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Understanding the interplay between pilot fuel mixing and auto-ignition chemistry in hydrogen-enriched environment

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Sandia National Laboratories

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Understanding the interplay between pilot fuel mixing and auto-ignition chemistry in hydrogen-enriched environment

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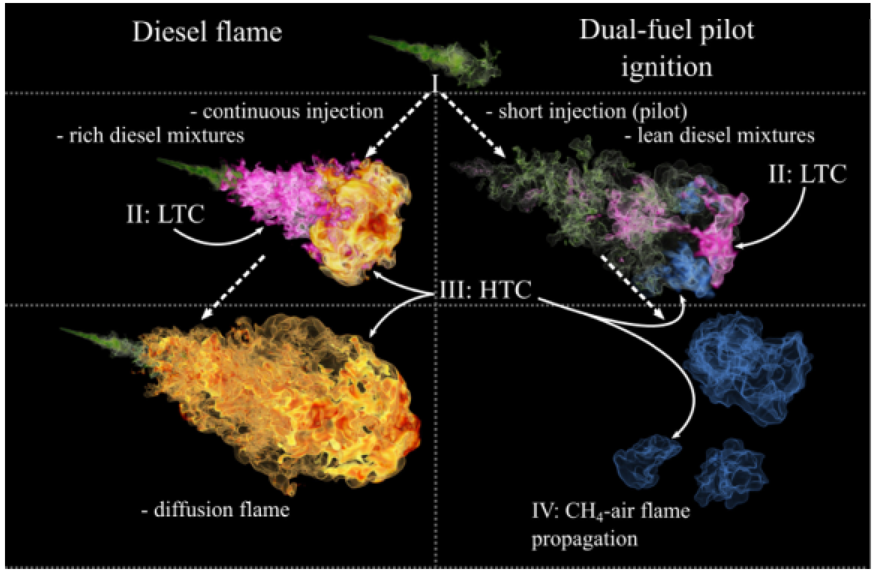
Diesel-Piloted Dual Fuel (DPDF) Combustion Strategy

Diesel-Piloted Dual-Fuel (DPDF) System

Combustion initiated by short pilot injection of highly reactive liquid fuel (diesel) into lean premixed primary fuel-air mixture charge.



• H. Kahila et al. (2019)

Inhibitive effect of H_2 on n-heptane auto-ignition chemistry

Combustion in a highly stratified environment

- Temperature: pilot-fuel vaporization cooling
- Equivalence ratio: partial mixing of pilot-fuel

→ Complex physical and chemical effects govern a spatio-temporal evolution of dual fuel auto-ignition process.

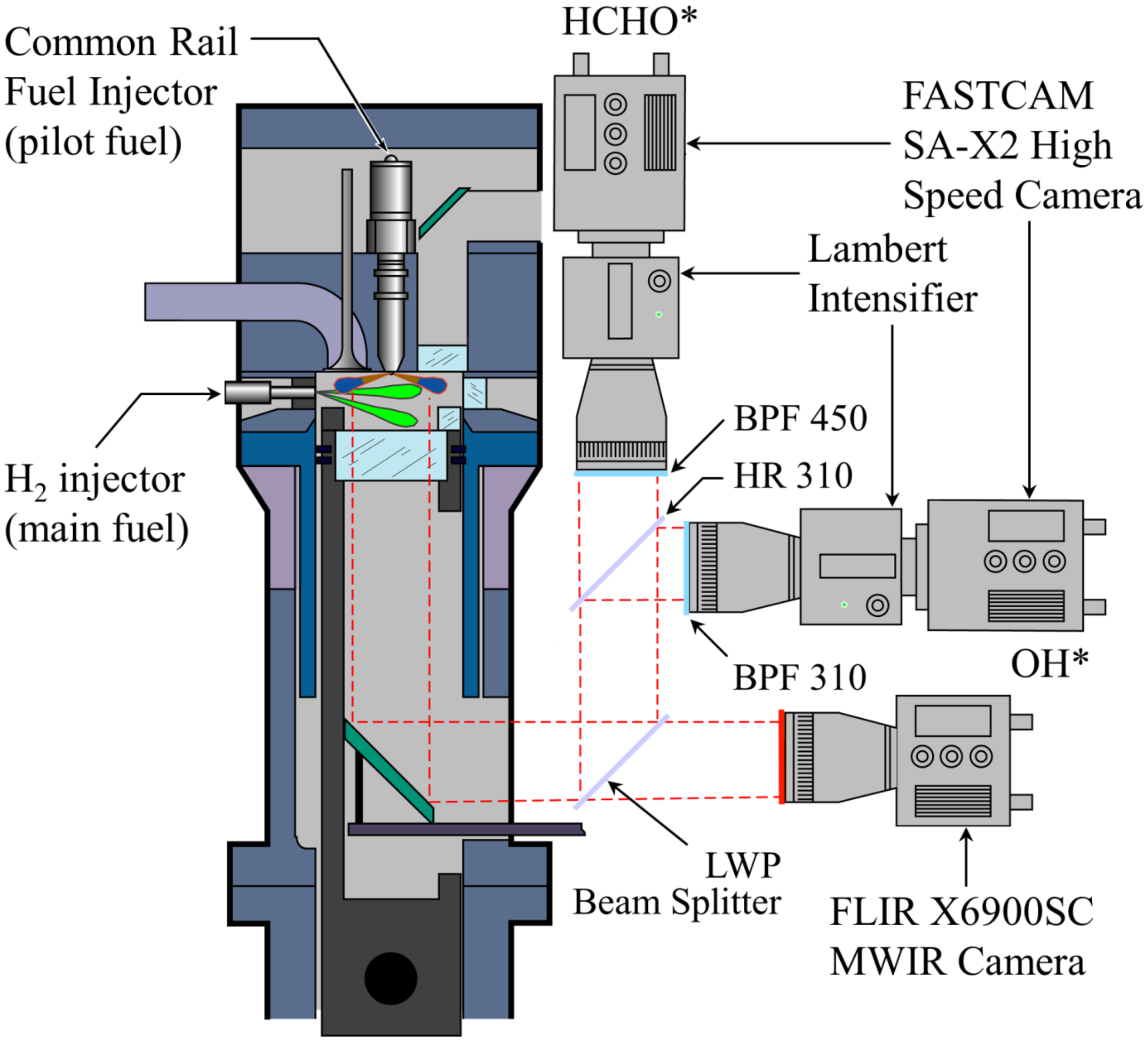
However, it is challenging to anticipate the dual-fuel combustion characteristics of H_2 as a primary fuel

: Low minimum ignition energy (**Pre-ignition**) vs Strong inhibition effect (**Longer ignition delay**)

Research Objective

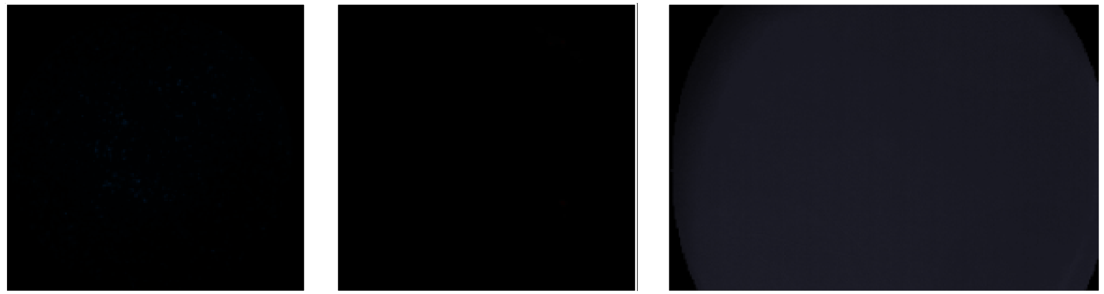
"Understanding the interplay between the physical and chemical processes that govern ignition of pilot fuel jet in the presence of lean-premixed H_2/air mixture, complemented with zero-dimensional chemical kinetics and one-dimensional spray dynamics simulation."

Experimental Setup



Schematic of heavy-duty optical engine with high-speed imaging setup

HCHO* OH* Infrared (IR)

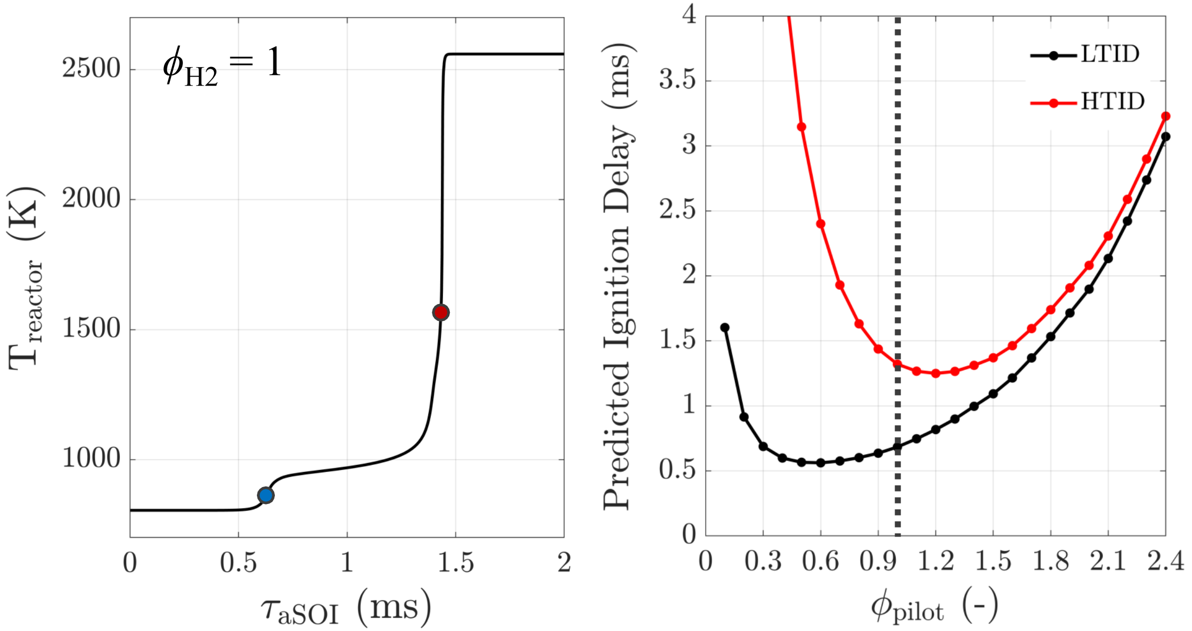


Operating Conditions

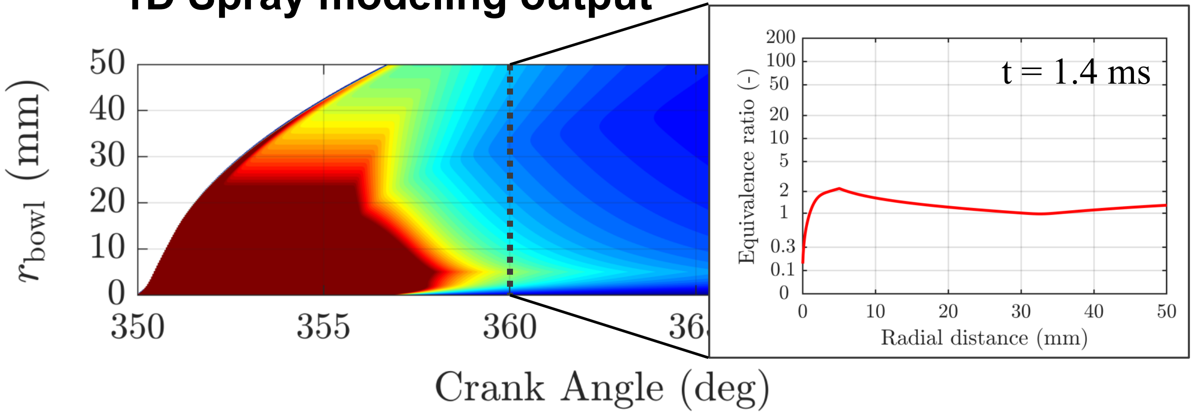
Intake conditions	100 ºC, 100 kPa, 21% O_2
Engine speed	1200 RPM (1 °CA ≈ 138 μs)
Fuel type	**Pilot fuel**: n-heptane **Main fuel**: Hydrogen
Injection timing	Pilot: 347 CAD (*TDC: 360 CAD) Main (H_2): 60 CAD (*homogeneous mixing)
Pilot fuel, Inj. parameters	**Case 1**: P_{inj}: 800 bar, t_{inj}: 760 μs (21 mg) **Case 2**: P_{inj}: 800 bar, t_{inj}: 500 μs (7.9 mg) **Case 3**: P_{inj}: 400 bar, t_{inj}: 760 μs (8.8 mg)
Main fuel, H_2 Inj. parameters	**ϕ_{H2}: 0 to 0.4 ($\Delta\phi_{H2}$ = 0.1)** P_{inj}: 40 bar, t_{inj}: 711 to 2844 μs

Experimental Setup

0D CHEMKIN output



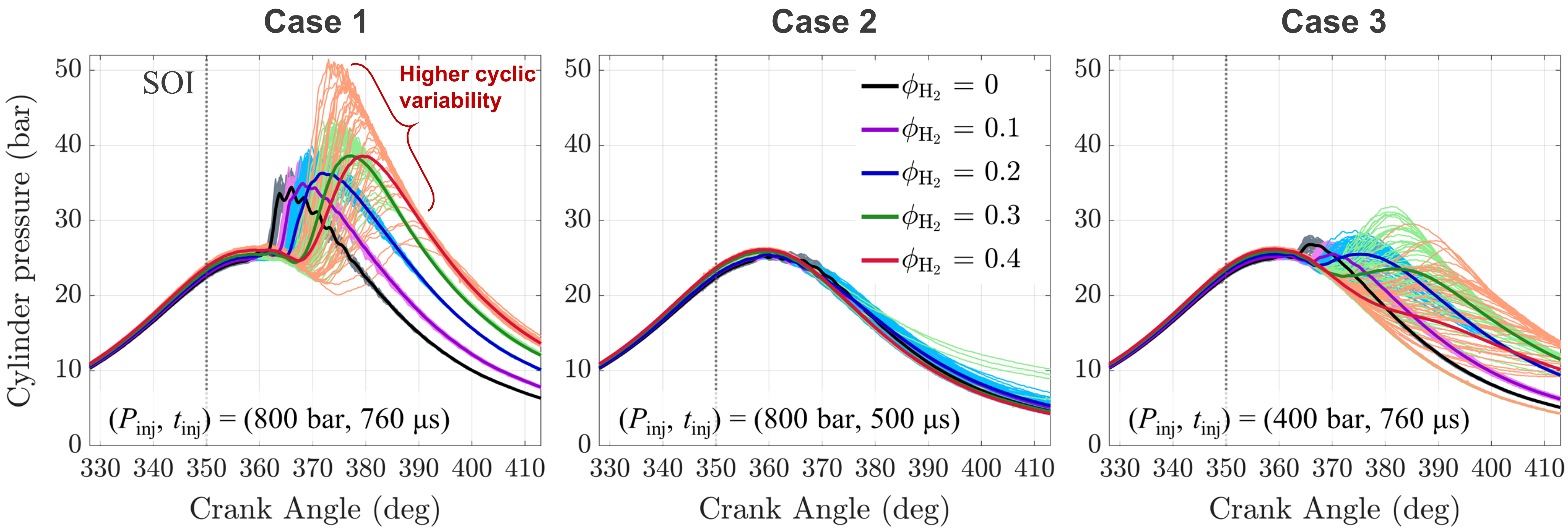
1D Spray modeling output



0D/1D Simulations

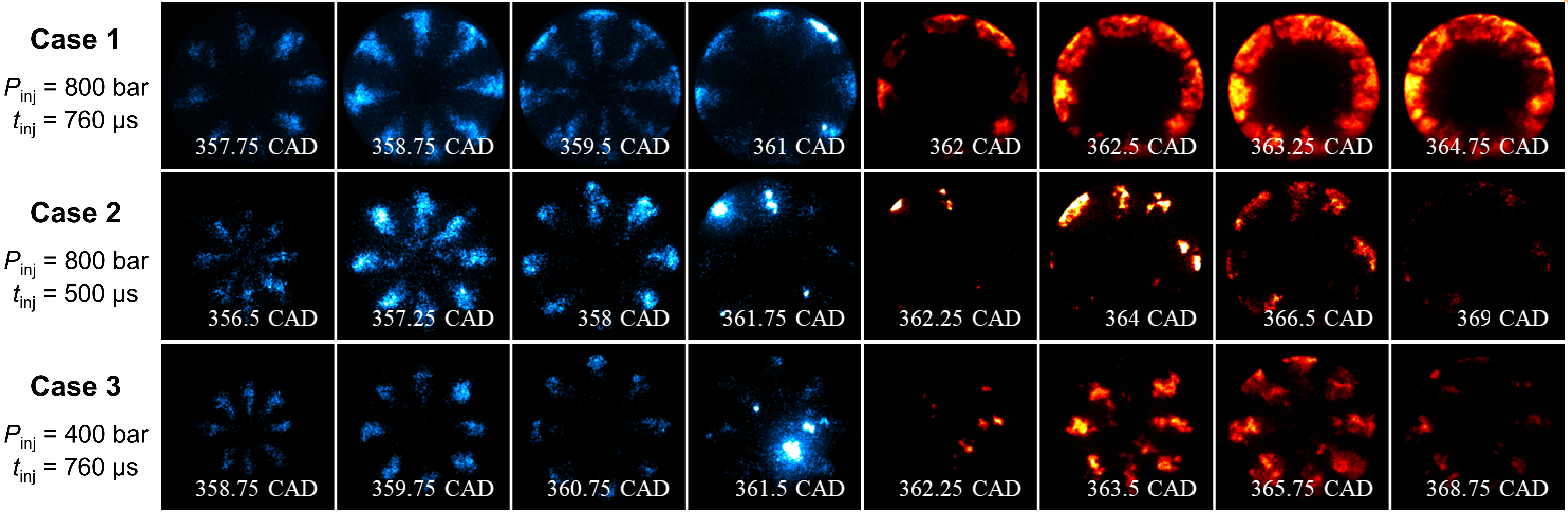
Chemical Kinetics Simulation	ANSYS CHEMKIN-pro software using 0D Closed Homogeneous Reactor (CHR) model, coupled with *LLNL detailed n-heptane mechanism ver. 3.1* (*accounted for the pilot fuel vaporization cooling effect)
Output (0D)	• *Temperature* • *Volumetric heat release rate* • *Chemical species* • *Reaction rates*
Computational Spray Modeling	1D jet model with a variable profile approximation for radial mixing and velocity distribution (also known as the *Musculus and Kattke model*)
Output (1D)	• *Equivalence ratio distribution* • *Jet penetration length* • *Mean velocity* • *Air entrainment rate*

Pressure traces with respect to the injection parameters



- Increasing the H_2 concentration results in two noticeable effects: **1) prolonged ignition delay** (inhibitive effect on pilot fuel ignition) and **2) higher cyclic variability** (low minimum ignition energy & ultrafast flame speed)
- The impact of reduced fuel mass (~60% relative to Case 1) in Case 2 and 3 manifests as a decrease in the maximum in-cylinder pressure and pressure rise rates.
- Contrary to Case 2, the longer injection can initiate successful ignition in most cycles except for few misfires at ϕ_{H2} = 0.4, while the influence of H_2 on pilot ignition delays is more pronounced in Case 3.

Two-stage auto-ignition process of pure pilot injection case



- For the single pilot fuel injection, first-stage ignition starts downstream of the eight fuel jets and propagates towards upstream, followed by near-wall, second-stage combustion.
- Reduced injection duration in Case 2 results in enhanced fuel-air mixing, leading to an earlier onset of LTHR near nozzle (~356 CAD) and a limited flame kernel development (fuel leaning out).
- Lower injection pressure and associated slower mixing contribute to: 1) the delayed onset of LTC (~359 CAD) and 2) second-stage ignition predominantly occurring upstream of the spray tip.

Impact of hydrogen on two-stage auto-ignition chemistry

Case 1

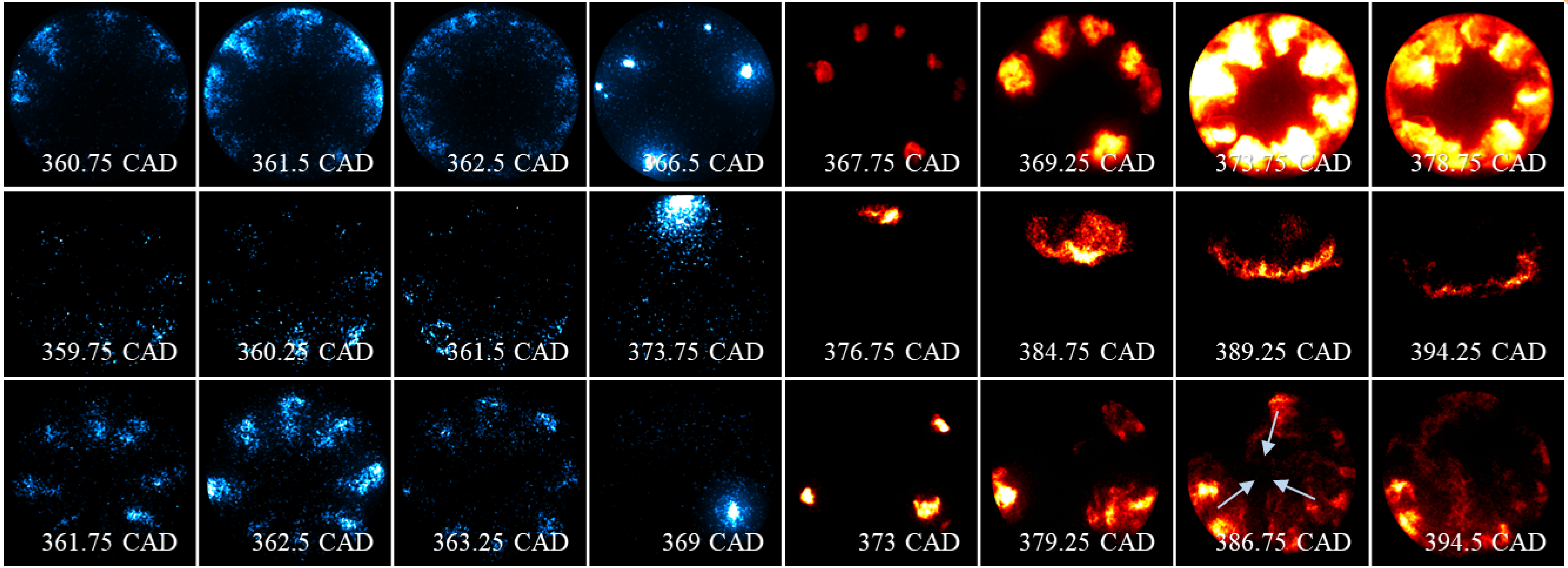
P_{inj} = 800 bar
t_{inj} = 760 µs

Case 2

P_{inj} = 800 bar
t_{inj} = 500 µs

Case 3

P_{inj} = 400 bar
t_{inj} = 760 µs



- In general, due to the strong inhibitive effect of H_2, an increased mixing time induces the delayed onset of low temperature combustion in the vicinity of the wall without recession, and not all pilot fuel jets proceeds to the second-stage auto-ignition.
- With reduced amount of pilot fuel injection (Case 2 & 3), the formation of flame kernel is significantly delayed and successfully initiated by few pockets with sufficient pilot fuel concentration.

→ ***"Importance of stochastic rich fuel pockets"***

Evolution of auto-ignition process: only pilot injection

Case 1

347.0 CAD

P_{inj} = 800 bar, t_{inj} = 760 μs

Case 2

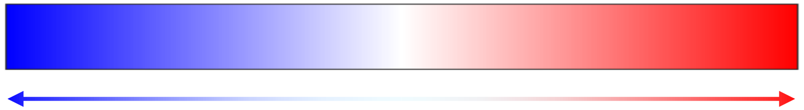
347.0 CAD

P_{inj} = 800 bar, t_{inj} = 500 μs

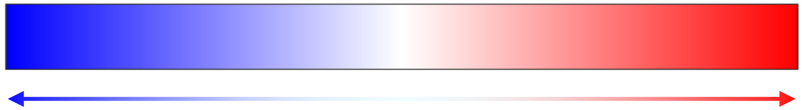
Case 3

347.0 CAD

P_{inj} = 400 bar, t_{inj} = 760 μs

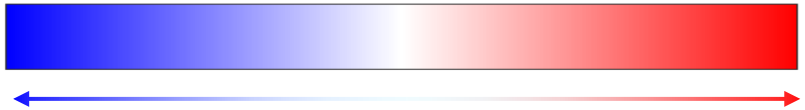


I_{HCHO*} I_{OH*}



I_{HCHO*} I_{OH*}

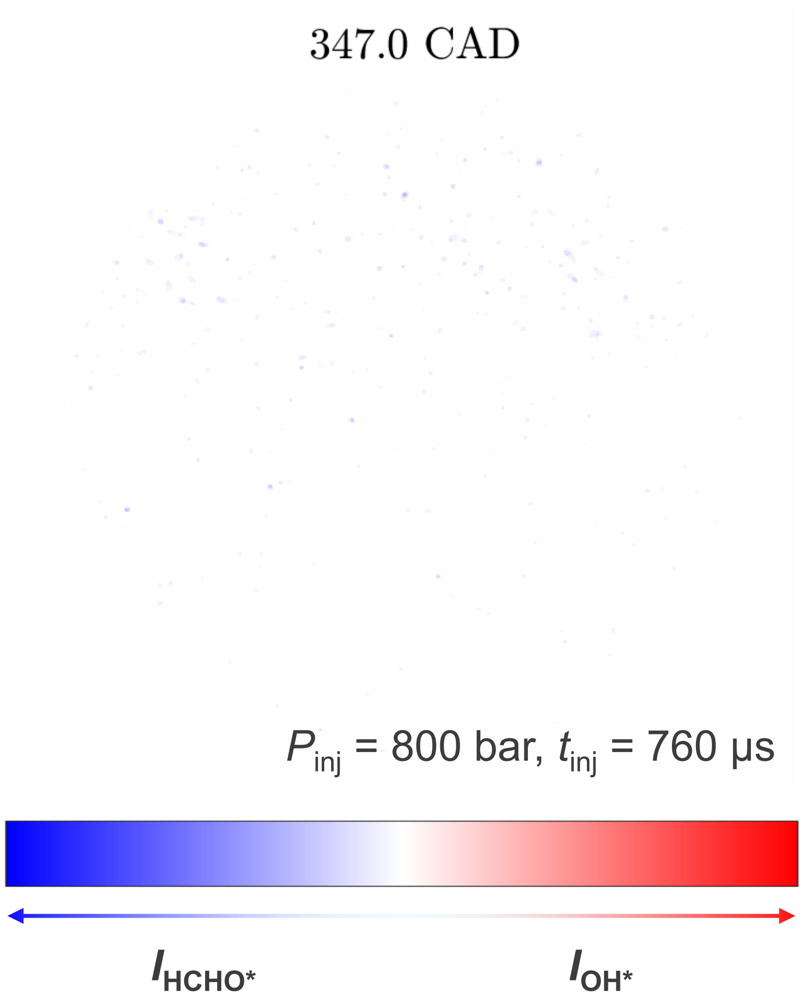
"LTC regime" **"HTC regime"**



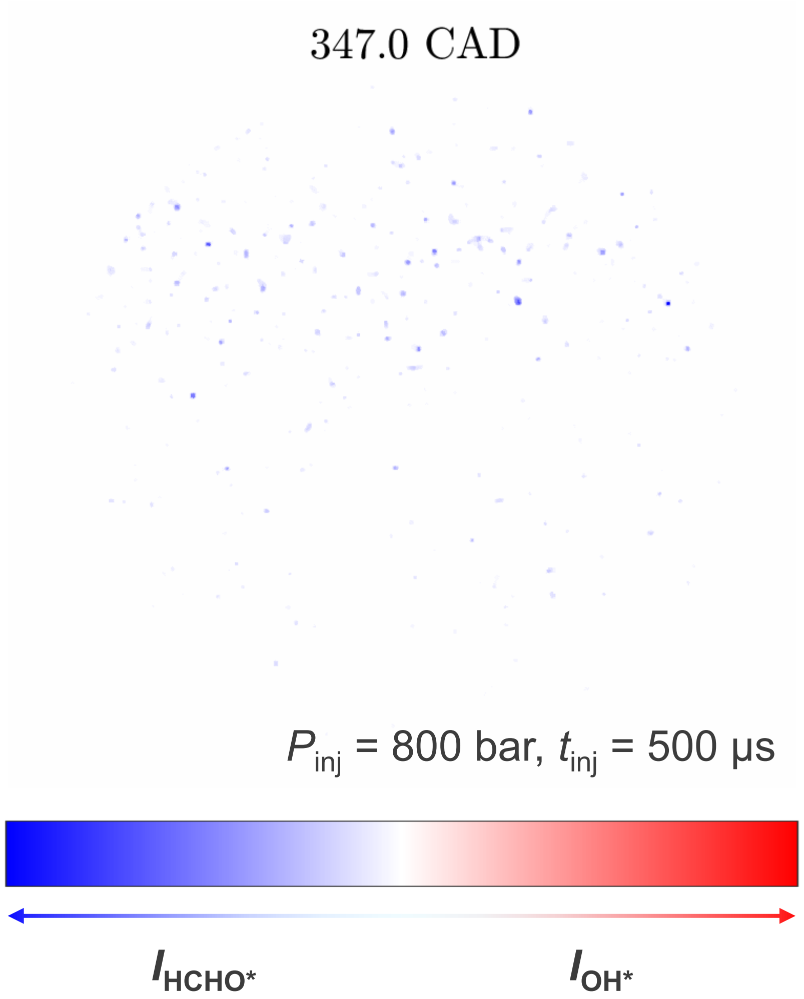
I_{HCHO*} I_{OH*}

Evolution of auto-ignition process: H_2 dual-fuel operation

Case 1

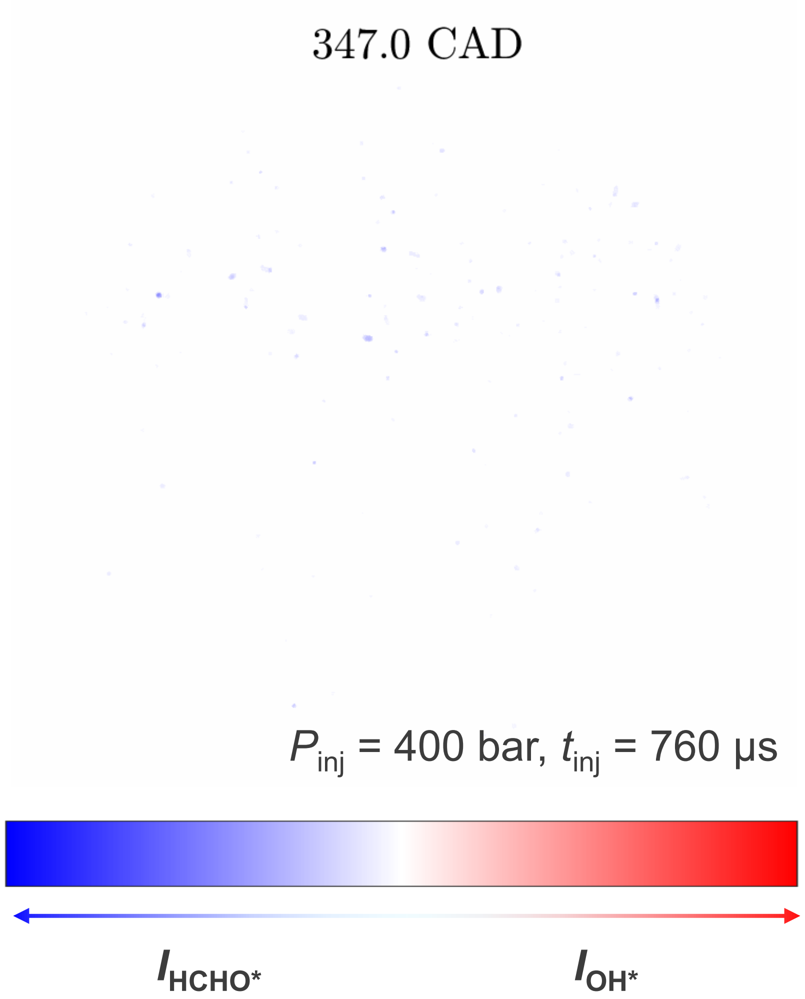


Case 2

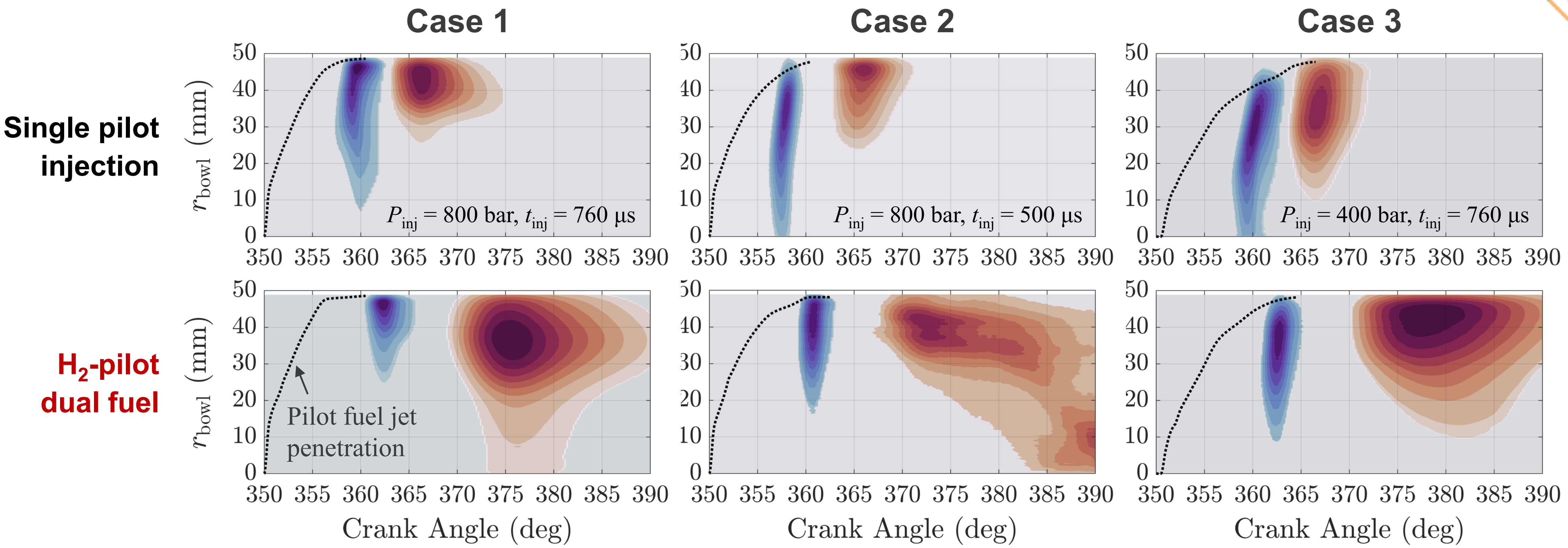


"LTC regime" **"HTC regime"**

Case 3

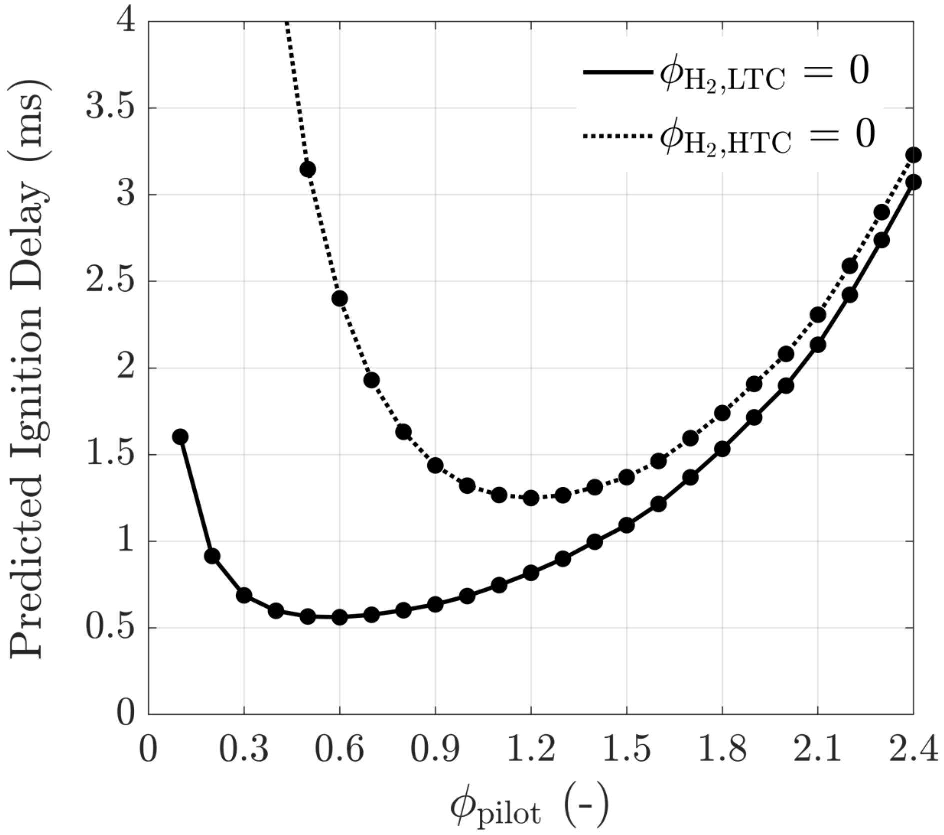


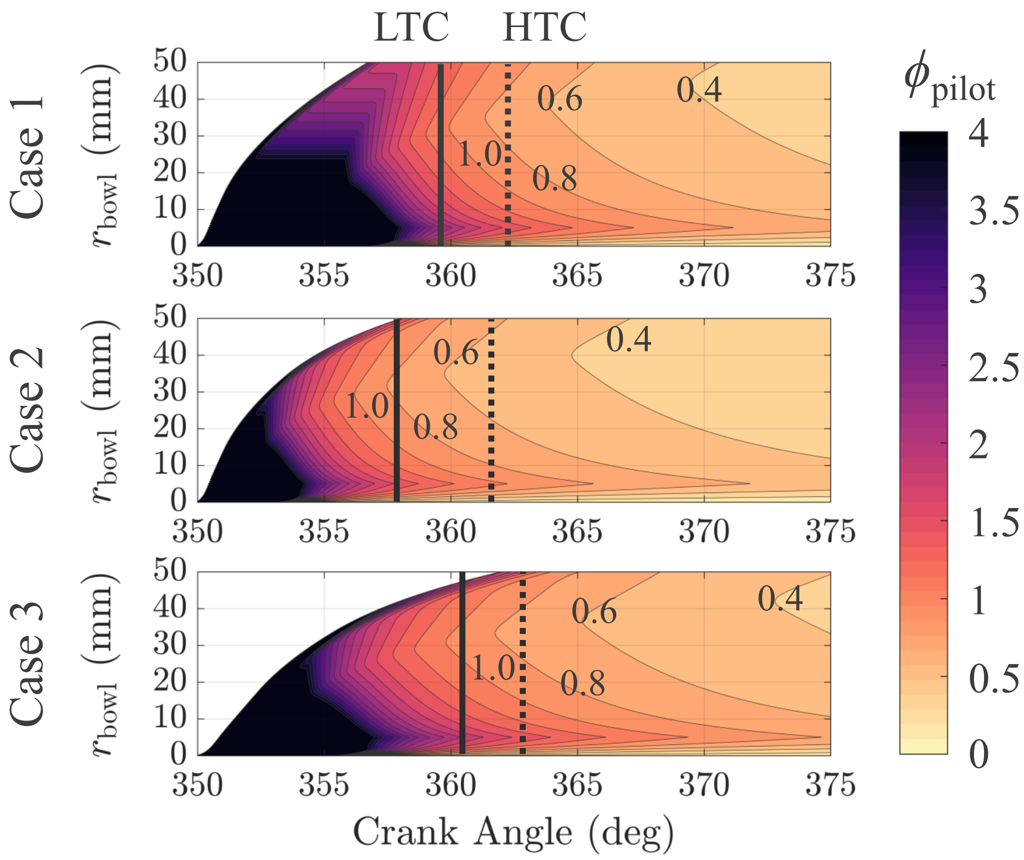
Spatio-temporal flame evolution with pilot jet penetration



- The changes in jet penetration with respect to pilot injection parameter result in variations in mixing time and pilot fuel concentration, followed by spatial changes in LTHR (HCHO*) and HTHR (OH*).
- In H_2 environment with reduced ambient density, faster jet penetration is noticeable but the inhibitive effect of H_2 delays the overall reaction, increases dwell time, and confines the reaction to near-wall regions.
- The injection rate profile of Case 3 is more conducive to maintaining rich fuel pockets, highlighting the significance of fuel jet evolution on the ignition process in hydrogen dual-fuel combustion.

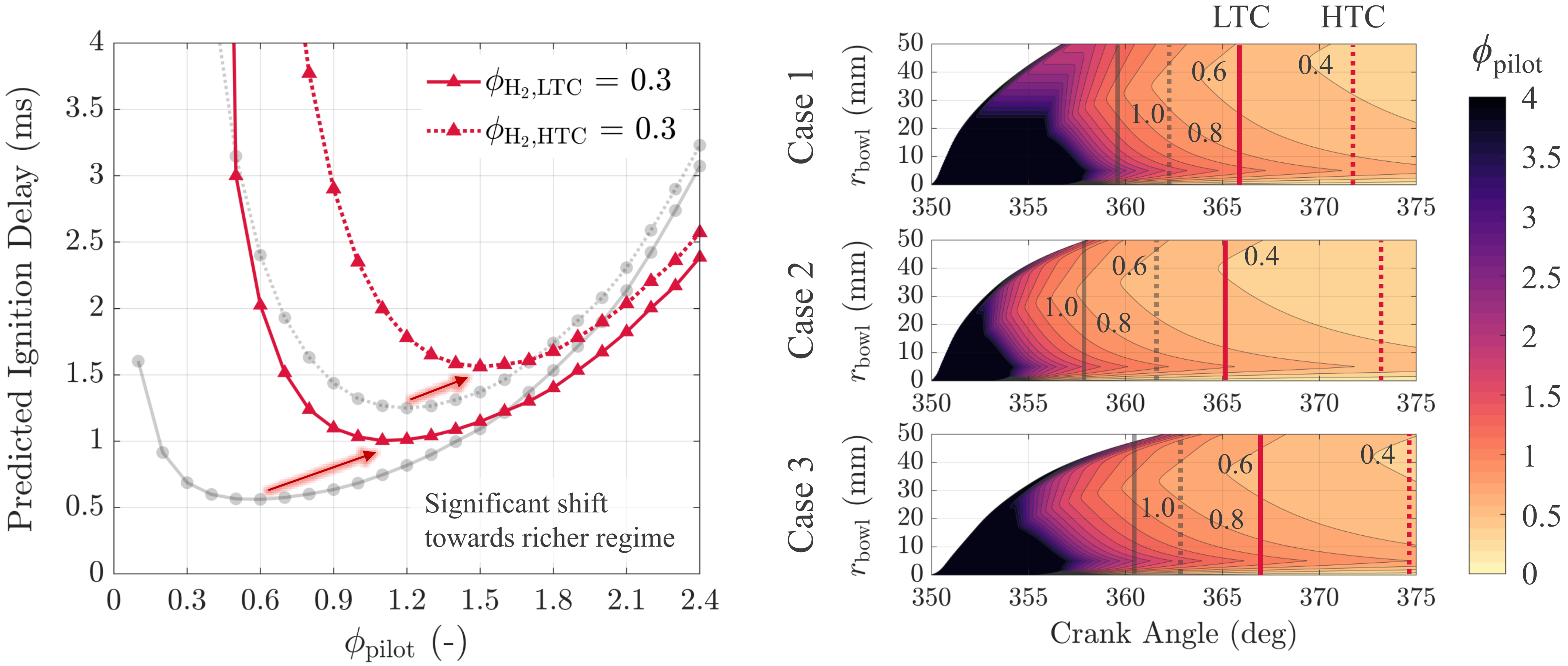
Physico-chemical interplay between pilot injection and chemical kinetics





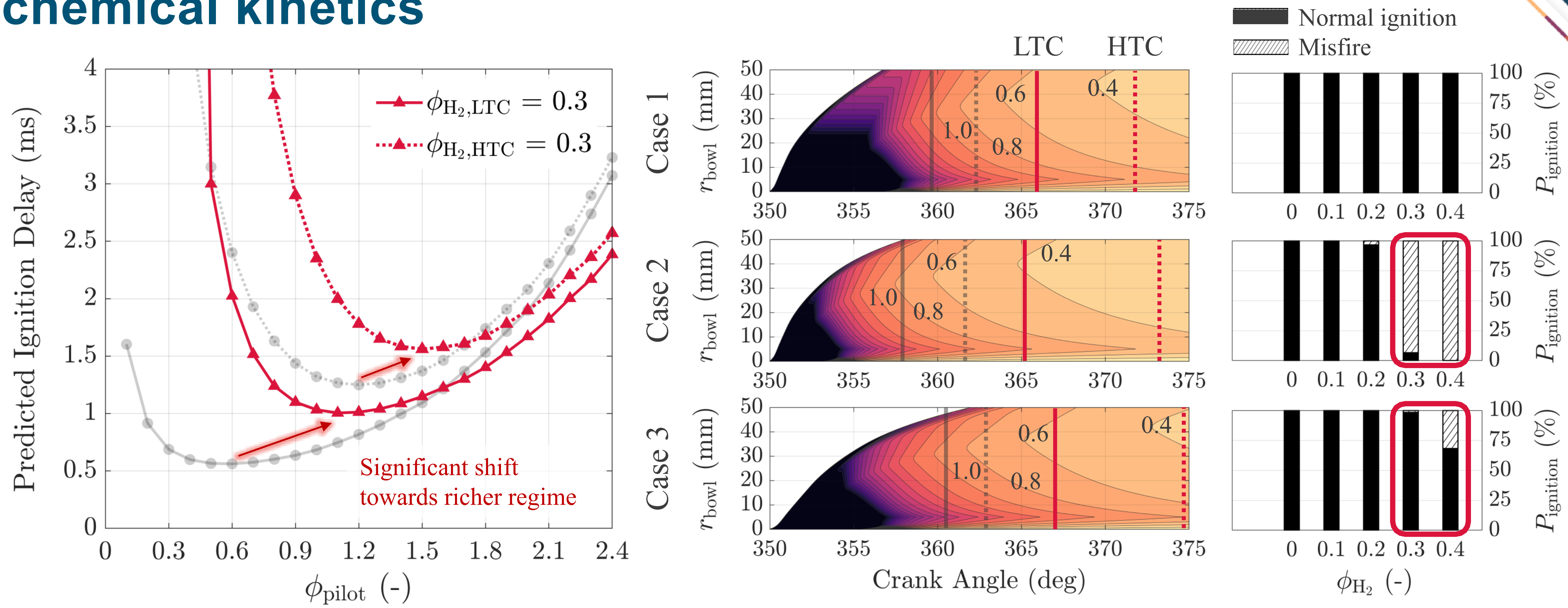
- The most-reactive mixture fraction (indicating shortest ignition delays) or highest pilot fuel concentration in the spray can possibly initiate the two-stage auto-ignition.
- With the pure pilot injection, a wide range of ϕ_{pilot} is available in the spray domain, which is not expected to limit the ignition process; except for the increased dependence on stochastic rich fuel pockets in Case 2.

Physico-chemical interplay between pilot injection and chemical kinetics



- The H_2 addition results in a significant shift of the most-reactive mixture fraction towards *richer regime* because of the low O_2 concentration ($[O_2]$) and radical scavenging by the primary fuel (H_2).
- Comparing all three cases, slower pilot fuel mixing induced by the lower injection pressure appears to enable more effective combustion with lower pilot fuel consumption, thus achieving a higher H_2 substitution rate.

Physico-chemical interplay between pilot injection and chemical kinetics



- Frequent misfires under rich hydrogen environment (Case 2) can be explained by the considerably low pilot fuel concentration across the entire jet area at the onset of low- and high-temperature ignition.
- Comparing all three cases, slower pilot fuel mixing induced by the lower injection pressure appears to enable more effective combustion with lower pilot fuel consumption, thus achieving a higher H_2 substitution rate.

Summary and Future Work

Summary

- Increasing the hydrogen content substantially delays the first- and second-stage ignition, followed by many misfires especially when the pilot injection parameter is inappropriate to create rich fuel pockets.
- Dual-fuel chemical kinetics simulations reveal that to overcome the strong inhibitive effect of H_2 under lean conditions, a pilot injection strategy should encourage significant local fuel concentration for reliable ignition.
- Supported by the 1D spray modeling and chemical kinetics simulation, higher H_2 substitution rates can possibly be realized by using larger injector orifices with lower injection pressures, while maintaining engine performance.

Future Work

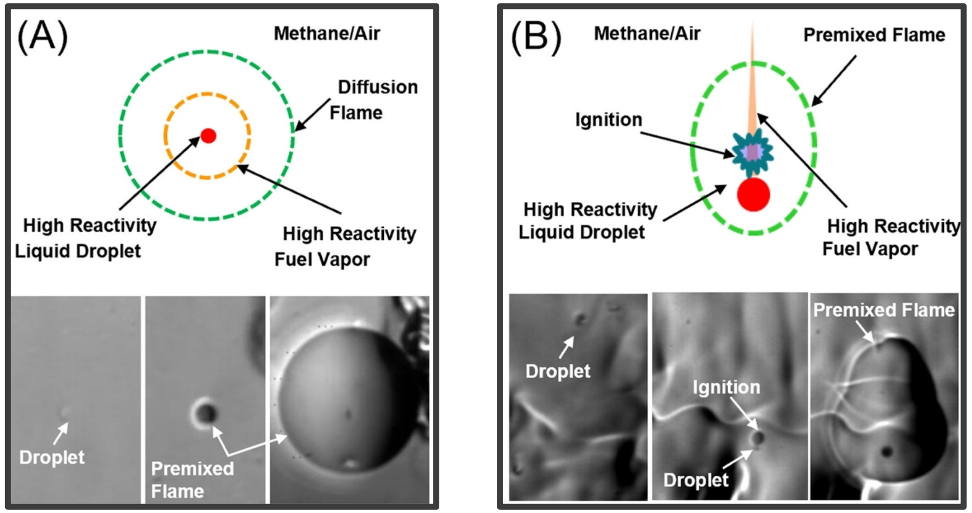
Homogeneous hydrogen mixture formation

- Measure the hydrogen mixing field with temperature field to quantify the tracer PLIF dataset (anisole or *p*-DFB).
- Combine H_2 mixing field diagnostics with PIV measurement for the flow-field characterization.

Oil-induced hydrogen pre-ignition

- Oil droplet injector to explore the impact of H_2 and the role of size and temperature on oil-induced pre-ignition.

Effect of diesel droplet size on flame evolution



- S. Bhoite et al. (2023)

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Any questions?

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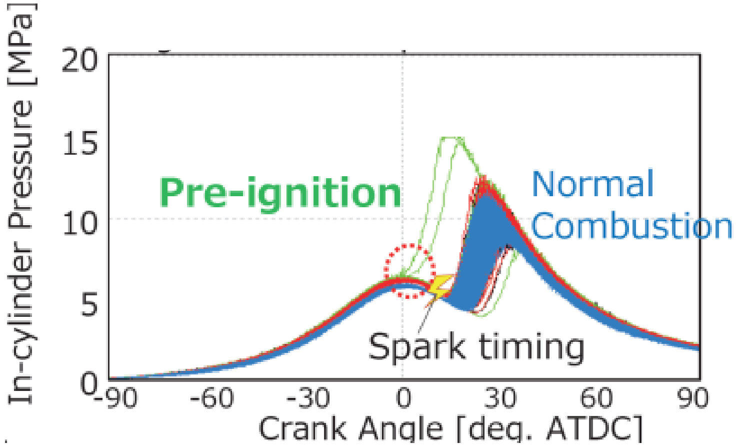
Hydrogen Pre-ignition Events

Sporadic Pre-ignition

Sources:

- Oil droplets
- Solid hot particles
- Carbonaceous deposits

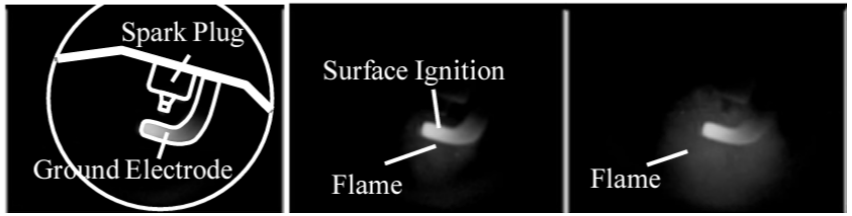
Little is known about the potential sources and related phenomenology; it seems to be caused by temperature increase during compression stroke.



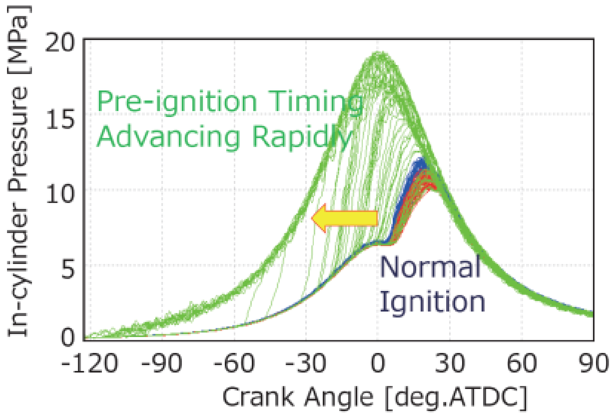
- Matsubara et. al, JSAE 20224660

Runaway Pre-ignition

- Occurs particularly at high load
- Spark-plug electrode or exhaust valves are the most common source
- May appear like a "thermal runaway", often requires fuel cut-off to stop.



- Matsubara et. al, JSAE 20234016



- Matsubara et. al, JSAE 20224660

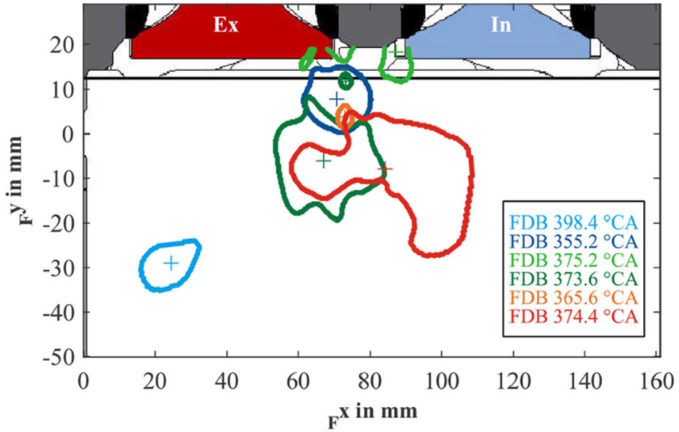
Back-fire

- Potential source of back-fire

: fresh mixture gets in contact with hot exhaust gas from previous cycle early during the intake stroke.

- A series of back-fire events

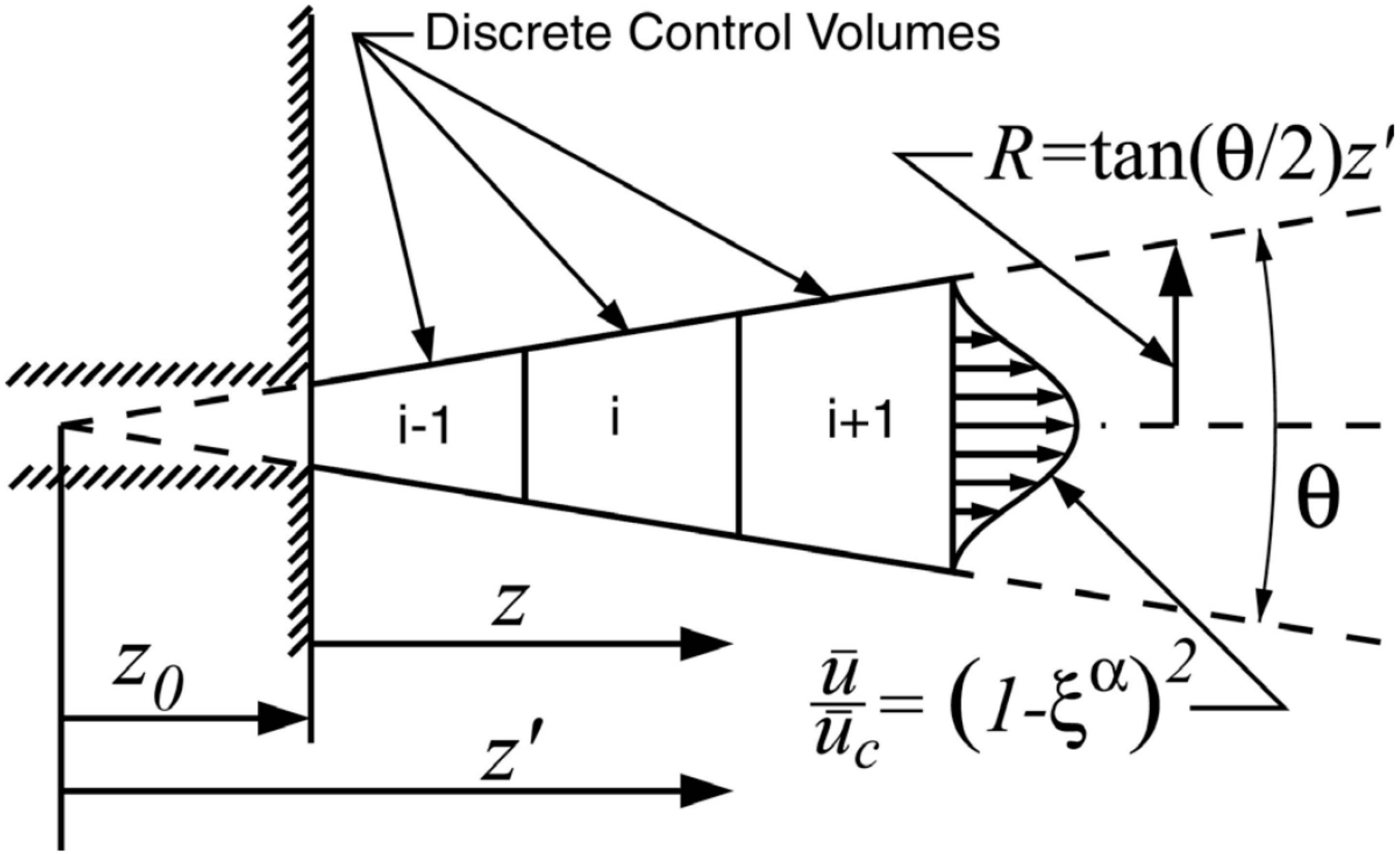
: back-fire heats up intake port mixture, subsequent cycles ignite almost immediately upon entering the cylinder.



- Eicheldinger et. al, IJER Vol 23, Issue 5

Musculus-Kattke 1D Jet Model

1D simplified jet model based on the control volume analysis encompassing mixing and transient jet development



Assumptions

1) The jet is not vaporizing.
(No evaporative cooling effect)

2) Incompressible flow

3) Turbulent viscous forces are neglected.

4) Axial mixing of momentum due to molecular and turbulent diffusion is neglected.

5) The net force due to any axial pressure gradient is negligible.

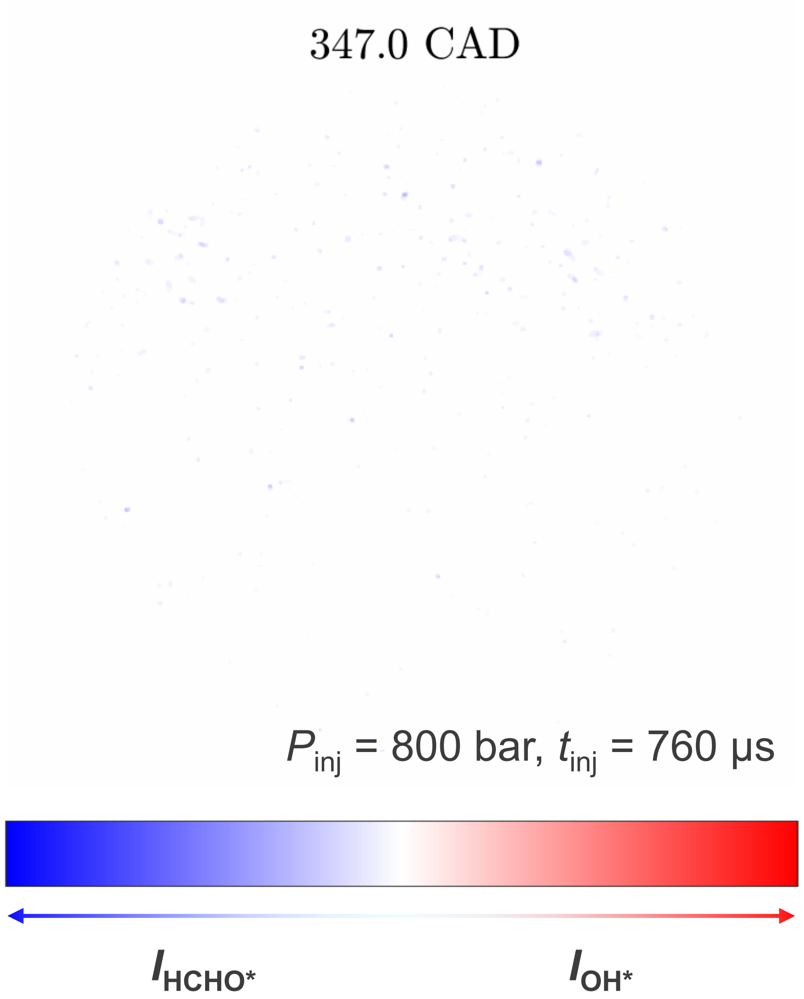
6) The jet spreading angle is constant.

7) The radial profile of mean axial velocity remains unchanged during the EOI transient.

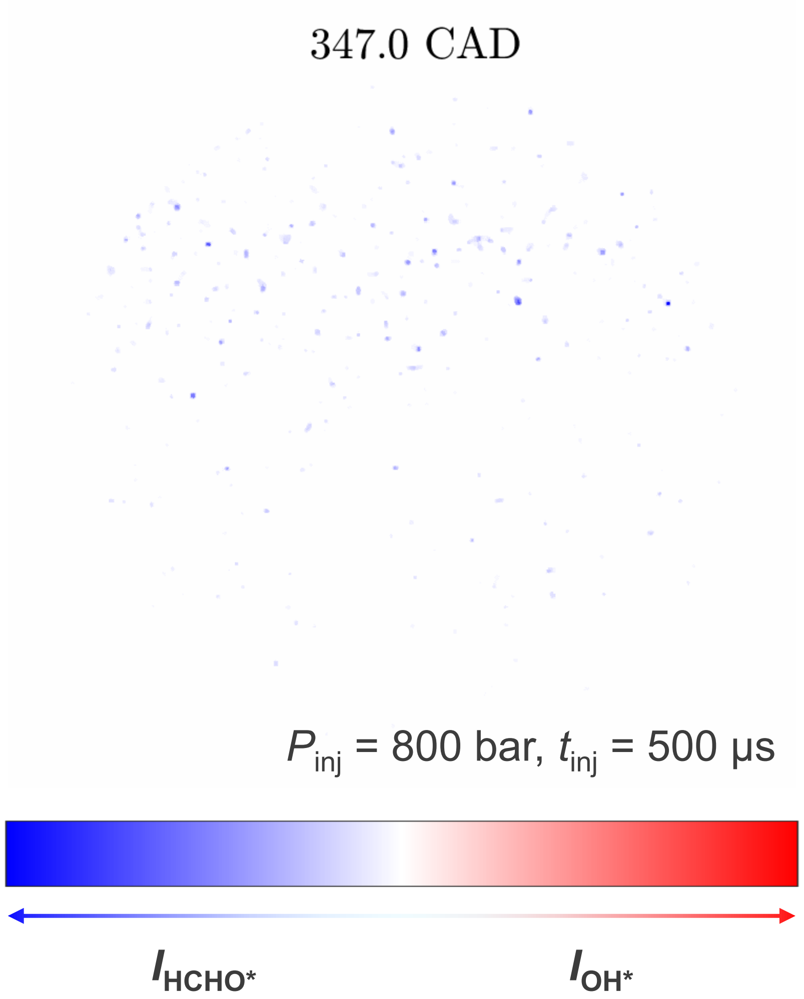
- M.P.B. Musculus and K. Kattke (2009)

Evolution of auto-ignition process: H_2 dual-fuel operation

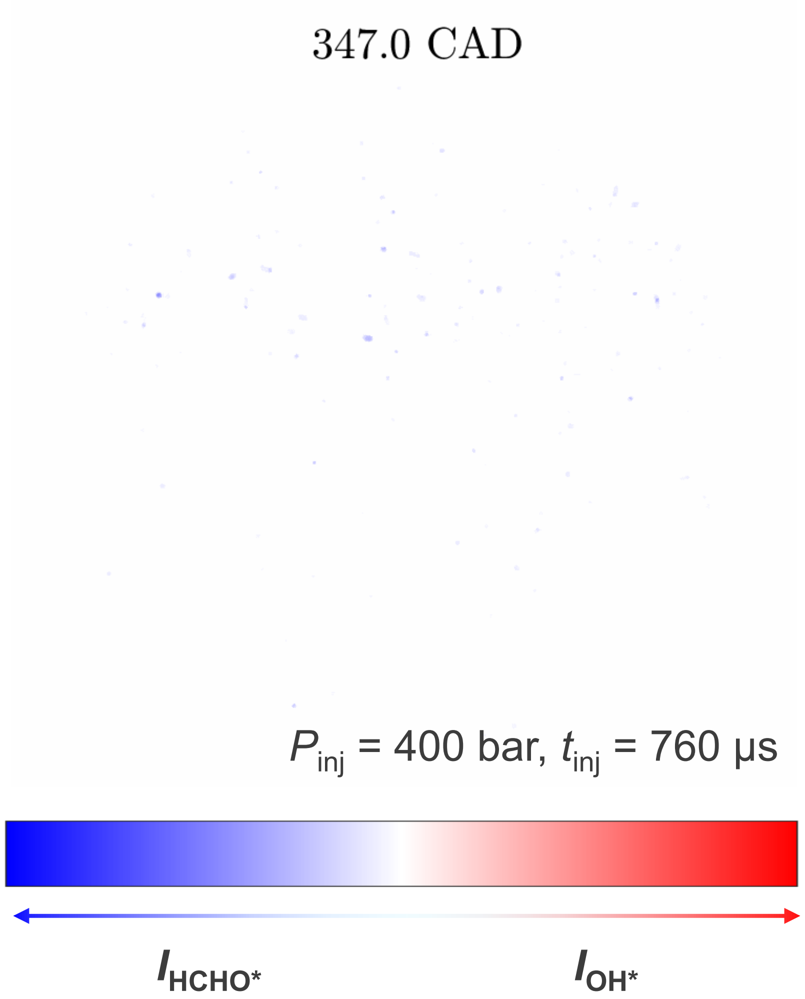
Case 1



Case 2



Case 3



"LTC regime" **"HTC regime"**