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TOWARDS CONCEPTUAL UNDERSTANDING OF PRE-IGNITION IN HYDROGEN INTERNAL COMBUSTION ENGINES

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BACKGROUND OF H2-ICE RESEARCH AT SANDIA

Results from an earlier light-duty H2-DI combustion program (discontinued in 2012) available on the ECN webpage

H2-DI program revived in FY22 with focus on difficult-to-electrify sectors – off-road, marine, rail, (heavy-duty)

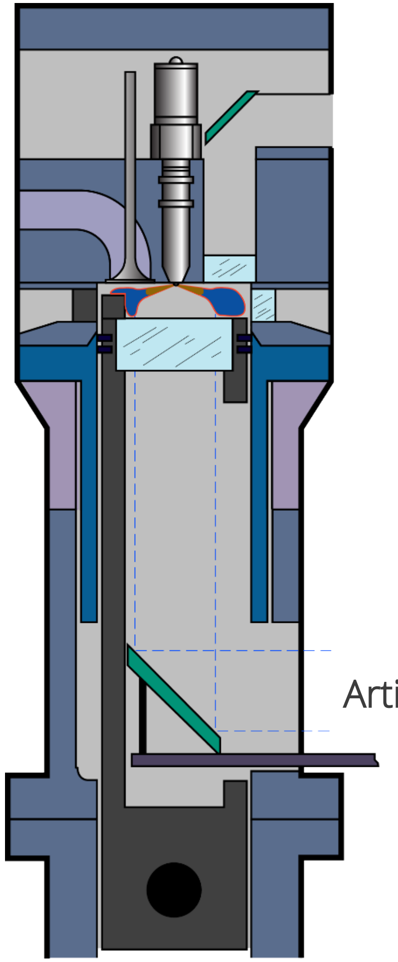
- **June 2022**: Focus on in-cylinder mixing and develop a framework for research of pre-ignition
- **2023-2024**: Program continues with industrial partners
- **Test-rig**: Sandia Heavy-Duty Optical Engine, 2.34 L/cyl., to be upgraded to Cummins 15L fuel-agnostic engine platform in Q4 2024
- Focus on **4-stroke medium-pressure H2-DI** technology with external ignition (spark, PC, etc.)
  - Off-road engines will likely be diesel-derivatives with a swirl combustion chamber

Addressing the greatest challenges:

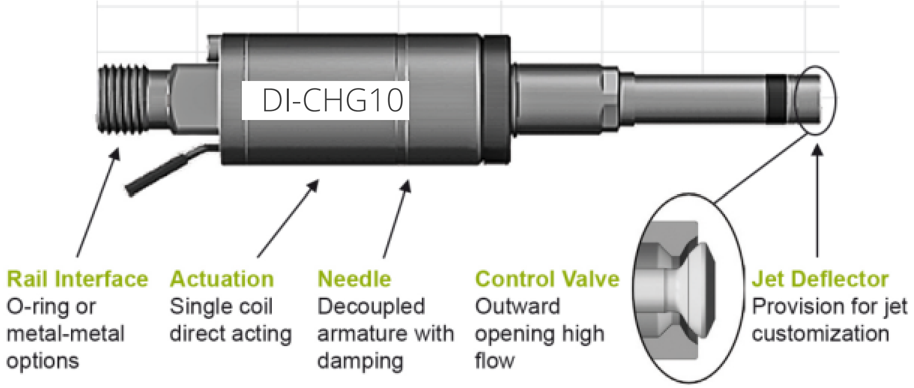
- **Power-density**
  - H_2 displacing air, ultra-lean operation to mitigate NOx
  - Requiring direct fuel-injection
  - Medium-pressure injection – avoiding on-board compressor
- **NOx emissions**
  - Direct-injection creates stratified mixture, increasing NOx formation and potentially creating hot-spots
  - No established guidelines for injector design and operating strategy
  - Predicting H2 in-cylinder mixing is very challenging to capture with CFD. Experimental validation data using modern injection hardware is limited.
- **Pre-ignition / Abnormal combustion**
  - Limiting the load, forcing ultra-lean operation, requiring sub-optimal spark timing
  - Plethora of possible sources: hot-spots, oil droplets, carbonaceous oil-residue, combustion residuals,…
  - Poorly understood, the dominant source may depend on engine design/operation
- **Advanced ignition systems potentially aggravate pre-ignition issues**

GENERAL APPROACH - OPTICAL IMAGING & NUMERICAL MODELING OF IN-CYLINDER CHEMICAL/PHYSICAL PROCESSES

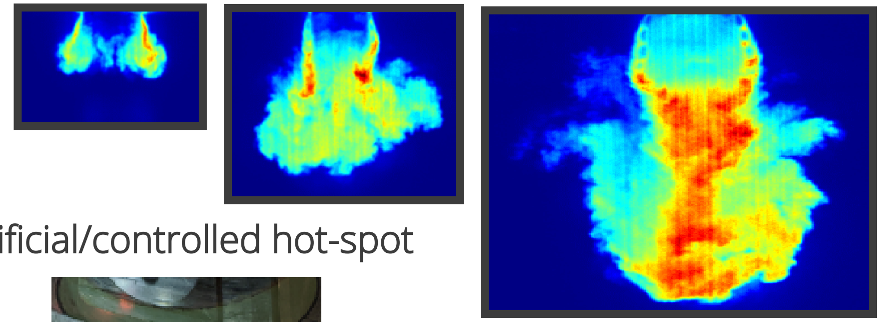
Heavy-duty (2.34 L/cyl.) optical engine



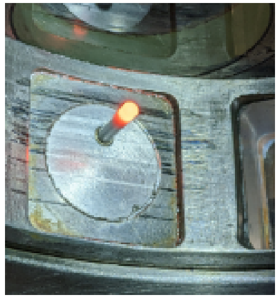
Phinia medium-pressure direct injector



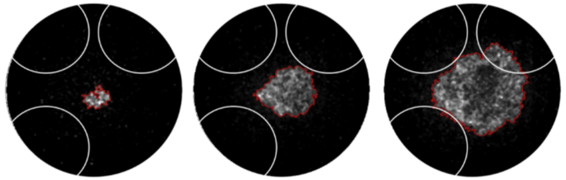
Laser-imaging of H2 jet evolution



Artificial/controlled hot-spot



Imaging of flame evolution



General approach

- Combine optical and planar laser-imaging diagnostics in an optical heavy-duty engine with computer modeling to close the knowledge gaps impeding H2ICE development
- Transfer fundamental understanding to industry through working group meetings, individual correspondence, and publications

Detailed approach:

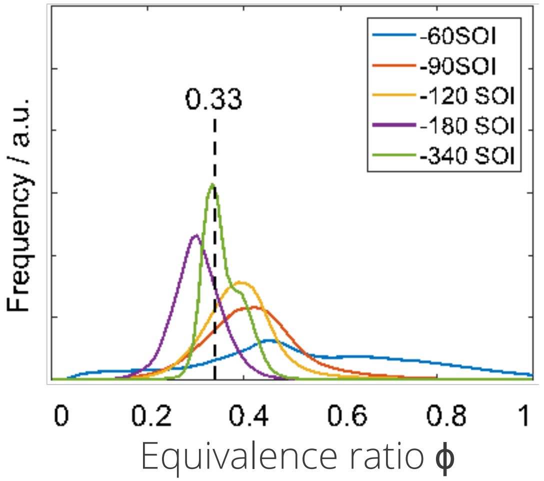
- Characterize impact of injector configuration, timing, and pressure on in-cylinder mixture formation and ensuing combustion evolution, using tracer-PLIF and PIV imaging
- Study pre-ignition mechanisms in the framework of induced pre-ignition – artificially induced controllable pre-ignition sources allow direct insight into the pre-ignition process and relevance of different mechanisms.

PAST ACHIEVEMENTS ON IN-CYLINDER MIXING (USING PHINIA INJECTORS)

Sample mixing dataset (1 operating cond.)

Piston-window view

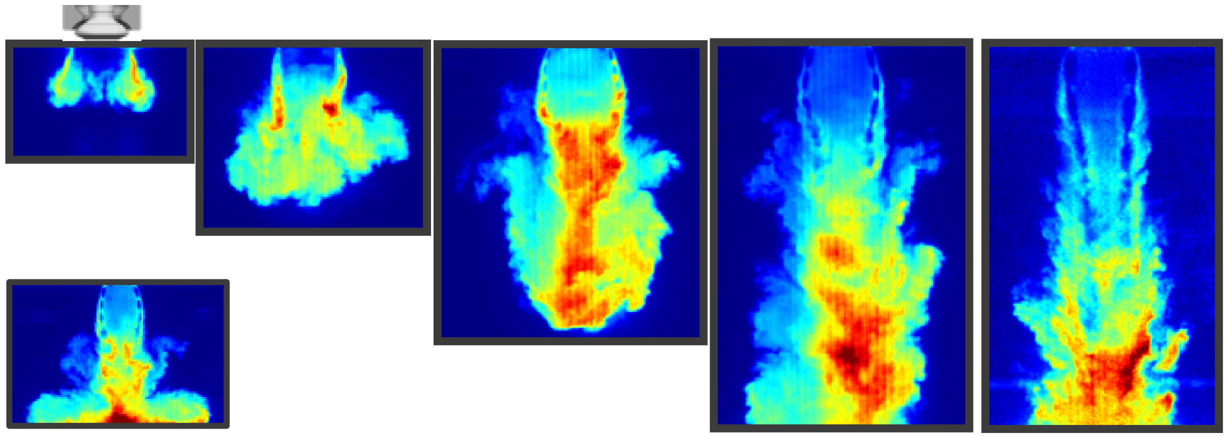
Mixture statistics



Database available on request, in process of publishing on ECN page

- Full engine geometry incl. intake/exhaust flow paths
- Simplified injector information as allowed by BorgWarner

Early jet evolution imaging



THE MECHANISMS OF PRE-IGNITION ARE POORLY UNDERSTOOD

Various potential sources of pre-ignition

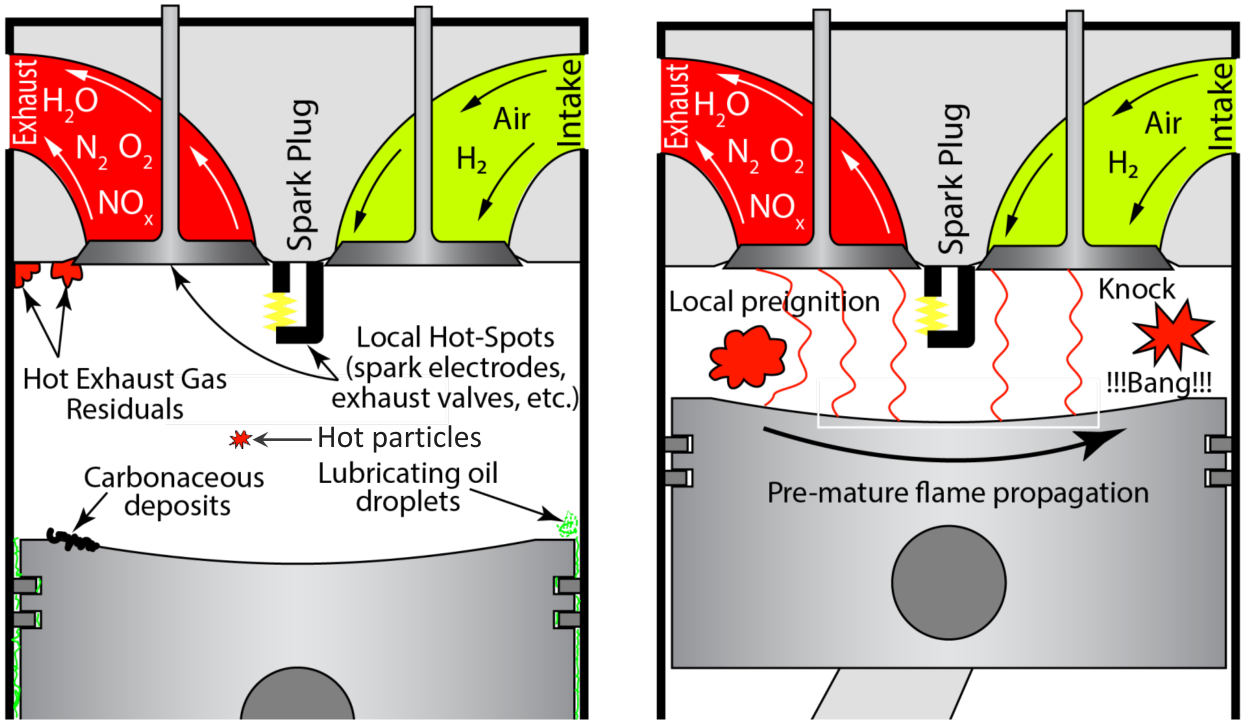
- Hot-spots – exhaust valves, spark electrodes
- Hot residual gases in crevices
- Glowing/hot particles or carbonaceous deposits
- Lubrication oil, oil ashes, etc..

Each mechanism can be dominant in different engines and under different operating conditions

- Decoupling different mechanisms is crucial to understand the physics
- Efficient mitigation by only reducing the dominant mechanism for particular engine
- Stochastic nature makes studies of pre-ignition challenging in a real engine – high probability of mechanical damage

➢ Idea: induce the pre-ignition under controlled conditions in the optical engine to allow studying the underlying phenomena

Conceptual schematic of H_2 pre-ignition mechanisms



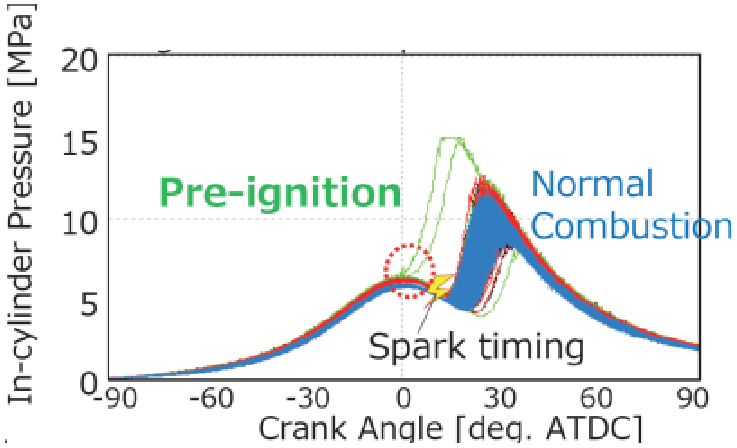
TYPES OF PRE-IGNITION

Sporadic Pre-ignition

Sources:

- Oil droplets
- Solid hot particles
- Carbonaceous deposits

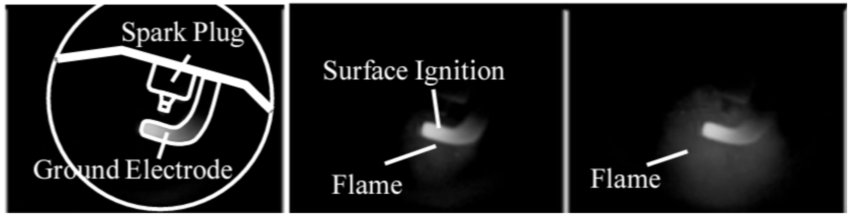
Little is known about the potential sources and related phenomenology; it seems to be caused by temperature increase during compression stroke.



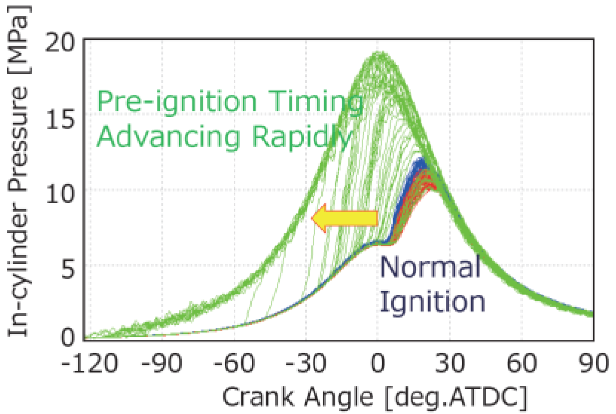
- Matsubara et. al, JSAE 20224660

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

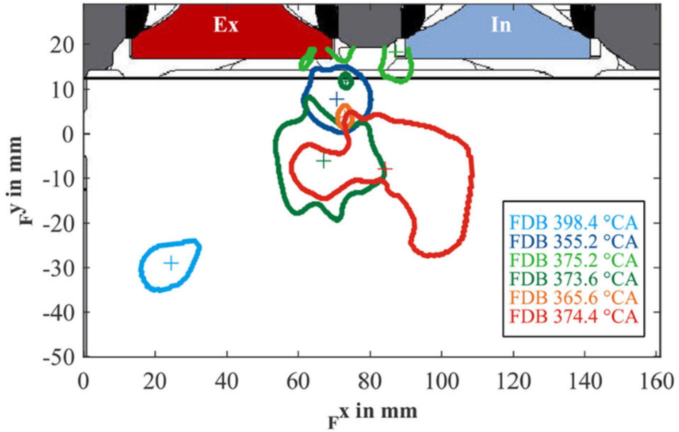
Back-fire

- 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

HOT-SPOT AND CATALYTIC SURFACE EFFECTS ON HOT-SPOT PRE-IGNITION - SETUP AND APPROACH

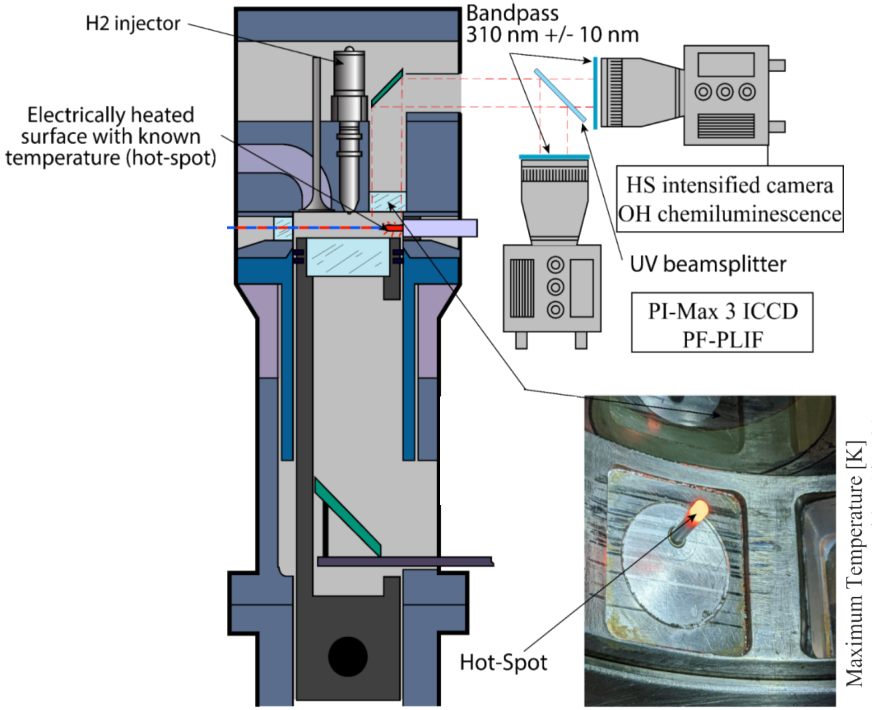
Goals:

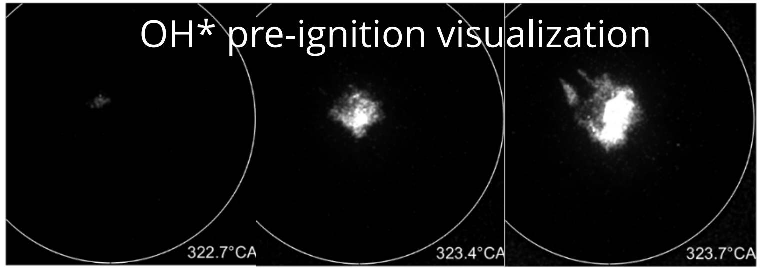
- Establish a framework that allows studying pre-ignition under controlled and repeatable conditions
- Understand **phenomenology of hot-spot pre-ignition**
- Understand the **role of catalytic effects** on hot-spot pre-ignition – applicability of Pt or Ir spark plugs?

Measurements conducted:

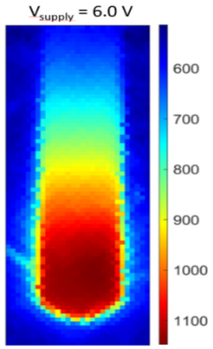
- Hot-spot (glow-plug) installed and it's temperature characterized during engine operation
- Tested the **pre-ignition timing and frequency** for different injection timings and surface temperature
  - 1200RPM and 600RPM, Φ=0.33
- Developed + **tested a Platinum-coated glow plug** to study the catalytic effects
  - 30nm Titanium adhesive layer
  - 500nm sputtered Platinum coating

Test-setup to visualize and characterize hot-spot pre-ignition using direct hydrogen injection

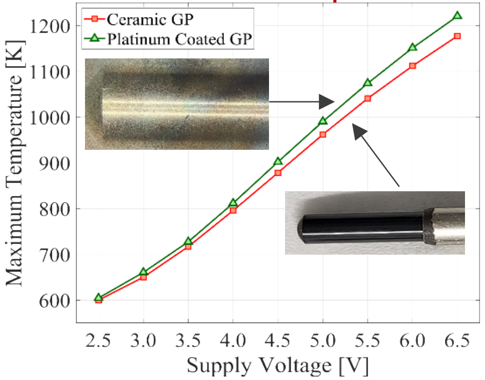


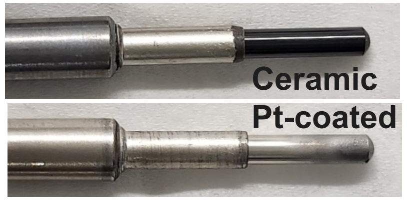


Glow-Plug temperature distribution



Max. surface temperature



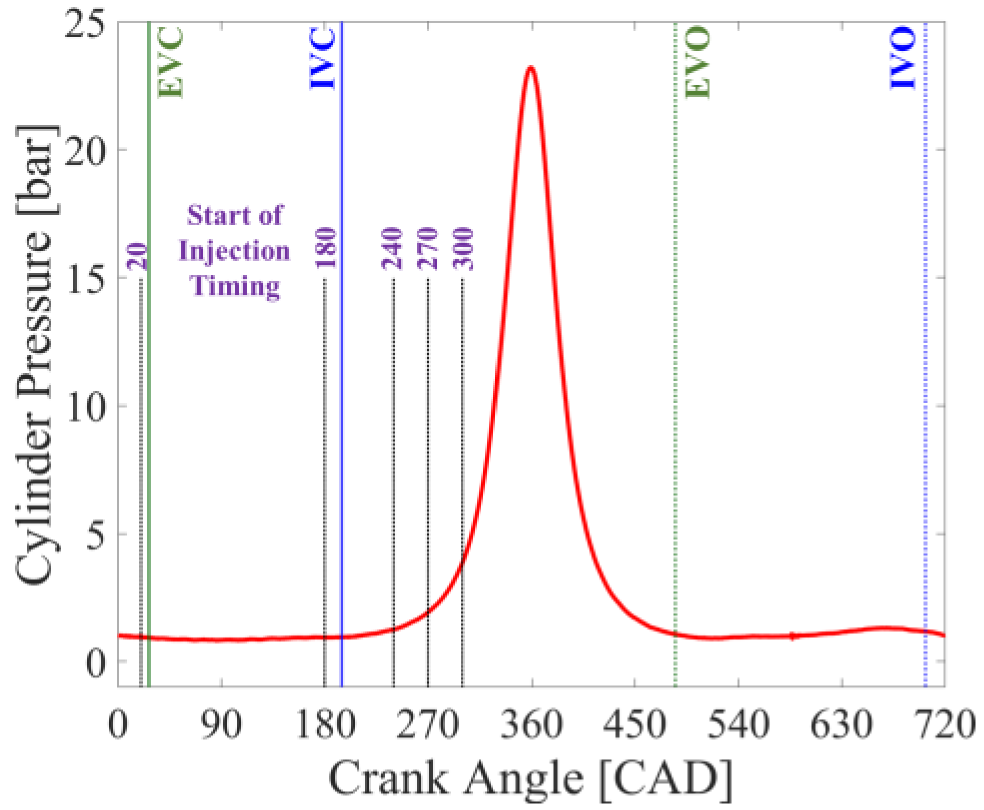


Brief Overview for Data Interpretation

5 Cycles that do not pre-ignite are grouped and shown at the very top

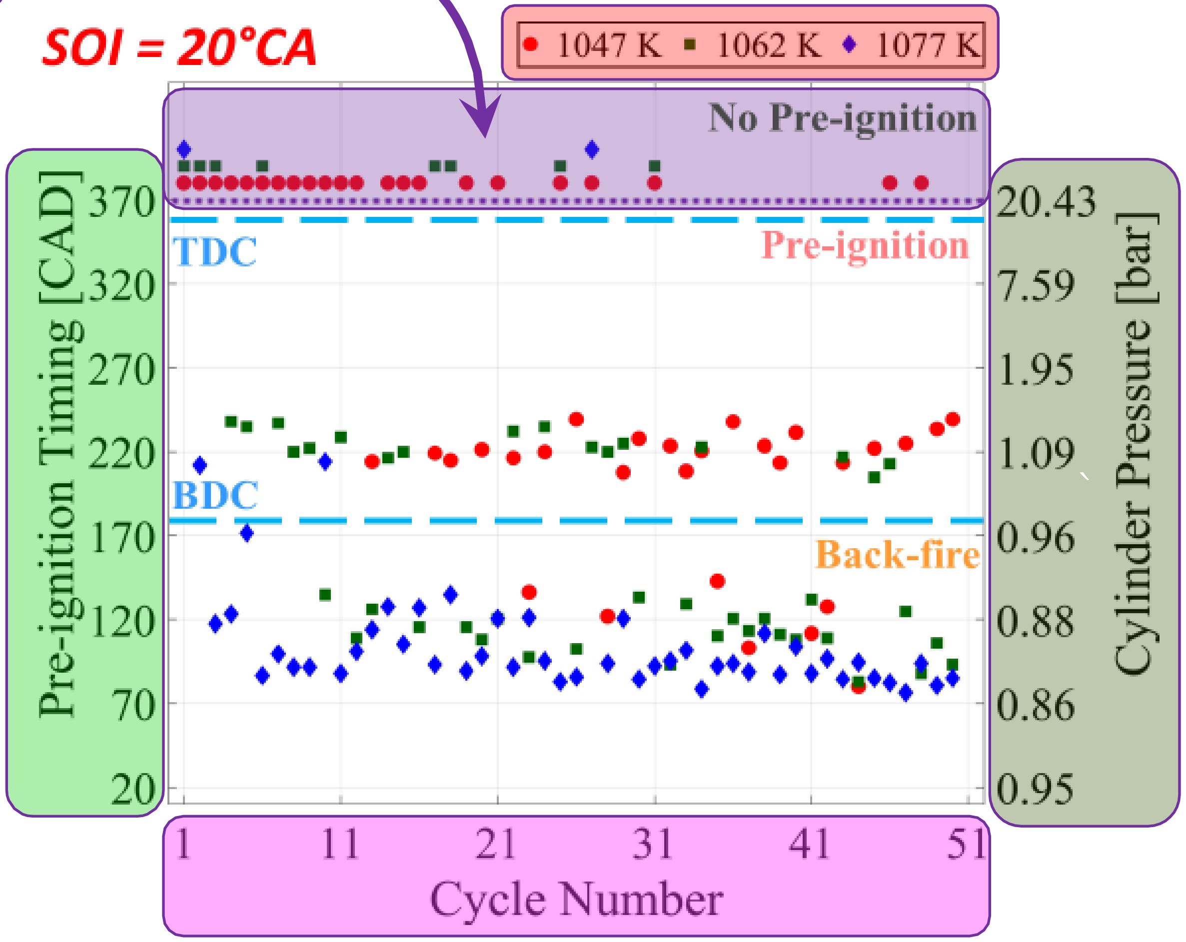
4 Legends indicate different GP temperatures

Valve timing & Cylinder pressure



SOI = 20°CA

2 Timing of pre-ignition based on OH* CL imaging



3 Indicative cylinder pressure corresponding to CAD timing (non-linear scale)

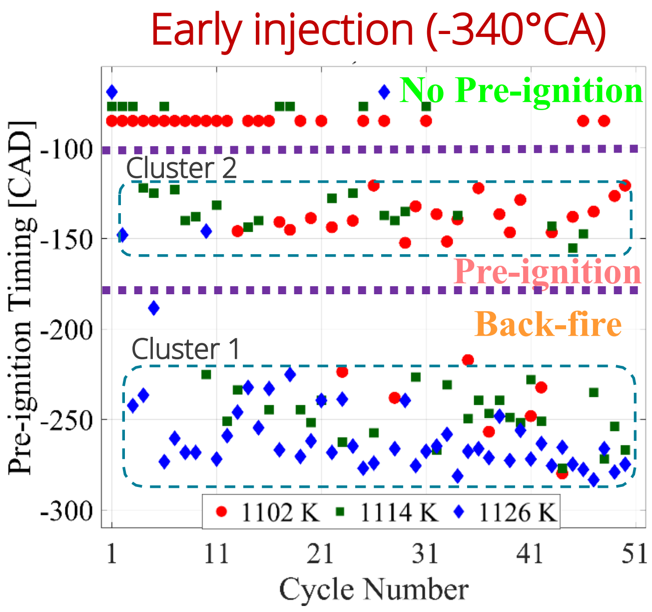
1 Sequential "fired" cycles in each test run (optical engine skip fire – 9:1)

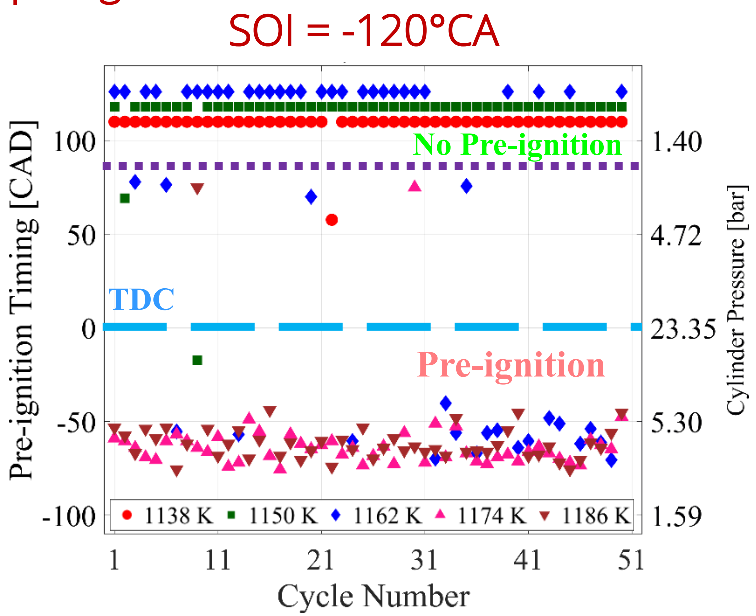
PRE-IGNITION TIMING IS CLUSTERED AWAY FROM TDC, PRE-IGNITION FREQUENCY EXTREMELY SENSITIVE TO HOT-SPOT TEMPERATURE

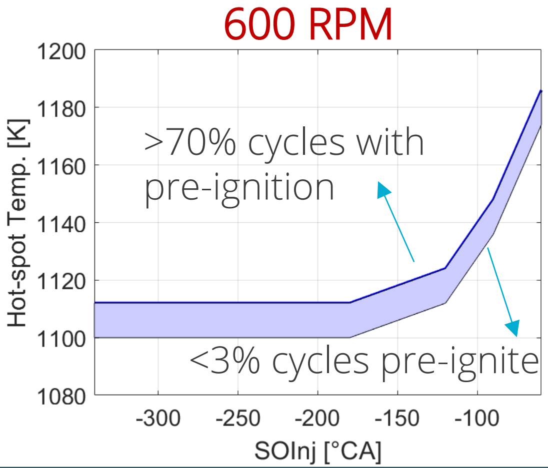
The pre-ignition timing is clustered into groups with similar timing:

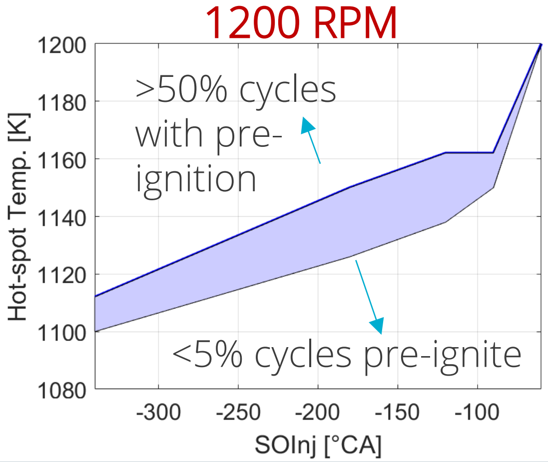
- Early injection: a cluster around -240°CA and around -120°CA.
- Later injection: a cluster around -60°CA, and some ignitions during the expansion stroke.
- Earliest pre-ignition timings governed by mixing – time it takes for the fuel to reach the hot-spot
- The variability of pre-ignition timing attributed to mixing variability – visualized by tracer-PLIF

Timing of pre-ignition









Pre-ignition frequency is extremely sensitive to hot-spot temperature

- 15-30 K temperature increase changes the engine operation from few-to-none pre-ignitions to nearly all cycles pre-igniting
- Likely associated with short residence time of gas near the exposed glow-plug surface. Future testing will explore the trends with more enclosed hot-spot.

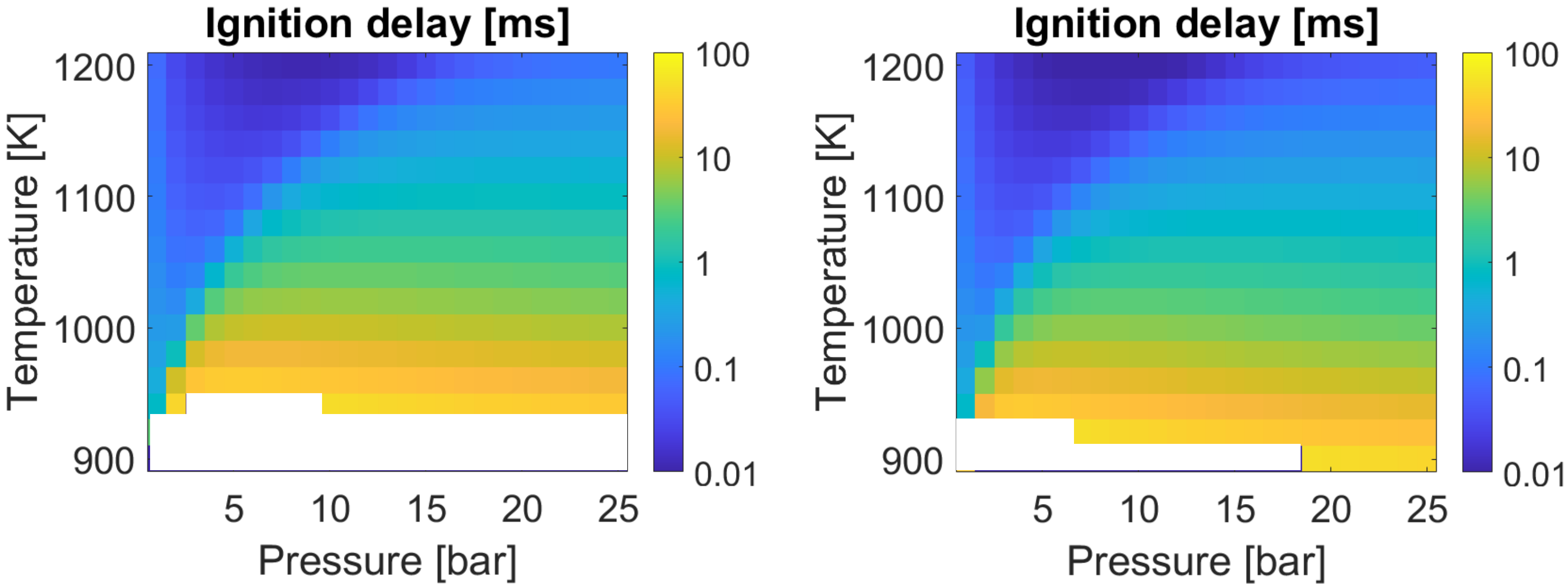
LOW-PRESSURE CHEMICAL PATHWAYS DOMINATE THE PRE-IGNITION TIMING

Can hydrogen chemical kinetics explain the early pre-ignition?

- Yes! Ignition delay drastically increases as a certain threshold of pressure is reached (at constant temperature)
- Explains why pre-ignition either happens early in the cycle, or does not happen at all
- Small sensitivity to mixture equivalence ratio
- **Injecting late in the cycle can effectively mitigate pre-ignition (provided that mixing is sufficiently fast)**

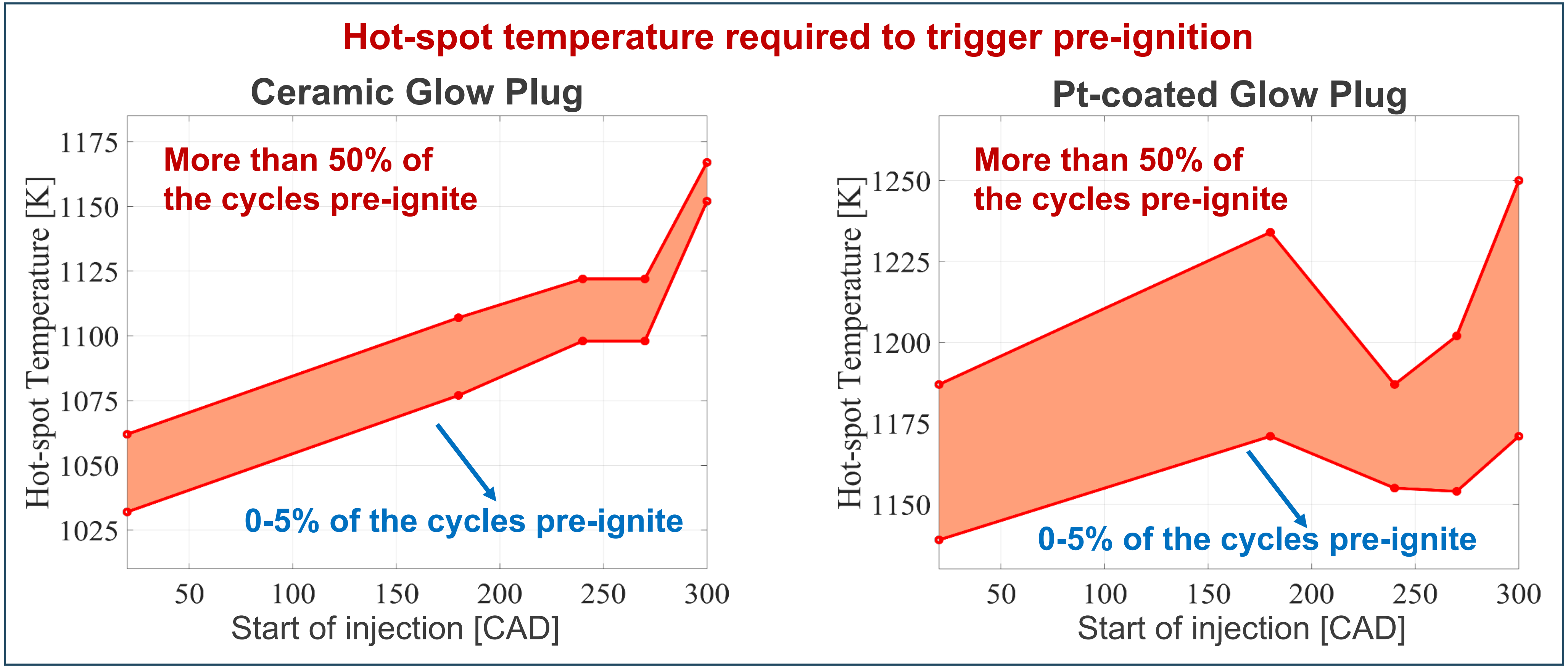
Closed homogeneous reactor simulations of H2 ignition delay for varied pressure/temperature

ϕ=0.3 ϕ=1.0



Kinetics mechanism: LLNL H2 detailed

CATALYTIC EFFECTS LIKELY NOT A PRE-IGNITION MECHANISM
INCREASED TEMPERATURE REQUIRED TO TRIGGER PRE-IGNITION



- Platinum-coated glow-plug required ~100K higher hot-spot temperature to induce similar pre-ignition frequency as the ceramic glow-plug
- Surface porosity and roughness (coated surface is appears smoother) are likely more impactful than the catalytic effects
- Use of Platinum or Iridium sparkplugs appears unlikely to impact pre-ignition

FUNDAMENTAL INSIGHTS INTO OIL PRE-IGNITION CHEMISTRY SETUP AND APPROACH

Goals:

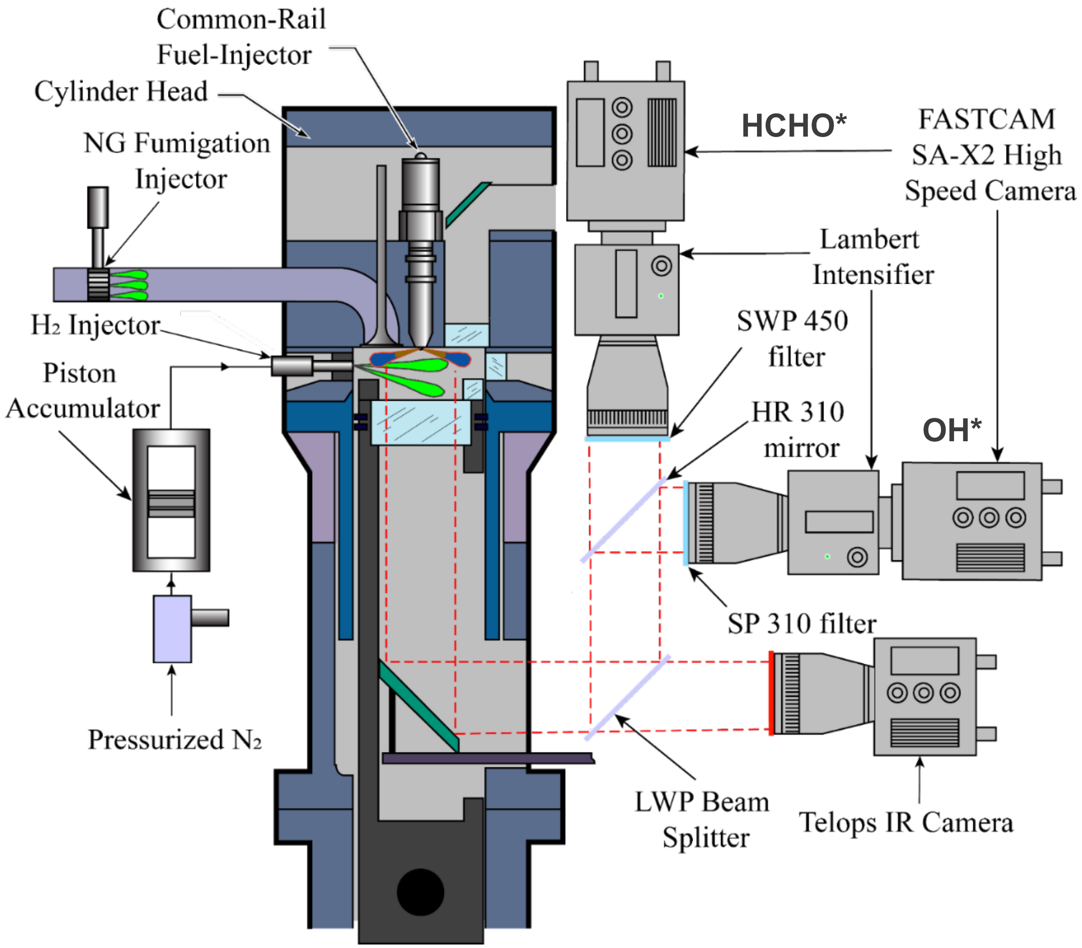
- First step towards understanding the phenomenology of oil-induced pre-ignition in H2ICE
- Simplified physics: oil pre-ignition = auto-ignition of HC in H2/air charge
- Understand the fundamentals of H2/HC autoignition chemistry before introducing more complexity

Approach:

- Premixed H_2 charge, inject HC fuel, at varied ϕ_{H2} and diesel injections properties
- Compare to old natural gas data
- 0D kinetics simulations for improved understanding

Cross-benefit: H2-diesel dual-fuel engines

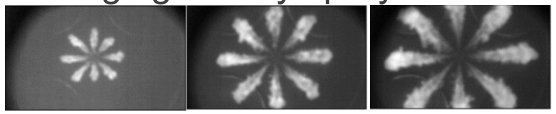
Setup to visualize all stages of diesel jet ignition in NG/air of H2/air charge



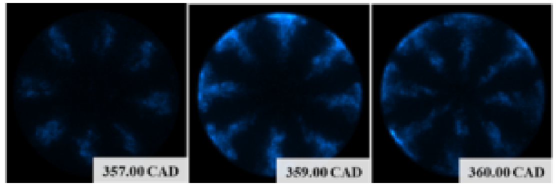
Conditions:

- Premixed H_2 (early DI) or nat. gas (fumigated) (homogeneity verified)
- Diesel direct injection (heptane as oil surrogate)
- 100°C intake temperature

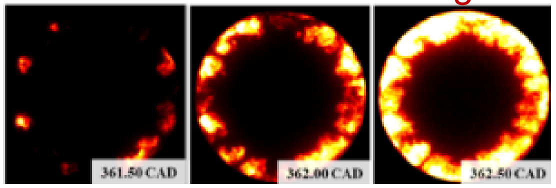
IR imaging – early spray evolution



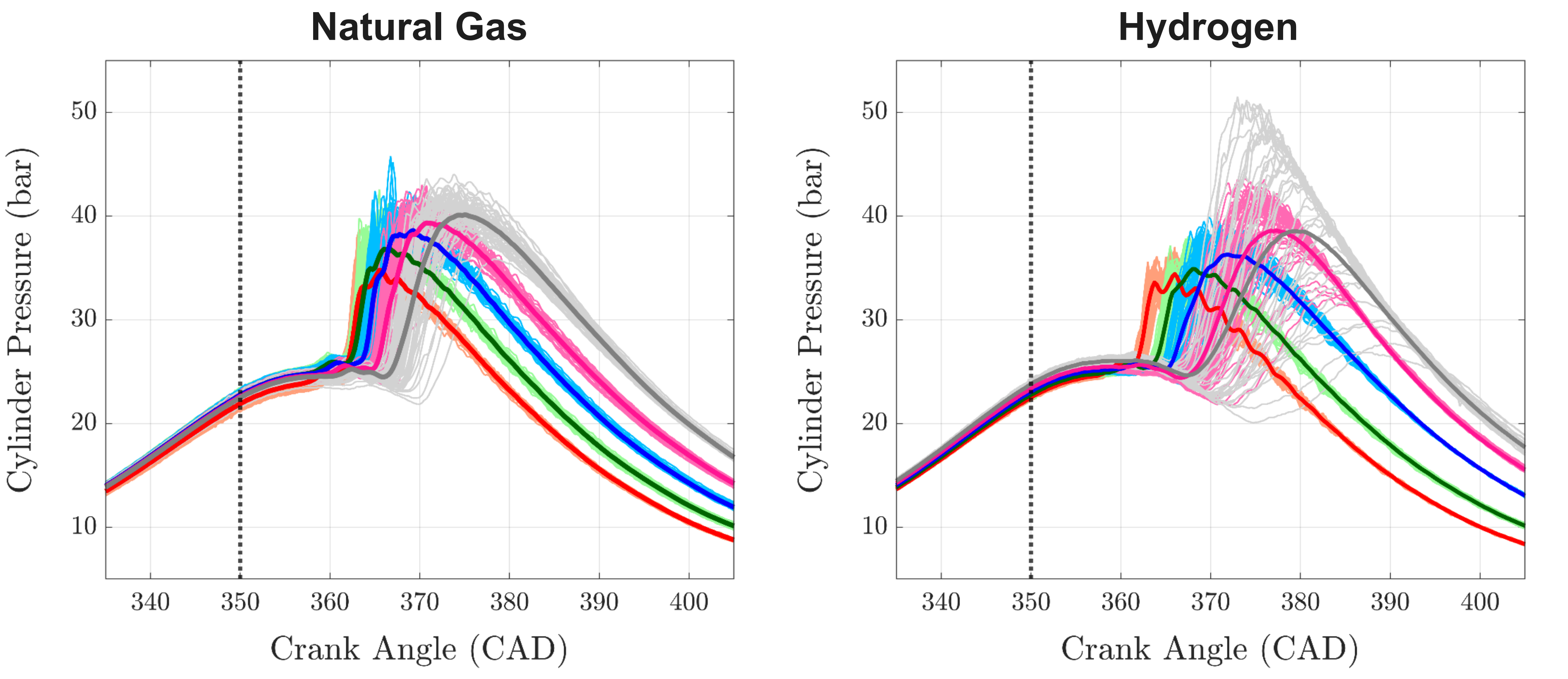
HCHO* chemilum. – cool flames



OH* chemiluminescence – ignition



HYDROGEN SIGNIFICANTLY DELAYS HYDROCARBON AUTO-IGNITION, EVEN RELATIVE TO NATURAL GAS



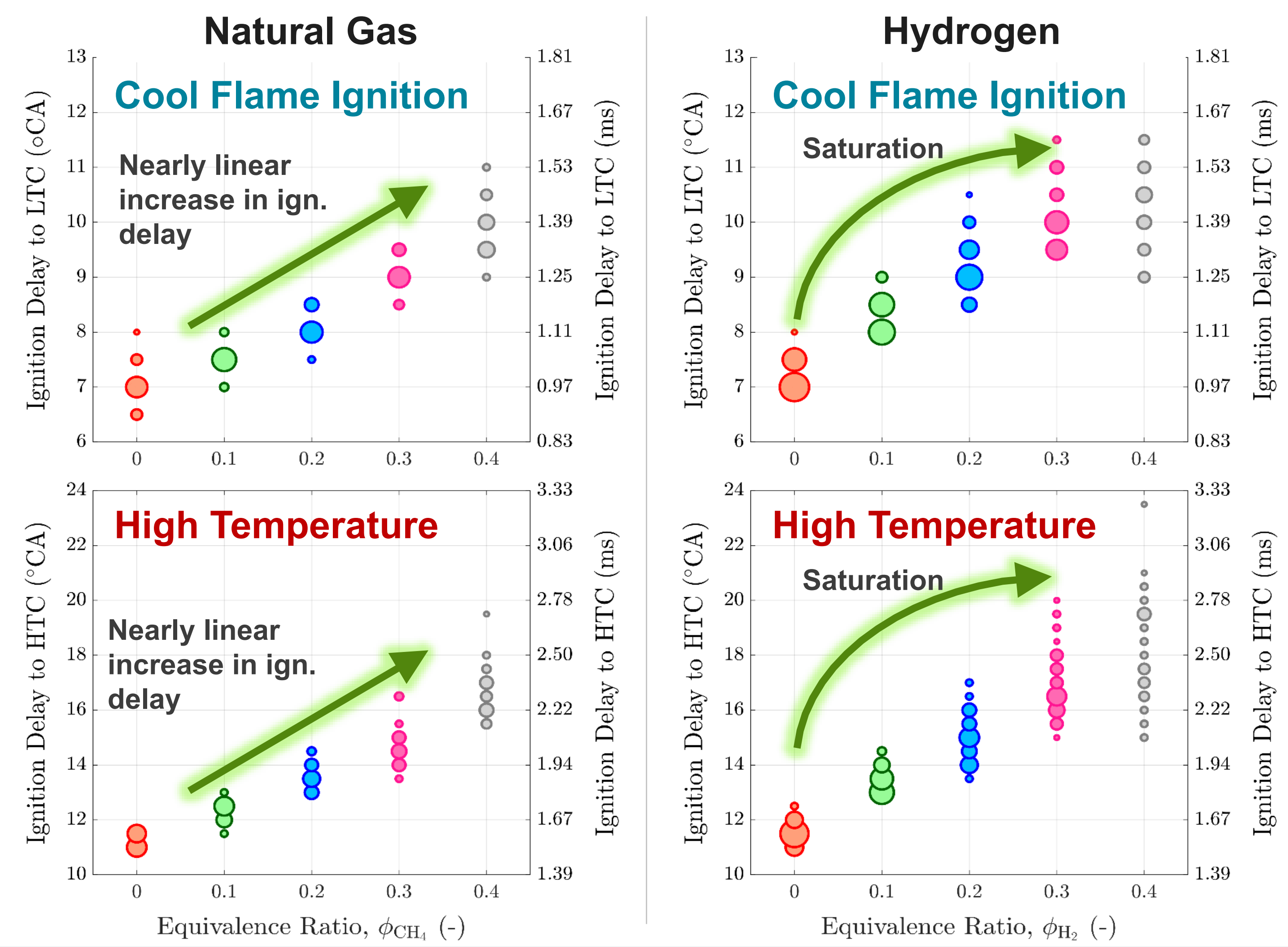
*Constant intake pressure and temperature

*Constant pilot injection (24mg), 7% energy at ϕ_{H2}=0.4

- Both natural gas and H2 strongly inhibit auto-ignition of hydrocarbons. H2 effect is more pronounced.
- Part of the natural-gas inhibition effect is due to the specific heat ratio → lower TDC temperature. No effect for H2.
- H2 dilutes air and reduces oxygen content more than natural gas (~15% prolonged ign. delay expected, ID ~ 1/[O_2])
- High cyclic variability of ID with H2 and fast flame speed – high variability of peak

H2 AND NATURAL GAS SIGNIFICANTLY DELAY COOL-FLAME REACTIVITY. H2 EFFECT SATURATES AT HIGH Φ_{H2}

Imaging-based evaluation of ignition delay (ID)



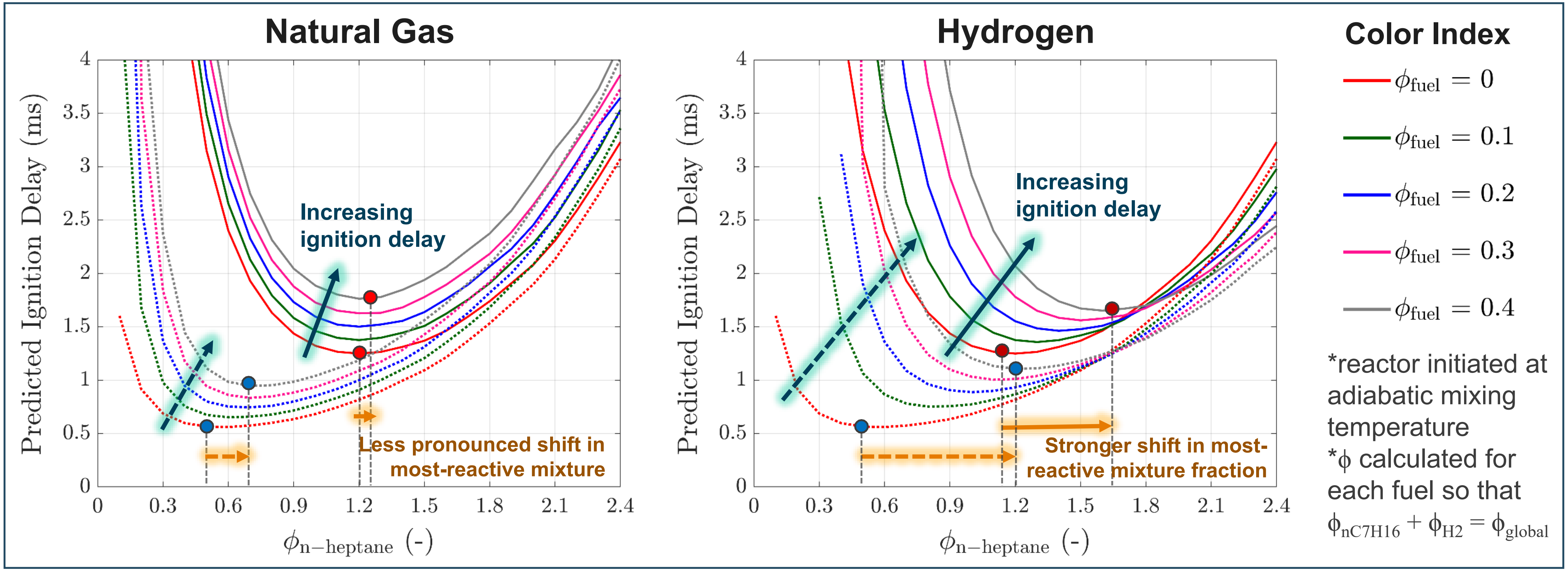
Cool-flame and high-temperature ignition are delayed

- Cool-flame delay ~50% of the total ignition delay increase
- Linear increase with ϕ_{NG}, saturation for ϕ_{H2} → unexplained

The observed increase in ID contradicts metal engine observations. Why?

- Physics of oil droplets vs. autoignition of atomized fuel?
- The role of oil additives? Large hydrocarbons in oil?
- Oil coking and particle formation?
- Ignition conditions outside the cool-flame chemistry regime?
- Engine thermal state associated with heat loss?

CHEMICAL KINETICS CONCUR WITH EXPERIMENTS. REDUCED IMPACT IN FUEL-RICH ZONES – RELEVANT IN DROPLET VICINITY



- A 0-D, *Closed Homogenous Reactor (CHR)* model to compare the chemical effects of premixed NG and H_2 on n-heptane auto-ignition - considering *adiabatic compression* and *fuel vaporization cooling*
- Reduced O_2 concentration and radical scavenging by primary fuel (NG/H_2) have strong impact on auto-ignition.
- H_2 strongly shifts the most-reactive mixture fraction to fuel-rich conditions.
- Weak inhibition effect at high ϕ_{nC7H16} may be favorable for oil-droplet ignition – rich mixture next droplet.

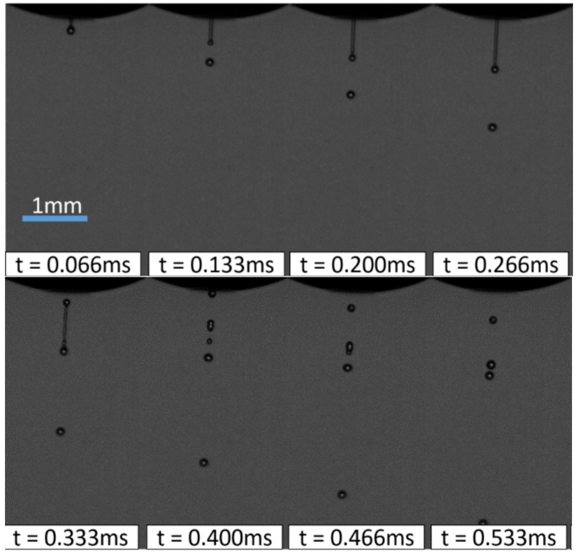
FUTURE PLANS TO ADDRESS OIL-INDUCED PRE-IGNITION:

Controlled and flexible introduction of oil droplets

- Impact of droplet size
- Impact of injection timing
- Oil composition effects on pre-ignition
  Oil-coking – injection into burnt gas

➢ **Flexible+controllable way to induce oil into the combustion chamber**

Oil-droplets from a single-hole injector

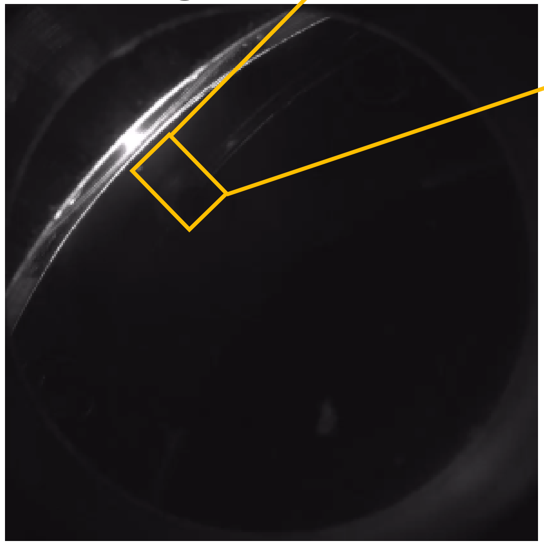


Preliminary results in operating engine

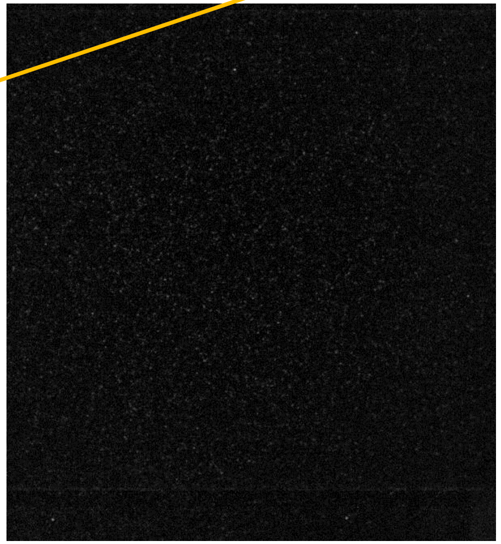
Operating condition
- CR = 10.3 : 1
- p_{BDC} = 1.7 bar
- T_{intake} = 140 °C
- φ_{H2} = 0.3

High-magnification camera

Low-magnification camera



OH* chemiluminescence



RESIDUAL-INDUCED PRE-IGNITION – PRELIMINARY RESULTS

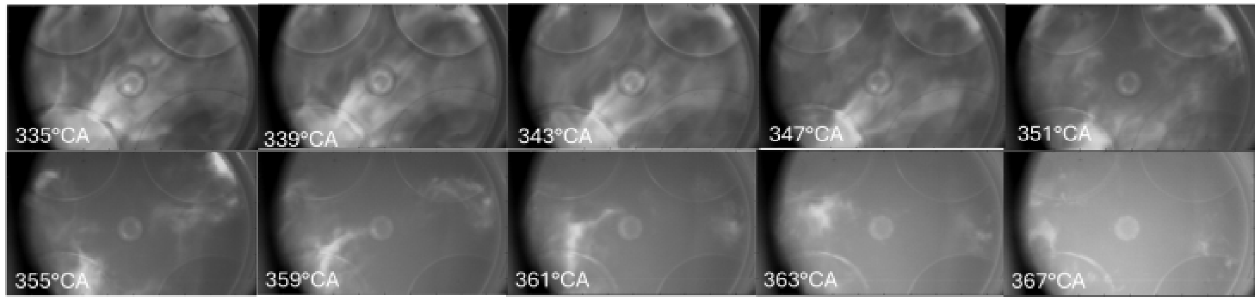
Approach:

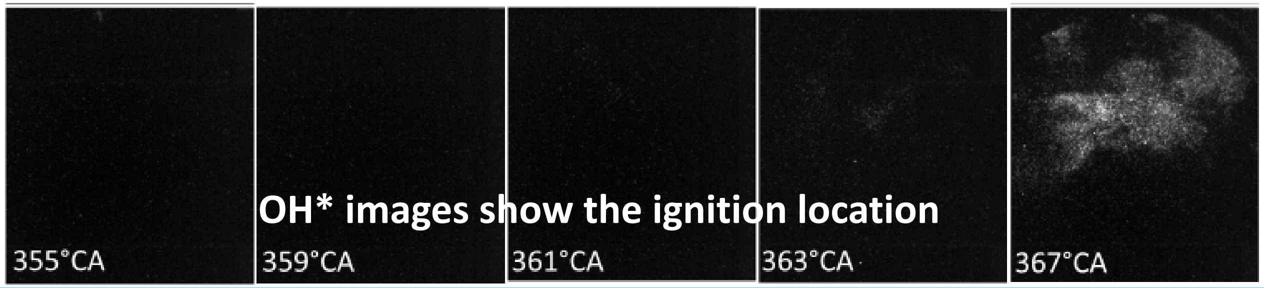
Controlled backfire by adjusting the temperature of combustion residuals and residence time

- Spark timing and equivalence ratio - temperature
- Intake-Exhaust pressure difference controls the residence time
- Fueled pre-chamber ensures fast combustion even for late spark timing

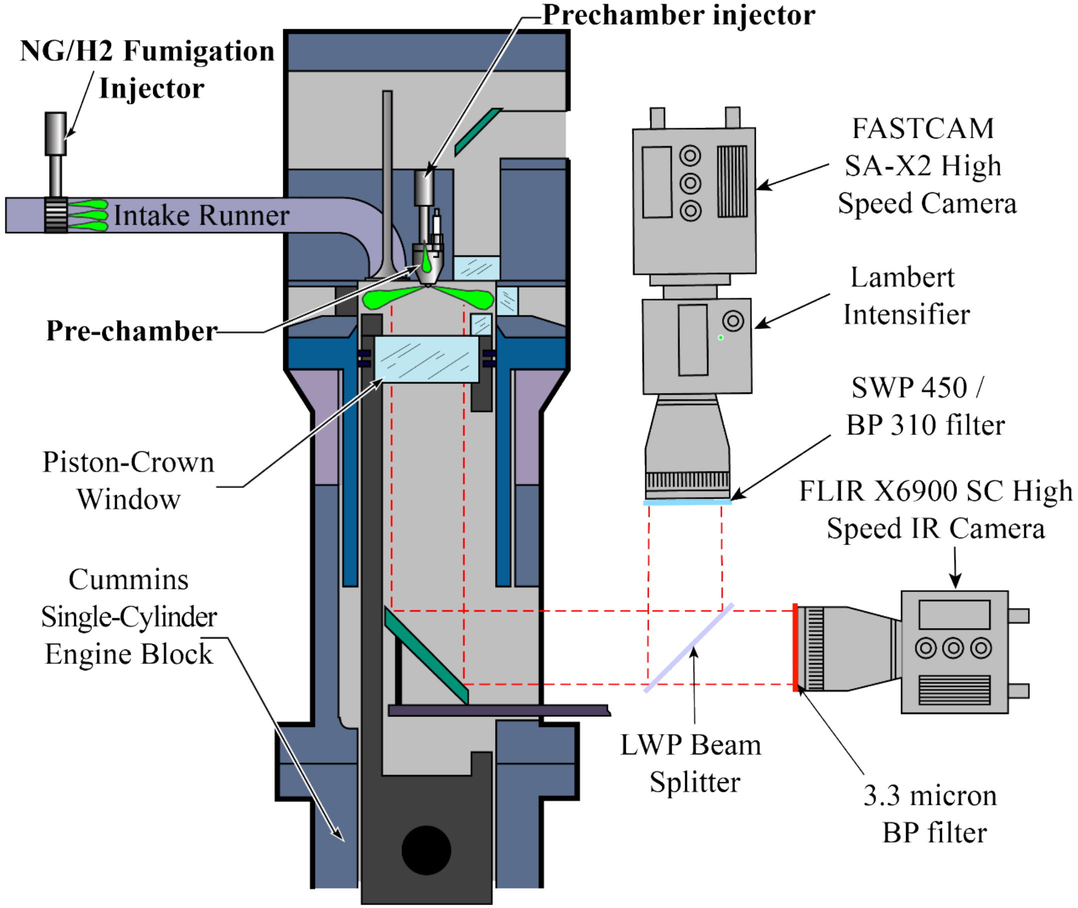
Visualization:

IR imaging shows location of residuals





Experimental setup



CONCLUSIONS

- **Sandia introduced a novel framework for studying pre-ignition in H2ICE**
  - Induced pre-ignition with a controlled and repeatable source
  - Explored the hot-spot pre-ignition, catalytic effects, oil-induced pre-ignition and combustion residuals
- **Hot-spot pre-ignition is strongly sensitive to in-cylinder pressure**
  - High pressure freezes auto-ignition reactions and slows pre-ignition
  - Late injection can mitigate hot-spot pre-ignition
- **Catalytic effects (Pt spark plugs) are likely not relevant in H2ICE applications**
- **Oil-induced pre-ignition is sensitive to local oil-vapor equivalence ratio**
  - Hydrogen has an inhibiting effect on lean hydrocarbon mixtures
  - Regions with high oil-vapor concentration (near droplets) might be more prone to trigger pre-ignition (need large-enough droplet)
- **Future research:**
  - Impact of oil droplet size on pre-ignition
  - The role of oil additives and oil coking
  - 0D/1D models describing residual pre-ignition and oil-droplet pre-ignition