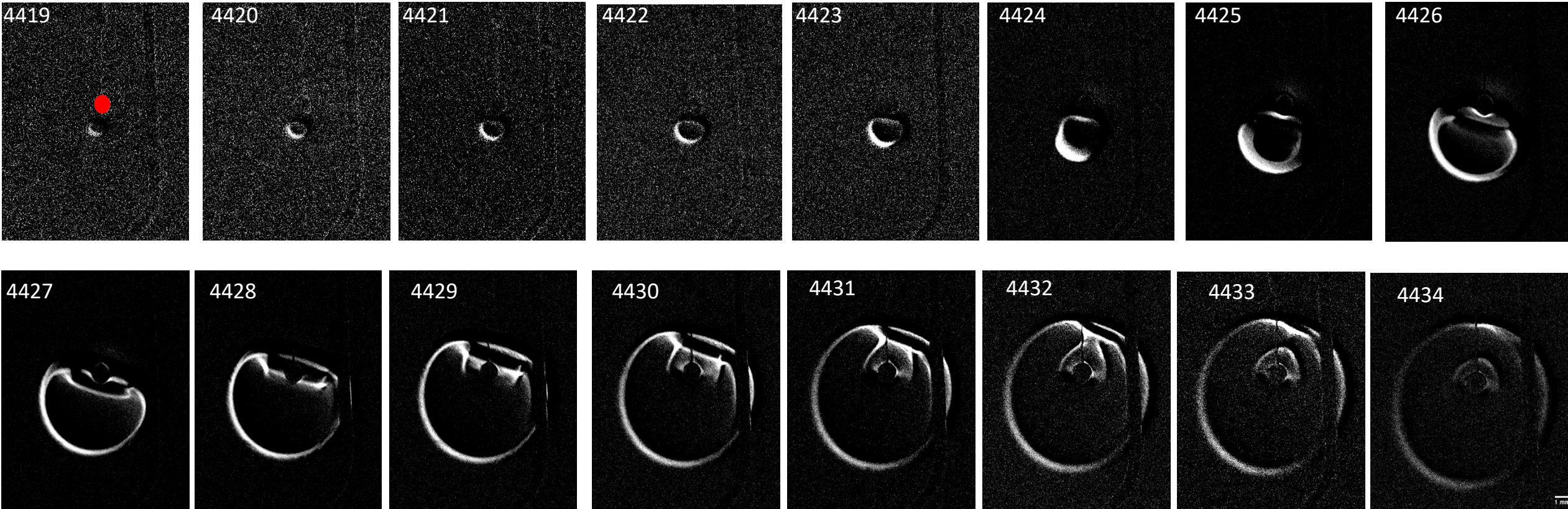
Δt = 6.7 ms

Initial flame acceleration toward the droplet, slight pause, then surrounds the droplet

2D projection of a 3D process

Hot-Flame Autoignition Dynamics

Run:Z026

Fuel: N-dodecane, P= 3 atm, T_{oven} = 650 K, Air(21% O_2)

$\Delta t = 0.3$ ms


Much faster than cool flame

Cool Flame Ignition and Propagation

- Interpretation of cool flame propagation in this spherical geometry is complicated
- Cool flame initiation occurs at a narrow region on the flammable spherical surface surrounding the droplet and it propagates both radially inward toward fuel rich conditions as well as along the flammable surface.
- The shadowgraph is a 2D projection of this complex flame-front evolution and depends on the flame origin location and the camera view angle

time

propagation
(along the curved flammable surface)

Front propagation (lean to rich mixture)

oxygen
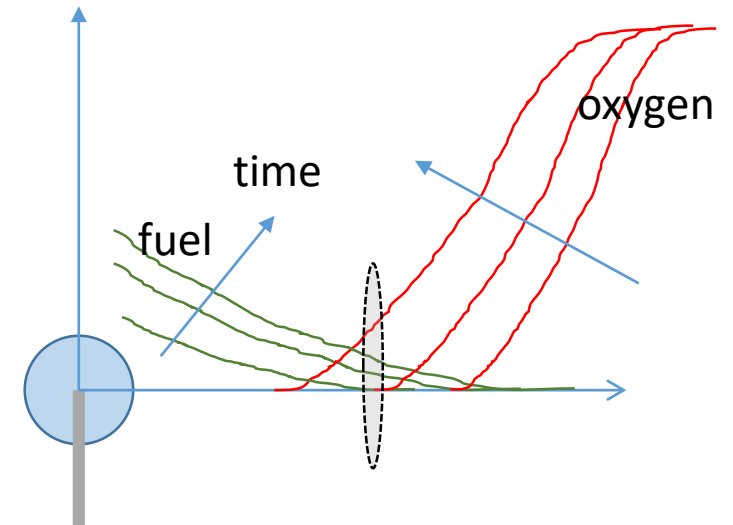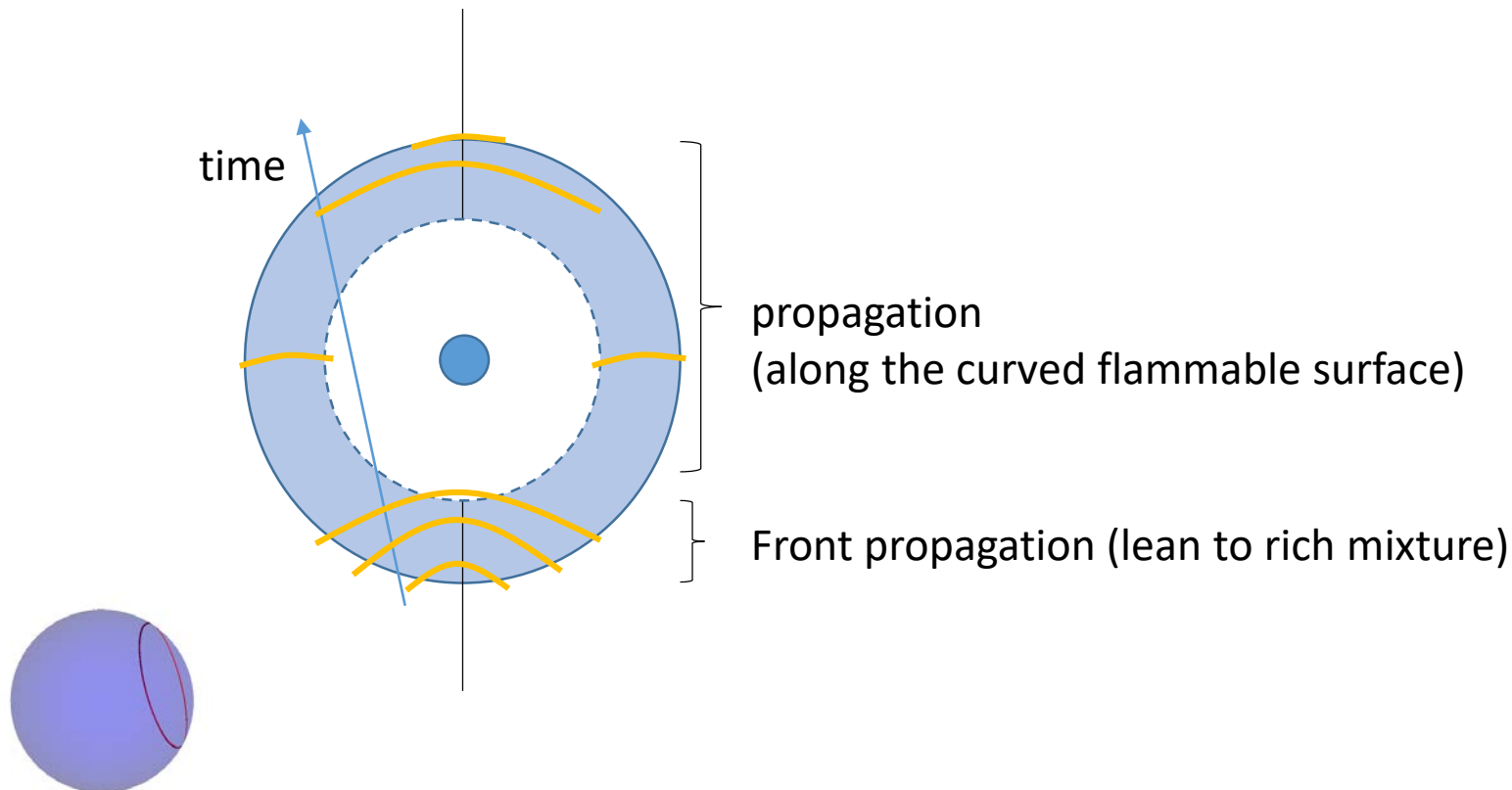
time

fuel

Cool Flame Ignition and Propagation

- Fuel: N-dodecane, P= 3 atm, T_{oven} = 650 K

- Cool flame location is tracked as function of time from inception until it reaches the droplet surface
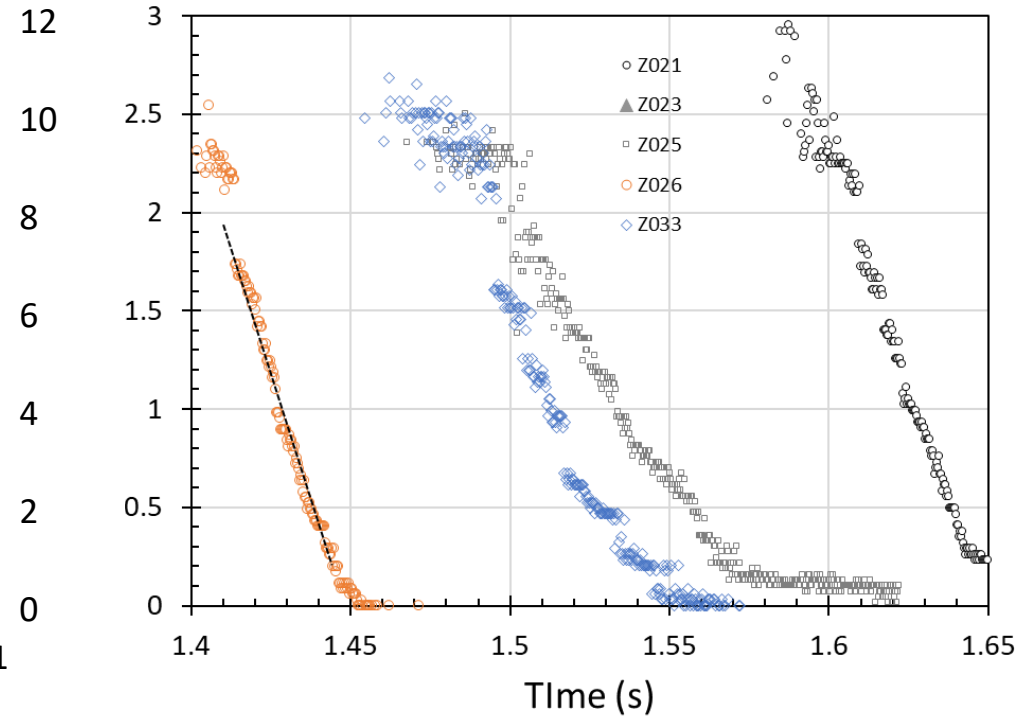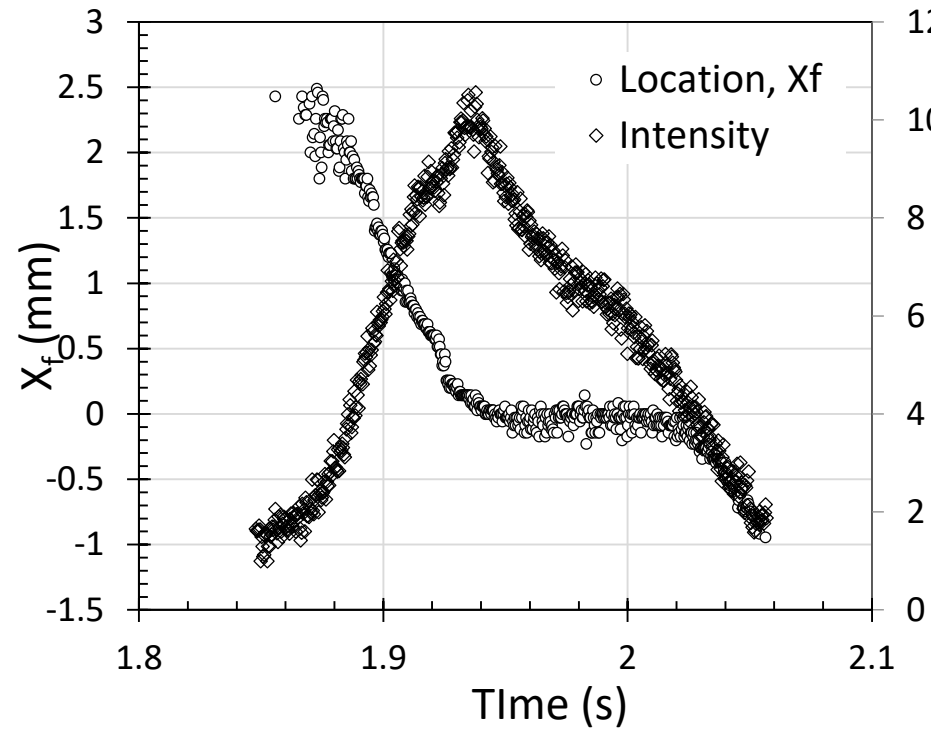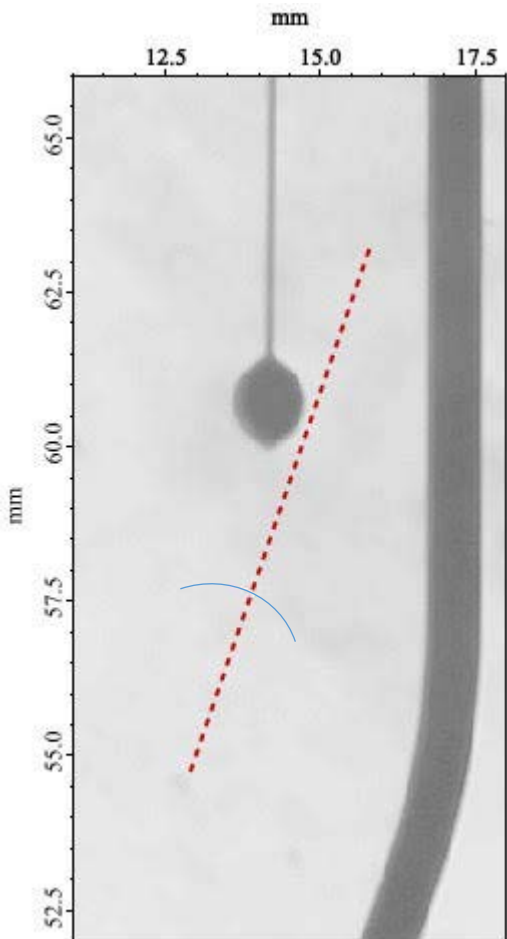
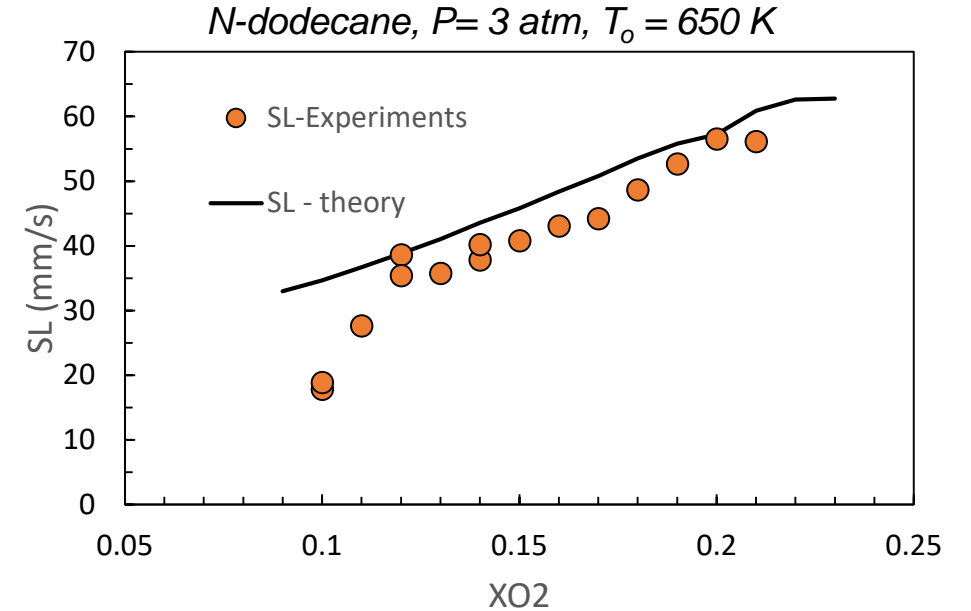A Theoretical model with simplified 6-step mechanism
yields an expression for CF spread velocity

No.	Reaction	A C7H16 and C8H18	A C10H22 and C12H26	T_a (K)
		Rate parameters		
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

N-dodecane, P= 3 atm, T_o = 650 K

$$S_L = \frac{T_f}{T_a(T_f - T_u)} \frac{\rho_f}{\rho_f} \sqrt{2 L_K D_f \, A \, e^{-(\frac{T_a}{T_f})}}$$

V. Nayagam, F.A. Williams, D.L. Dietrich, Combustion Theory and Modelling (2021-accpted)

Concluding Remarks

o N-dodecane droplet autoignition characteristics were experimentally investigated for the first time in a microgravity environment.

o First and second induction times, as well as initial cool flame propagation speed were obtained as a function of ambient oxygen concentration in an O_2/N_2 environment at fixed pressure (3 atm) and temperature (650 k).

o First induction time is insensitive to oxygen variations, while the second induction time varies as $X_{O_2}^{-2.6}$, for the range studied.

o Homogeneous mixture calculations can be used to correlate the first induction time, but the second induction time depends on the effective equivalence ratio that seems to vary with the ambient oxygen concentration.

o A simplified theory seems to correlate the cool flame propagation speed, when the cool flame temperature is specified (from homogeneous calculations)