Exceptional service in the national interest

DORMA001

Heavy-Duty H2 Combustion

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Combustion Research Facility

FY 2023 DOE Vehicle Technologies Office Annual Merit Review
Decarbonization of Off-Road, Rail, Marine and Aviation
Program Manager: Gurpreet Singh

DORMA001 OVERVIEW: HEAVY-DUTY H2 COMBUSTION

Timeline

- Project provides research that supports industry's H2 engine development projects
- Project directions and continuation are evaluated annually
- Project initiated in FY2022, FY2023 first time under review at AMR

Budget

- Project funded by DOE/VTO:
  FY2022: $400k
  FY2023: $450k

Partners

- BorgWarner, Argonne National Laboratory, University of Duisburg-Essen, Polytechnic University of Valencia, Danish Technical University
- Project lead: Sandia (Srna)

Barriers

(based on feedback from industry partners)

- Inadequate understanding of H2-ICE in-cylinder processes
  - Mixing and combustion, CFD simulation → suboptimal efficiency and higher NOx emissions
  - H2 pre-ignition root-causes → expensive hardware R&D and power density limitations
  - Flame-wall interactions and quenching → oil consumption and increased wall-heat losses
  - Advantages/disadvantages of advanced ignition systems (pre-chamber) → potential for pre-ignition, benefits?, combustion evolution
- Air management system requirements for ultra-lean operation
- Mitigation of engine-out NOx emissions and development of low-cost aftertreatment
- Multi-fuel operation using single hardware configuration
- Predictive simulations of H2ICE combustion process

DORMA001: RELEVANCE/OBJECTIVES

Relevance

Hydrogen Internal Combustion Engines (H2ICE) are being actively developed by most (all) OEMs for decarbonization of difficult-to-electrify sectors

H2ICE market entry as early as 2023-2027

Market share projections by several U.S. OEMs indicate that for applications that require high-power density, have difficult cooling/packaging requirements, or need to operate in extreme ambient environments, H2ICEs are likely to gain and retain a significant market share to 2050 and beyond

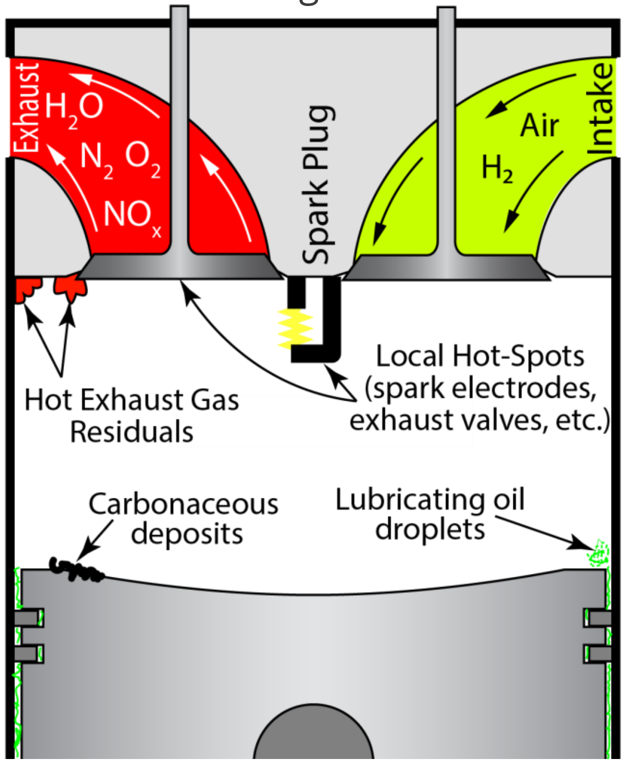
Long-Term Objective

Close the knowledge gaps pertaining to H2ICE in-cylinder processes and control strategies to allow industry to design and build cost-effective, high power H2 engines with emissions below zero-impact level

H2ICE – FUNDAMENTAL R&D KNOWLEDGE GAPS

Current OEM perspective:
Urgent need to bring a H2ICE product on the market quickly (PFI, modifying existing engines, efficiency is secondary)
Second generation H2ICE will be developed with focus on performance and emissions (DI, optimized configuration, etc.)

Understanding pre-ignition/knock mechanisms is key to successful mitigation



Challenges	Knowledge Gaps
Preignition & knock: mitigation and detection	Phenomenological understanding of key pre-ignition mechanisms
Injection and mixing: full optimization, NOx mitigation	In-cylinder mixing validation data Predictive CFD modelling Injector design guidelines
Flame/wall interactions Heat-loss, material thermal stress	H_2 near-wall quenching/reactions Accurate heat-loss models
Predictive simulations of H2ICE combustion process	Kinetics of H2/NG/renew. diesel fuel blends
Multi-fuel operation using single hardware configuration	Combustion strategies & controls
Reduced power density relative to diesel counterparts, efficiency	Strategies for increasing power density & efficiency
NOx emission in certain operating points	Alternative NO_x mitigation strategies (e.g. H_2O inj.)

Impact
Efficiency, range, emissions, cost, accelerated development

Improvements to existing products through component retrofit

DORMA001 MILESTONES

Long-Term Objective

Close the knowledge gaps pertaining to H2ICE in-cylinder processes and control strategies to allow industry to design and build cost-effective, high power H2 engines with emissions below zero-impact level

FY2022 (completed)

1) Database of in-cylinder H2-DI mixture-formation in a heavy-duty optical engine, using modern medium-pressure DI hardware
2) (internal goal, not tracked) Establish connection between injection parameters, in-cylinder mixture formation, early flame-kernel evolution and combustion cyclic variability
3) Engineering correlations linking the H2 pre-ignition likelihood to temperature of an electrically heated surface (artificial hot-spot) within the combustion chamber.

FY2023 (in progress)

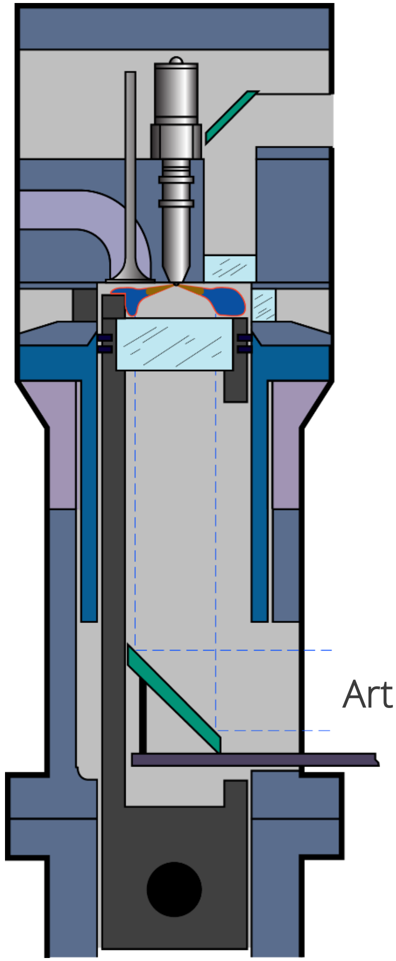
1) Evaluate in-cylinder mixing depending on injector nozzle configuration and the impact of engine swirl
2) (internal goal, not tracked) Engineering understanding of pre-ignition driven by surface catalytic effects and oil droplets.
3) (internal goal, not tracked) Develop framework to study hot-residual-gas pre-ignition under controlled and repeatable conditions

DORMA001: COLLABORATION & COORDINATION WITH OTHER INSTITUTIONS

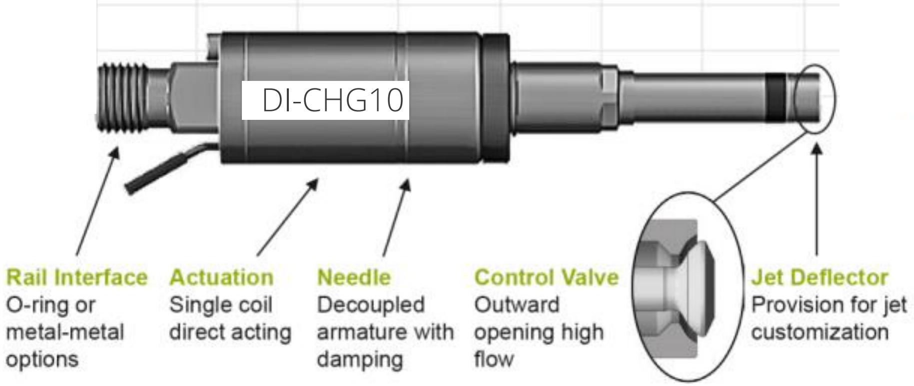
- All work has been conducted under the Advanced Engine Combustion Working Group in cooperation with industrial partners
  - Cummins, Caterpillar, DDC, Mack Trucks (Volvo), GE, Paccar, Gamma Technologies
- New research findings are presented at biannual meetings and directly to industry
- Tasks and work priorities are established in close cooperation with industrial partners
  - Both general directions and specific issues
  - Regular exchange with industry's H2ICE R&D engineers about our results (3-6 month period): Cummins, Caterpillar, BorgWarner, Bosch, Gamma Technologies, Wabtec, Paccar, Toyota Motor Company
- Government/University collaborations support experimental and simulation activities
  - University of Duisburg-Essen – in-cylinder H2 mixture formation
  - Polytechnic University of Valencia – H2 pre-ignition research and CFD of H2 and pre-chamber combustion processes
  - Argonne National Laboratory – CFD of H2-DI in-cylinder mixture formation

DORMA001: APPROACH - OPTICAL IMAGING & NUMERICAL MODELING OF IN-CYLINDER CHEMICAL/PHYSICAL PROCESSES

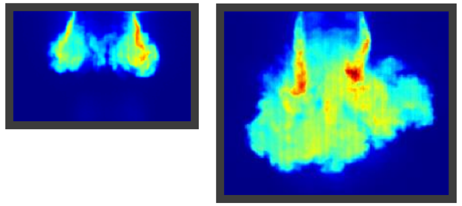
Heavy-duty (2.34 L/cyl.) optical engine

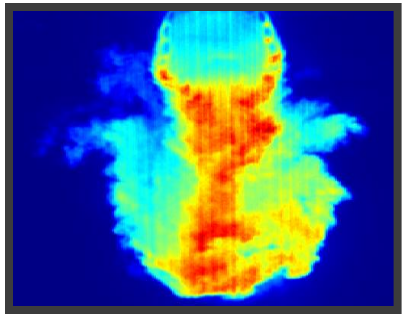


BorgWarner medium-pressure direct injector

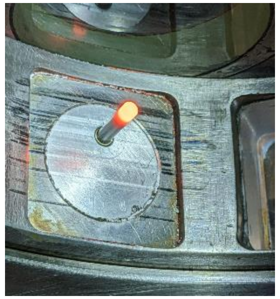


Laser-imaging of H2 jet evolution

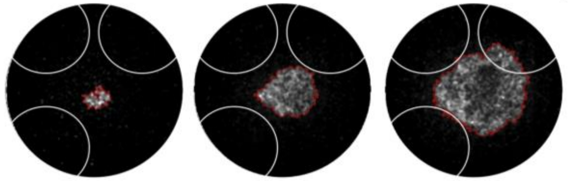




Artificial/controlled hot-spot



Imaging of flame evolution



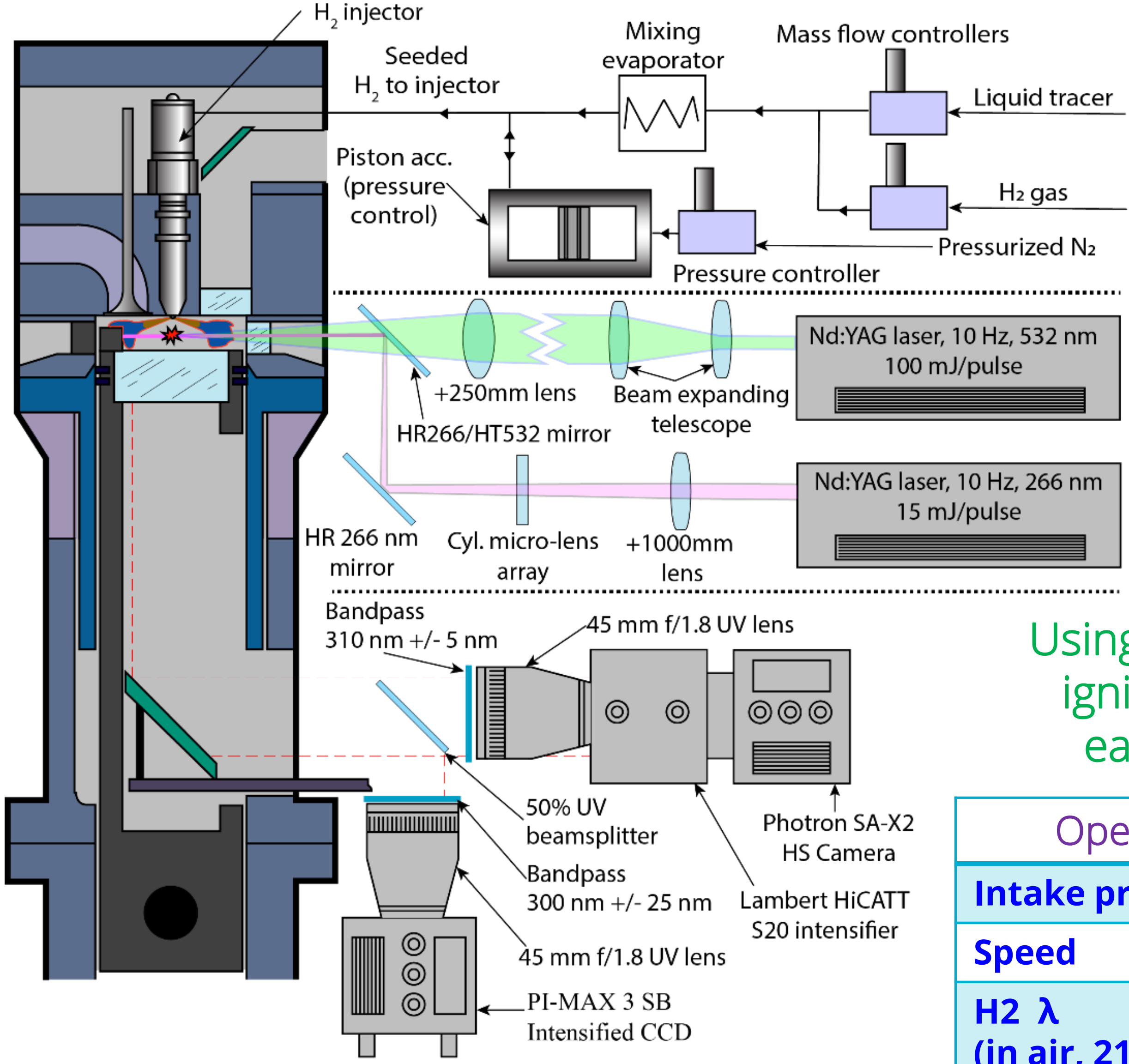
General approach

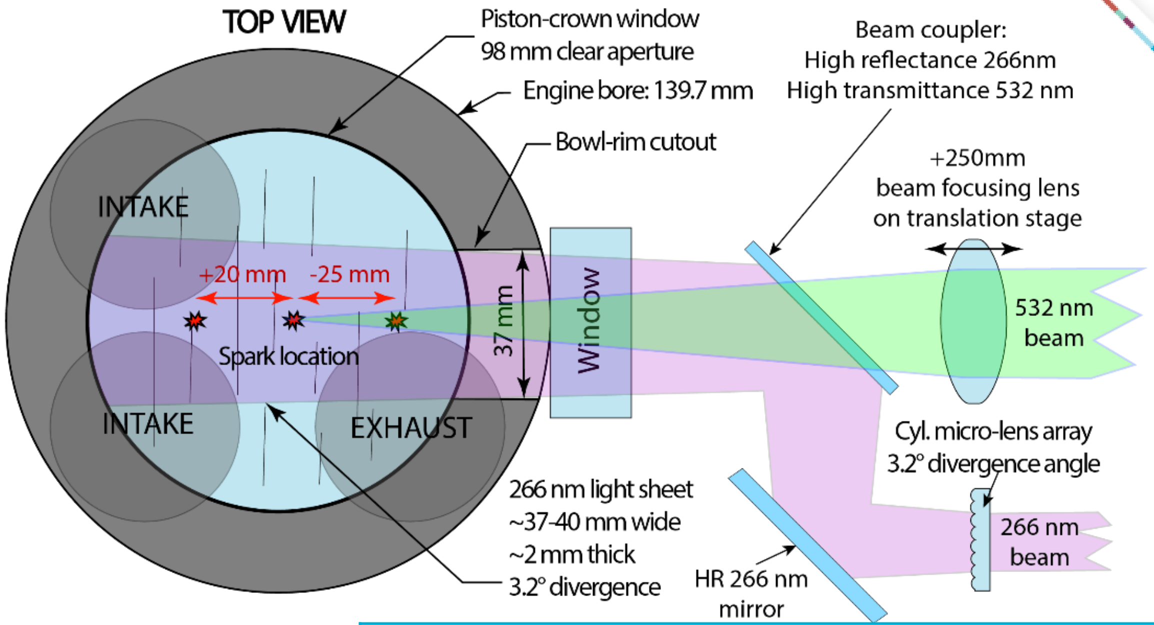
- Combine optical and planar laser-imaging diagnostics in an optical heavy-duty engine with computer modeling to close the knowledge gaps impeding H2ICE development
- Transfer fundamental understanding to industry through working group meetings, individual correspondence, and publications

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.

DORMA001: TECHNICAL ACCOMPLISHMENTS AND PROGRESS: CHARACTERIZATION OF IN-CYLINDER MIXING AND FLAME EVOL.





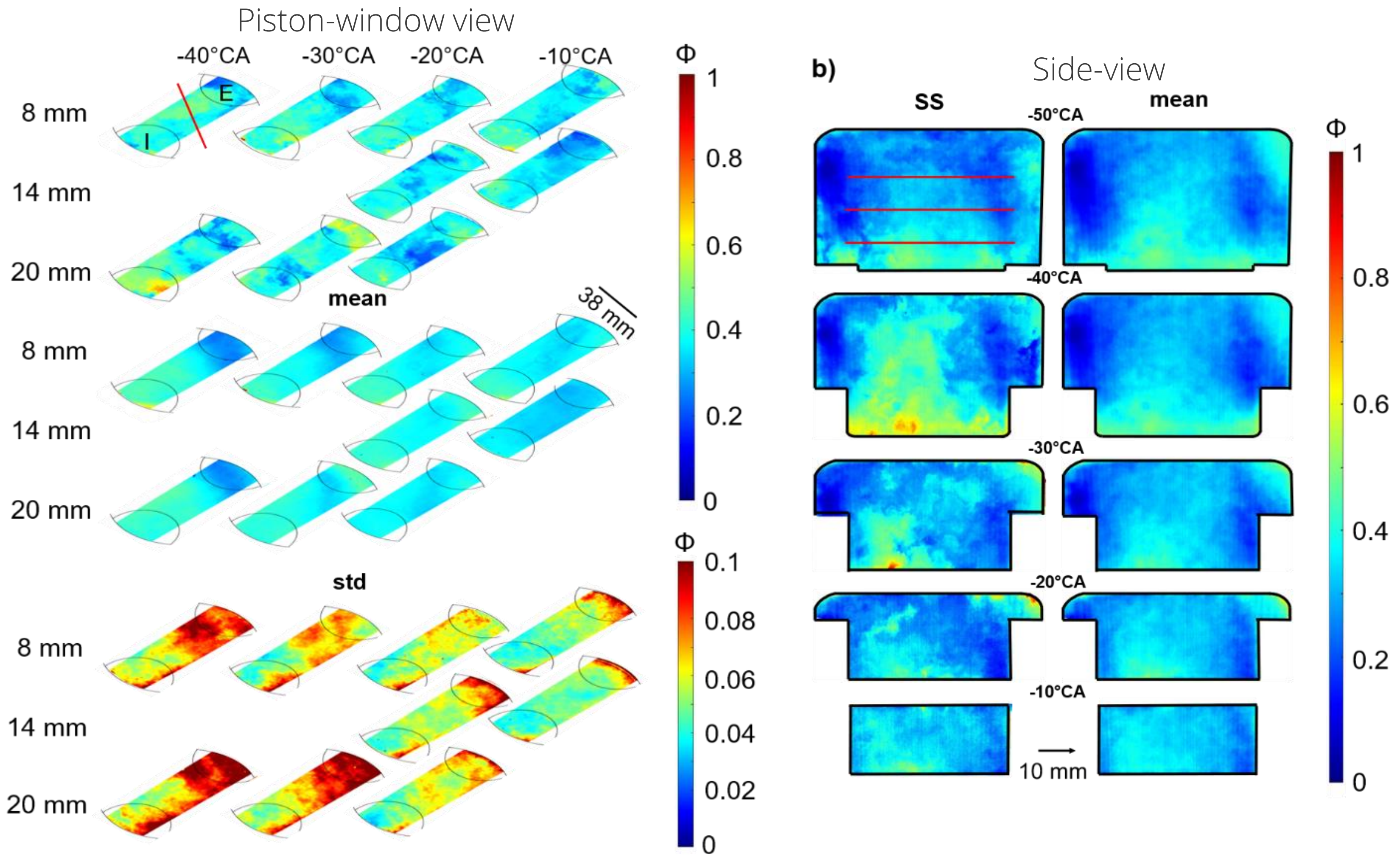
Using laser ignition, the ignition location can easily be changed

Operating conditions	
Intake pressure	1 bar
Speed	1200 RPM
H2 λ (in air, 21% O2)	3

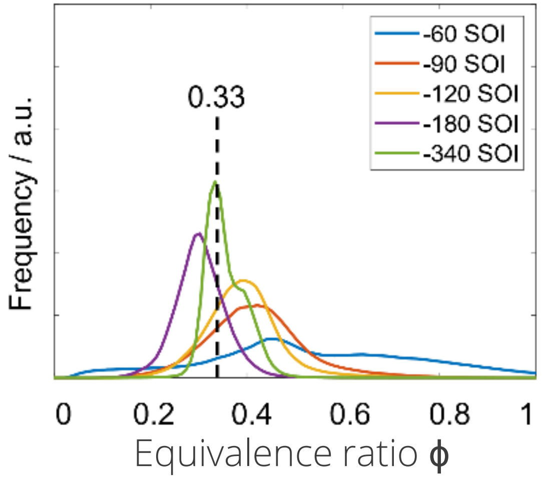
Measurements matrix	
Injection timing [CAD]	(-340°, -180°, -120°, -90°, -60° bTDC)
Injection press. / duration	40 bar / 2.27 ms 20 bar / 4.40 ms
Spark timing	-20 °, -10°
Light sheet	14mm below firedeck
Spark location	14mm below firedeck: Center of cylinder +20/-25mm from center

IN-CYLINDER MIXING DATABASE INCLUDES FULL QUANTITATIVE 3D INFORMATION ABOUT MIXTURE AT SPARK TIMING, INCL. STATISTICS

Sample dataset for a single operating condition: SOI = -120°CA, P_{inj} = 40bar



Mixture statistics

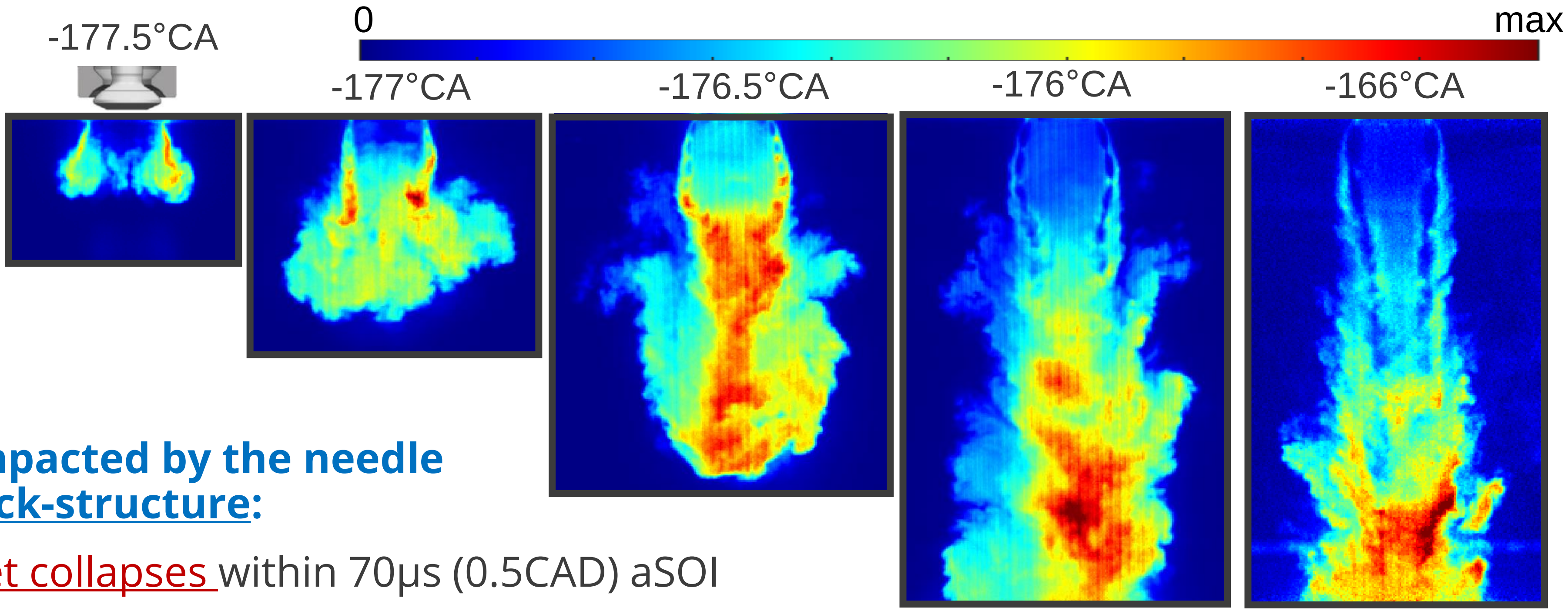


Database available on request, in process of publishing on ECN page

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

TRACER-PLIF IMAGING OF EARLY JET EVOLUTION REVEALED A COLLAPSED JET WITH SIGNIFICANT INTERNAL SHOCK STRUCTURE

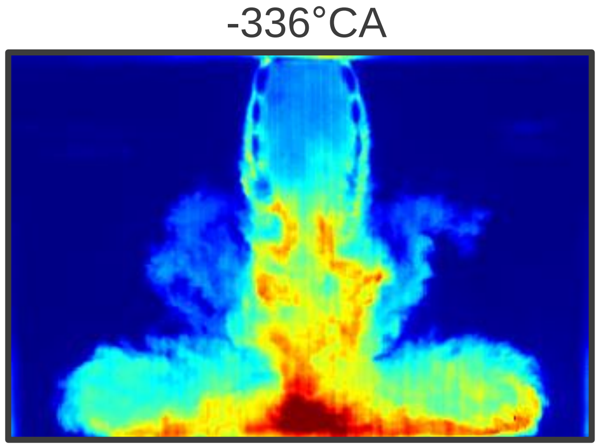
(qualitative imaging for
early jet evolution)



The jet pattern is impacted by the needle motion and the shock-structure:

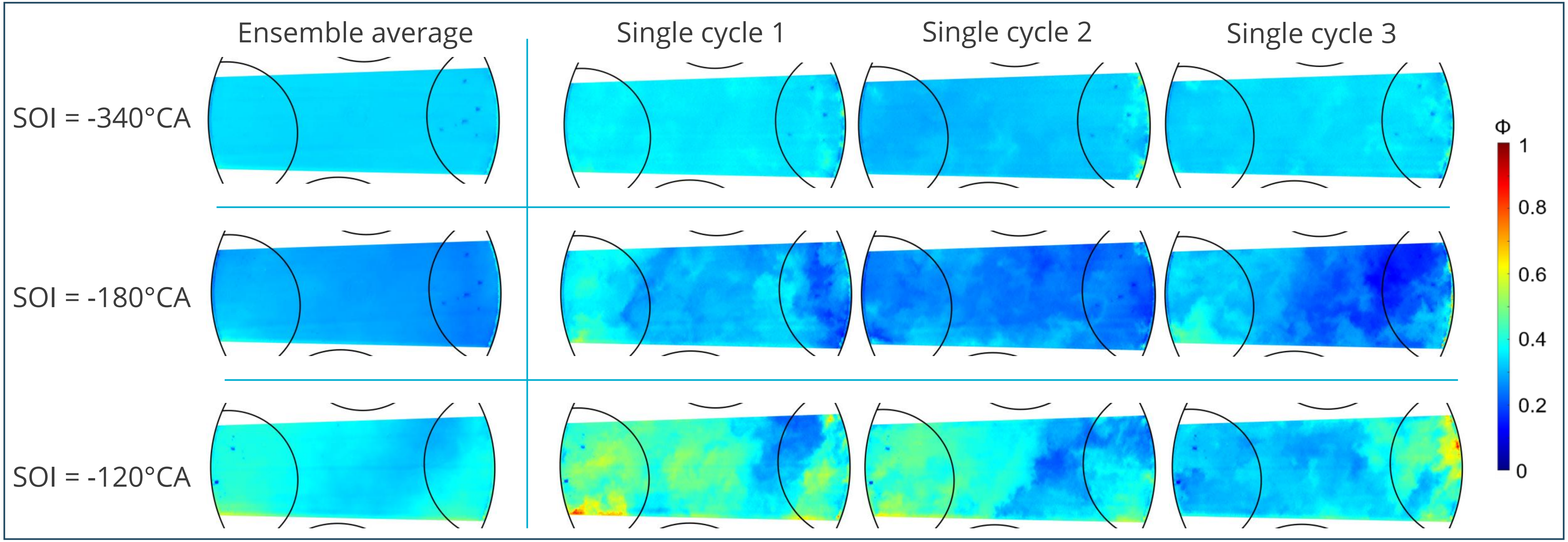
- The hollow-cone jet collapses within 70μs (0.5CAD) aSOI
- Under-expanded shock pattern extends for a significant distance from the nozzle
- Jet behaves similarly as a single-hole jet – fuel penetrates along the injector axis, impinges on piston and recirculates

Reproducing the shock pattern and jet collapse is a challenge for CFD. This data can help validate numerical modelling.



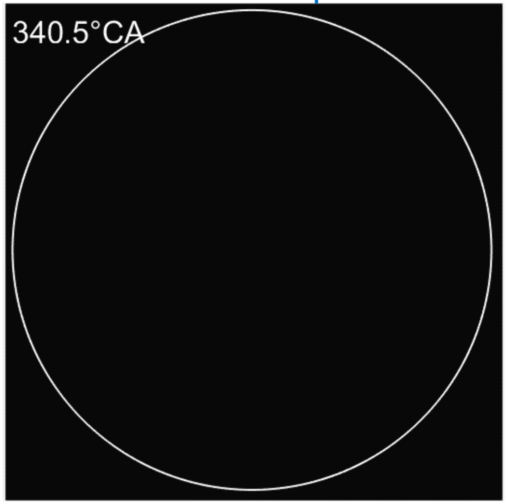
HIGH CYCLIC VARIATION IN MIXTURE DISTRIBUTION MAY HAVE IMPLICATIONS FOR NO_X AND COMBUSTION CYCLIC VARIABILITY

- Mixture becomes increasingly stratified with delayed injection timing
- High cyclic variability of local mixture even for early injections, which are near-homogeneous in ensemble average
  - Implications for NOx modelling, RANS CFD simulation, optimal spark location, combustion variability
  - **Optimization of injector configuration and engine flow needed for more repeatable and faster mixing**

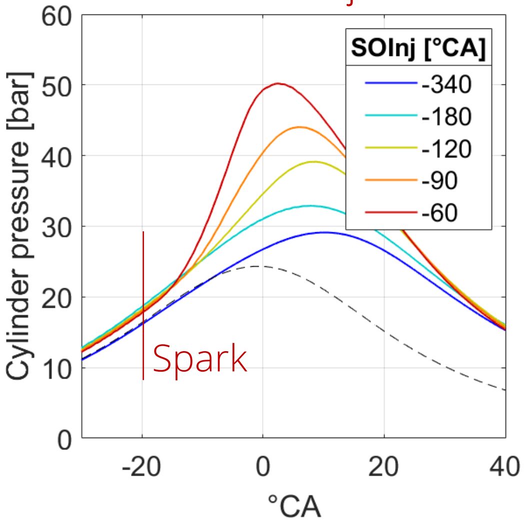


THERMODYNAMIC TRACES AND COMBUSTION STATISTICS

OH* H2 combustion video with laser spark



Averaged in-cylinder pressure central spark, P_{inj} = 40 bar



Injection timing significantly impacts combustion speed and peak pressure:

- Injection during intake – H2 displaces part of air
- **Higher turbulence and mixture stratification with late injections accelerate combustion, but do not deteriorate the CoV (IMEP)**
- Correlation between mixture and flame evolution will reveal further insights

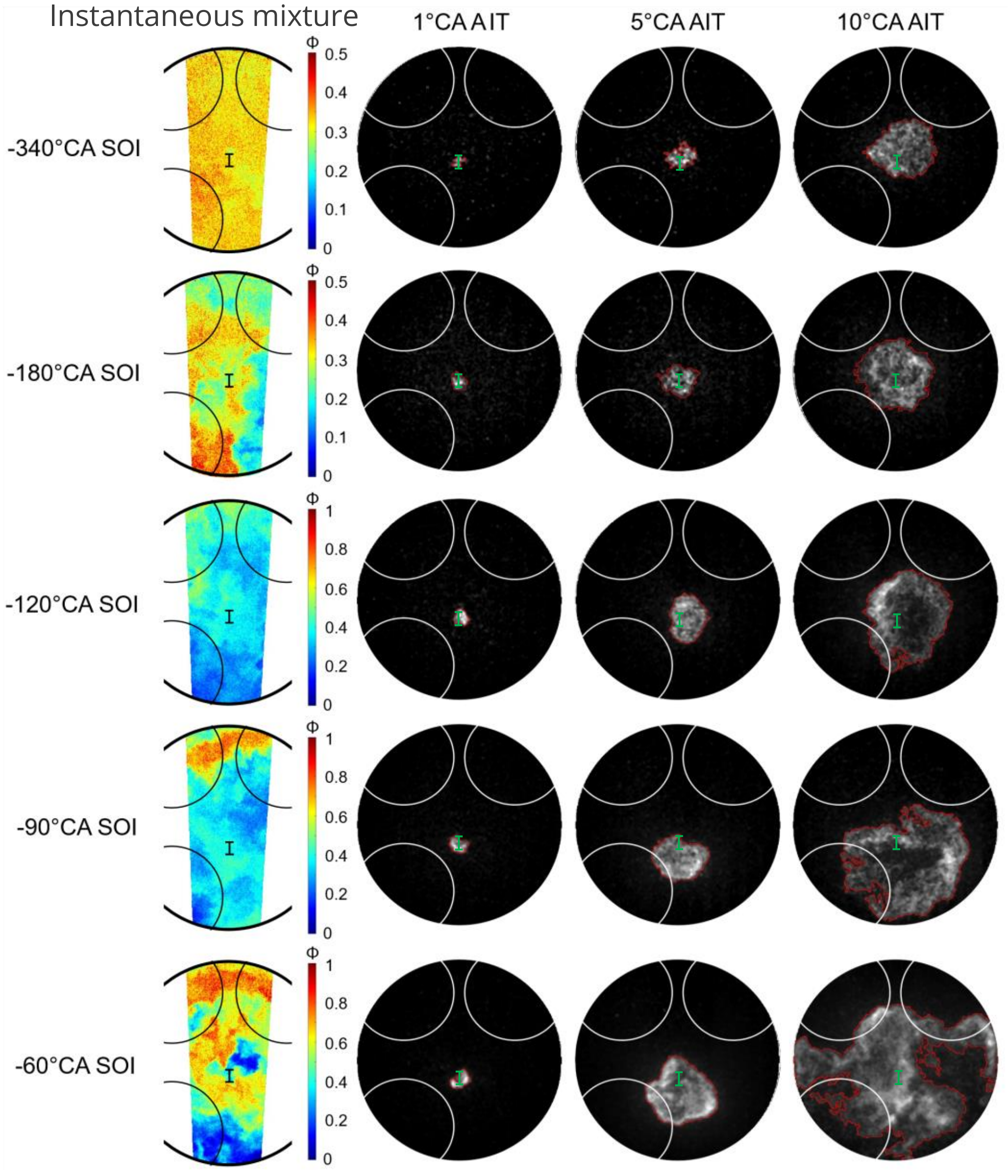
Statistics of IMEP and COV (P_{ini} = 40bar, ignition at -20°)

SOI	Spark position	IMEP	CoV (IMEP)
°CA	**mm**	**bar**	**%**
-340	+20	3.67	8.43
	central	3.82	1.64
	-25	3.7	2.81
-180	+20	3.28	19.72
	central	3.64	1.86
	-25	3.44	5.3
-120	+20	3.82	1.03
	central	3.76	1.03
	-25	3.72	1.85
-90	+20	3.86	1.06
	central	3.81	1.45
	-25	3.83	1.45
-60	+20	3.74	1.72
	central	3.77	1.96
	-25	3.92	1.96

Overall, combustion is very repeatable

Some ignition locations, with early injection, showed higher CoV

FAST EARLY FLAME KERNEL EVOLUTION TRANSLATES INTO SHORT COMBUSTION DURATION AS OBSERVED FROM PRESSURE TRACES

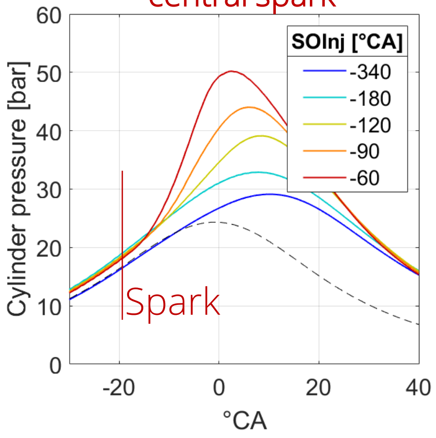


AIT – after ignition timing

Significantly faster early flame evolution with late injections

- **Stratification and injection turbulence effect**
- Directly translates into shorter combustion duration

Averaged in-cyl. pressure central spark



Local mixture does not solely govern flame evolution

- Flame evolution may not be concentric even with early injections
- Weak correlation between local fuel-mixture and flame propagation speed
  - Flow effects, convection
  - Out-of-plane mixture impact
- Some combinations of injection and ignition location create significant cyclic variability in direction of initial kernel propagation

Need to combine mixing and flow-field (PIV) diagnostics

FLAME PROBABILITY MAPS SHOW CLEAR IMPACT OF LOCAL MIXTURE ON EARLY FLAME KERNEL PROPAGATION SPEED

Flame probability map: **1)** binarize individual images; **2)** sum all binary images; **3)** divide by number of cycles

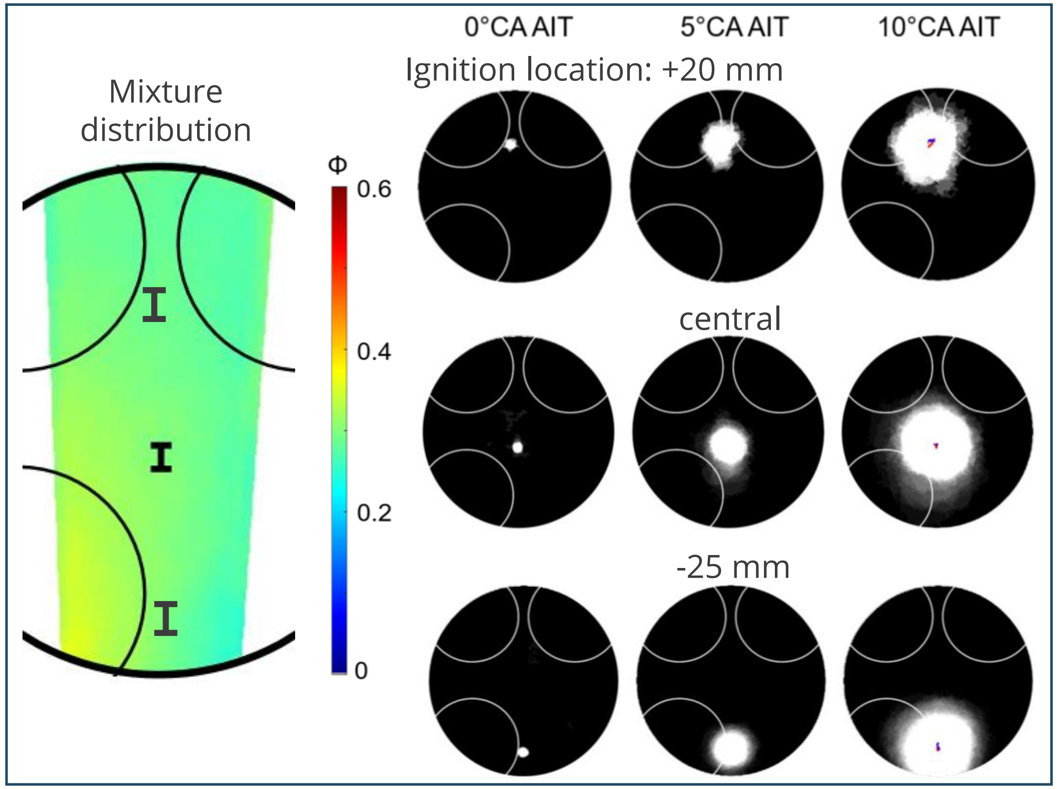
→ Visualization of cyclic variability of flame kernel evolution, and the speed of kernel growth

→ Connect mixing with speed of flame kernel growth, show any repeatable flame convection by flow

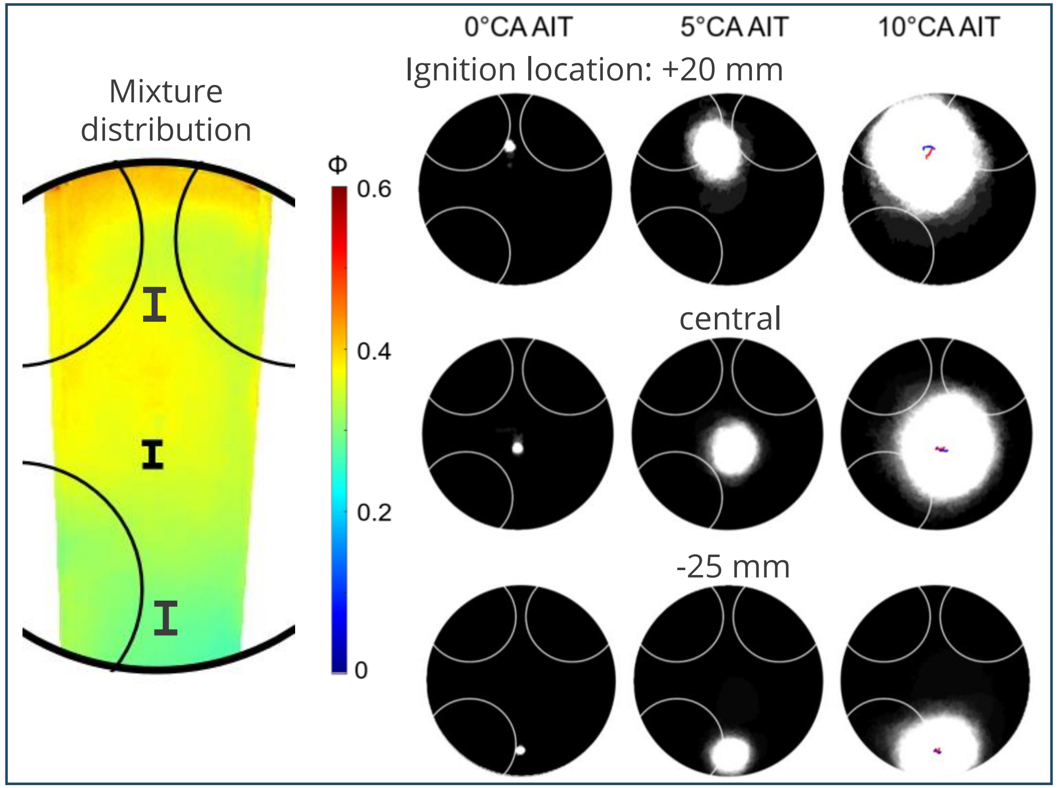
→ Minor effect with injection at -180°CA, strong impact with later injections (-120°CA).

→ Clear indication of importance of optimized engine configuration and calibration

SOI = -180°CA

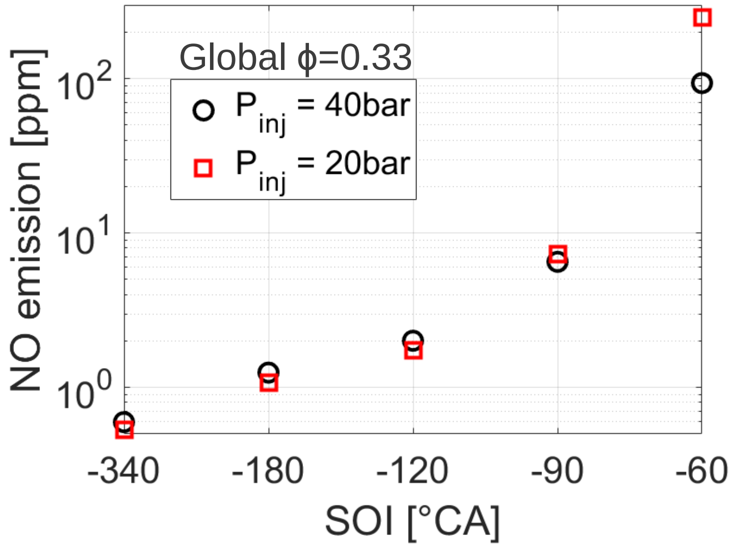


SOI = -120°CA



NO_X – CLEAR CORRELATION BETWEEN LOCAL MIXING AND NO_X EMISSIONS, ULTRA-LOW EMISSION POSSIBLE

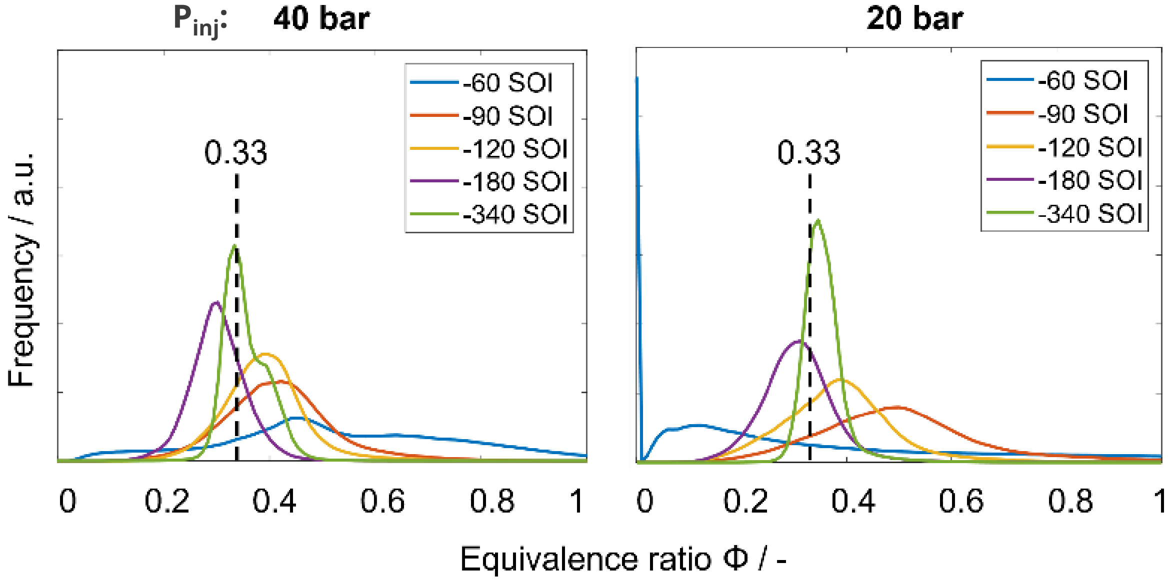
Engine-out NOx emission



Sub-ppm NOx emission possible with early injections

- Fast rise of NOx emission with delayed injection
  - 10 ppm equals about 0.09 g/kWh – still quite low
- Effect of injection pressure visible with late injections – slower mixing

PDF of in-cylinder mixture at ignition



Direct correlation between NOx and in-cylinder mixture established

- Opens the use of the mixing/combustion CFD validation database for validation of NOx formation models
- Critical equivalence ratio for NOx formation is established at ϕ~0.5
- Opportunities for development of 0D/1D engineering models

HOT-SPOT PRE-IGNITION – SETUP AND APPROACH

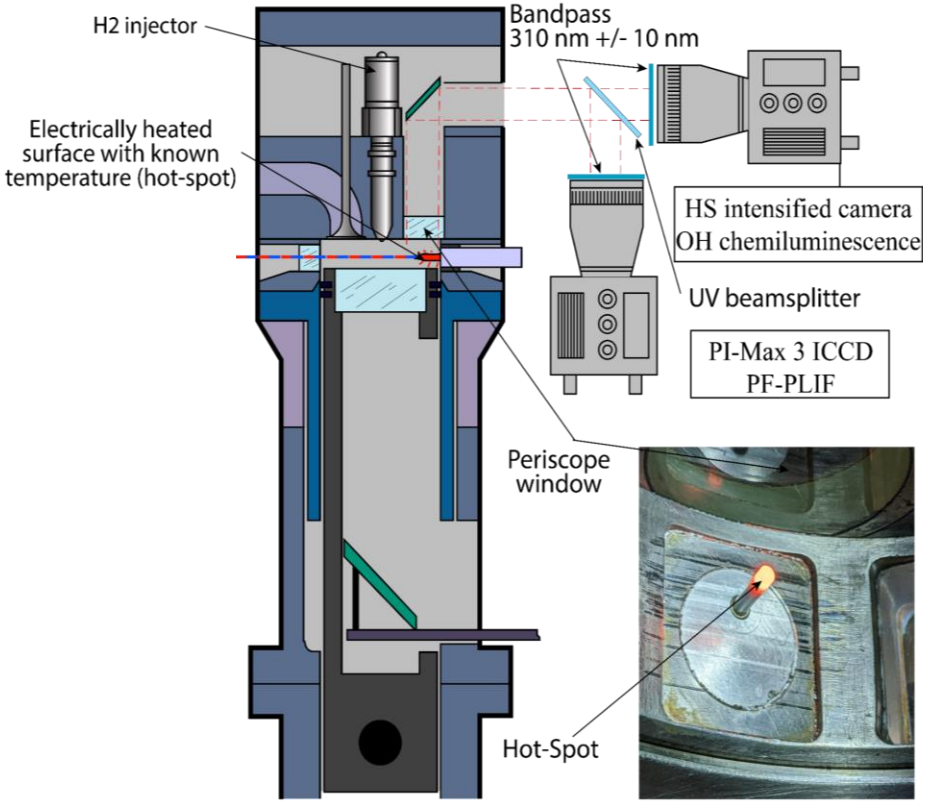
Goals of this research:

- Establish a framework that allows studying pre-ignition under controlled and repeatable conditions
- Understand **phenomenology of hot-spot pre-ignition** – understand the relevance of this mechanism in H2ICE

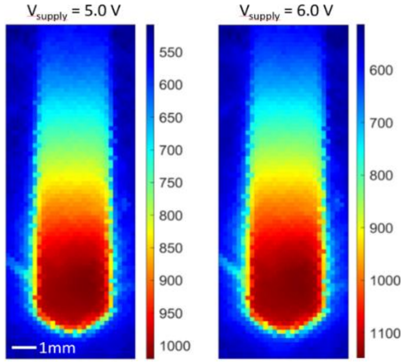
Measurements conducted:

- 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
  - low injection pressure
  - Φ=0.33
- Tracer-PLIF measurements
  - Mixing around the glow-plug
  - Used to characterize temperature stratification induced by the glow plug

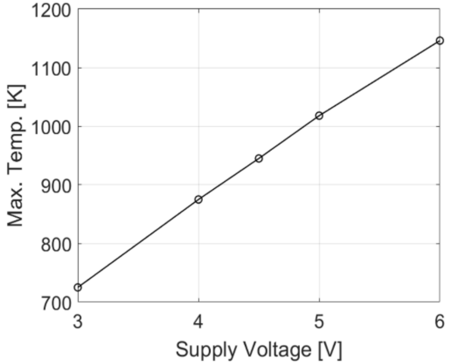
Test-setup to visualize and characterize hot-spot pre-ignition using direct hydrogen injection

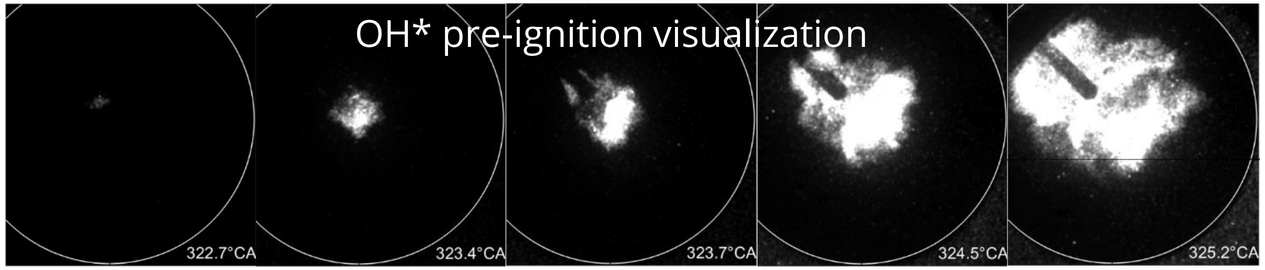


Glow-Plug temperature distribution



Max. surface temperature



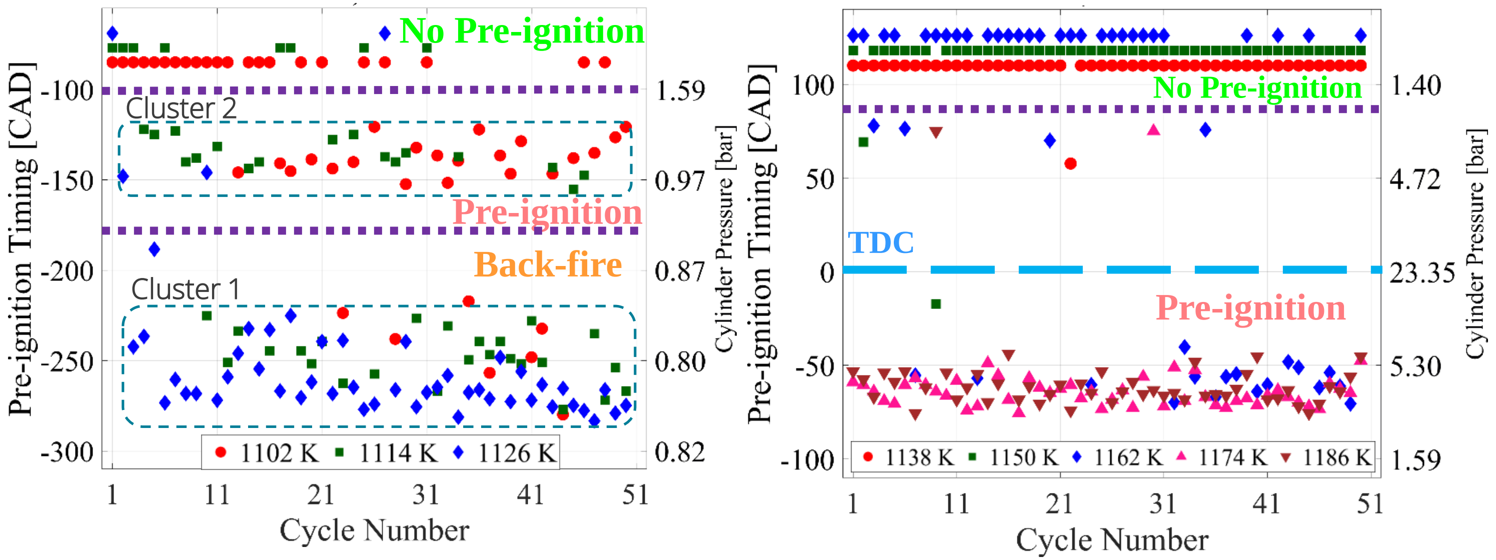

OH* pre-ignition visualization

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:

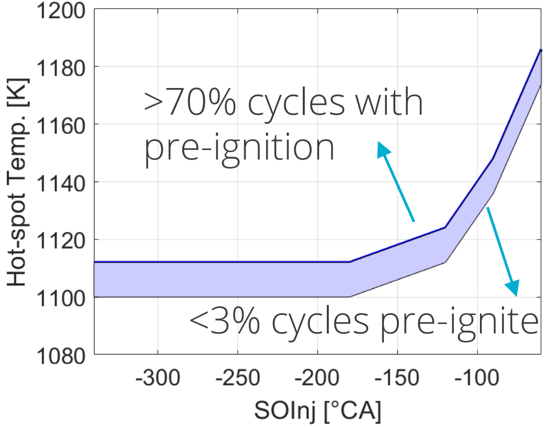
- Early injection: a cluster around -240°CA and around -120°CA.
- Later injection: a cluster around -60°CA, and some ignitions during the expansion stroke.
- Earliest pre-ignition timings governed by mixing – time it takes for the fuel to reach the hot-spot
- The variability of pre-ignition timing attributed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

Timing of pre-ignition

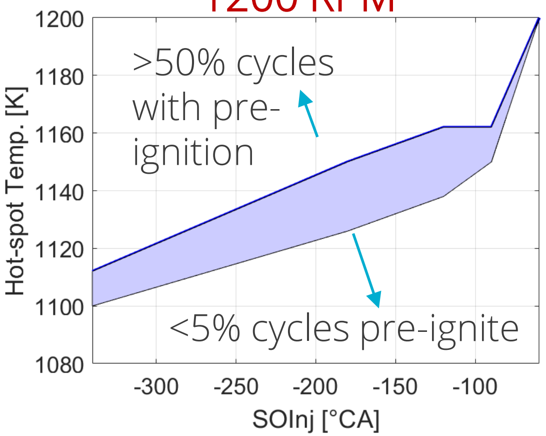

Early injection (-340°CA)

SOI = -120°CA

600 RPM



1200 RPM



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

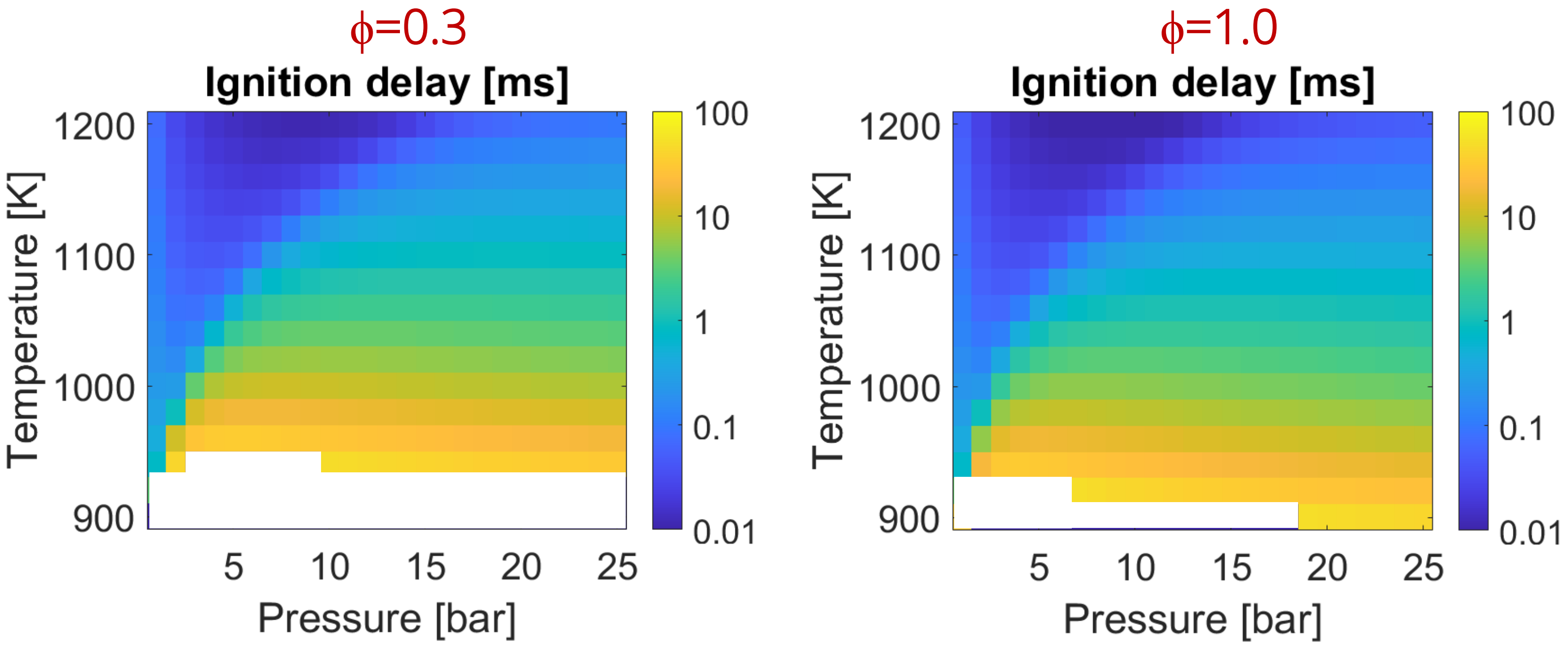
- 15-30 K temperature increase changes the engine operation from few-to-none pre-ignitions to nearly all cycles pre-igniting
- Likely associated with short residence time of gas near the exposed glow-plug surface. Future testing will explore the trends with more enclosed hot-spot.

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



Kinetics mechanism: LLNL H2 detailed

REMAINING BARRIERS/FUTURE PLANS:

Future plans:

Continue addressing the in-cylinder mixture formation and pre-ignition challenges, expand the scope to investigate ignition systems and wall-heat loss

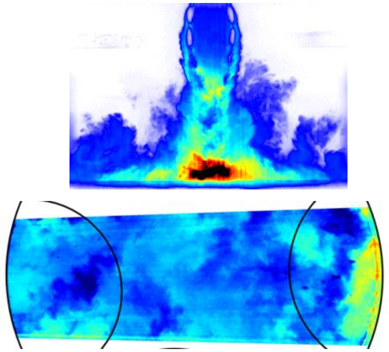
- Co-optimization of injector pattern, operating strategy and combustion chamber geometry based on imaging of in-cylinder mixture and velocity fields, and flame evolution
- Science-base and engineering correlations describing propensity of different pre-ignition mechanisms under varied operating conditions
- Collaboration with lubricant suppliers to develop low-pre-ignition oil formulations
- Characterize pre-chamber ignition in-cylinder combustion processes and it’s effects on pre-ignition
- Develop H2ICE wall heat transfer engineering models (with support of advanced CFD/DNS)

Longer-term plans

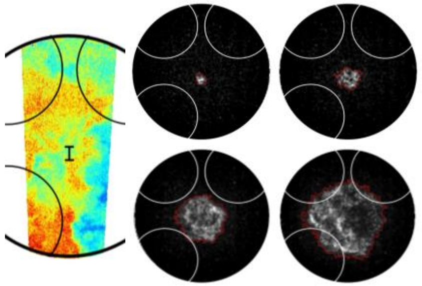
- Upgrade the HD optical engine facility to feature interchangeable tumble and swirl combustion chamber geometries to streamline optical engine hardware with H2ICE development trends
- Continued support of industry by conducting research aligned with H2ICE development trends: combustion chamber design, injection technology (pressure, injector configuration), ignition technology (spark, pre-chamber, dual-fuel),…

**Any proposed future work is subject to change based on funding levels*

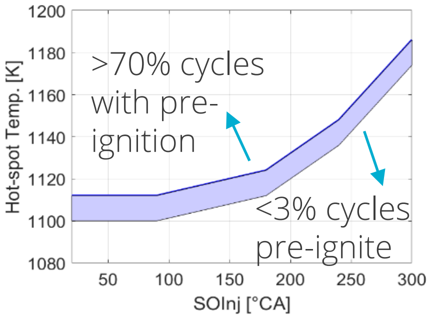
SUMMARY – DORMA001 – HEAVY-DUTY H2 COMBUSTION



Developed a database of H2-DI in-cylinder mixture formation using a modern medium-pressure injector, for validation of CFD simulation and 1D engineering models. High cyclic variability of local mixture even with early injections has implications for NOx formation and combustion cyclic variability, prompting future research to optimize injector configuration in synergy with in-cylinder flows.



Experiments with varying ignition location and injection strategy in conjunction with quantification of local mixture revealed the importance of optimized combustion chamber arrangement, and expanded the mixing database with fired engine operation results. High impact of in-cylinder flow on flame development was revealed, prompting future measurements to include PIV flow diagnostics.



Characterized the pre-ignition frequency relative to hot-spot temperature and injection timing → temperatures exceeding 1100K are needed to trigger pre-ignition, and pre-ignition occurred primarily at low in-cylinder pressure. Kinetic simulations explained the phenomenological observations and highlighted a potential mitigation pathway using late DI and high intake pressure.