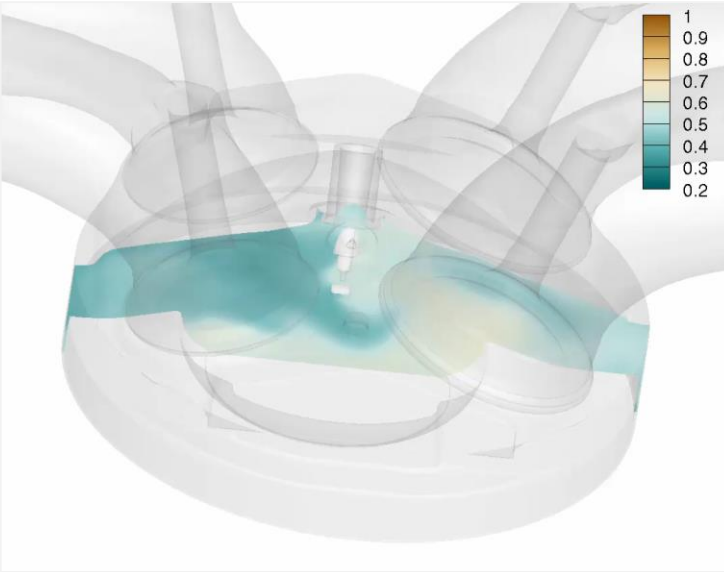
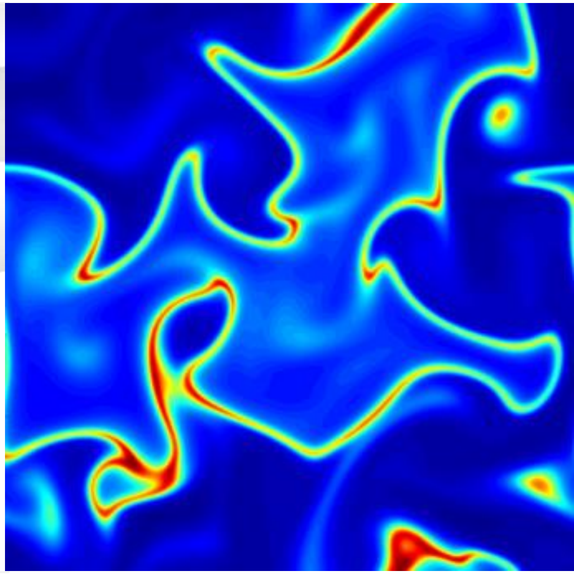
LARGE EDDY SIMULATIONS OF MULTI-CYCLE SACI COMBUSTION WITH AND WITHOUT PARTIAL FUEL STRATIFICATION





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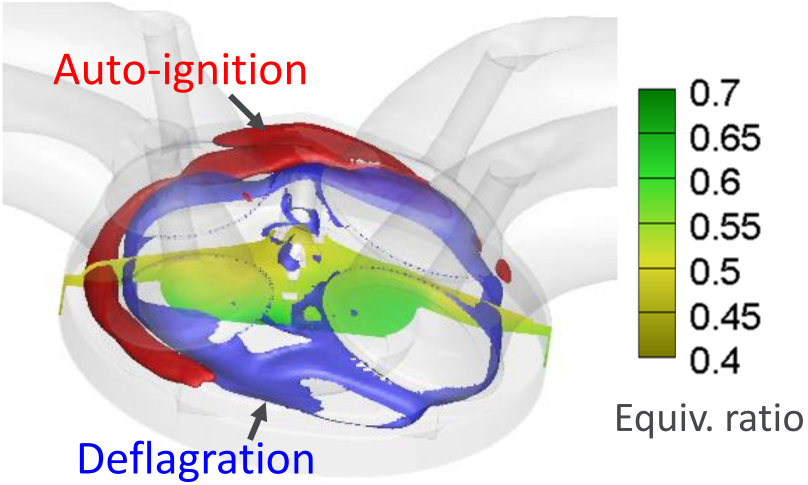
- Magnus Sjöberg (Sandia National Lab) for *experimental data*
- Convergent Science for *software licenses*
- ANL’s LCRC clusters for HPC resources

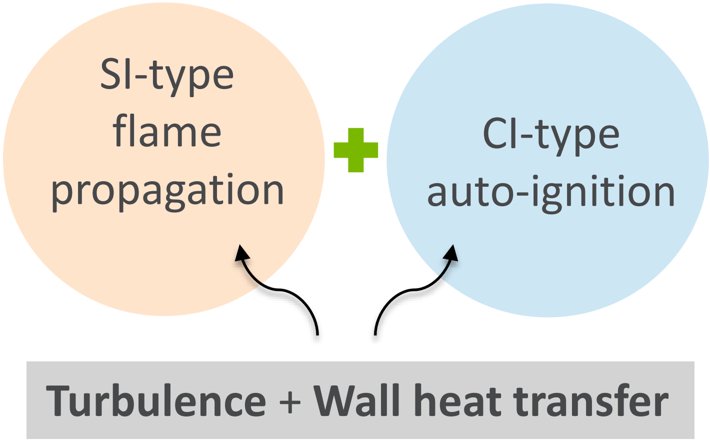
Co-Optimization of
Fuels & Engines

CHALLENGES IN MULTI-MODE COMBUSTION MODELING

- Lean/dilute spark-assisted compression ignition (**SACI**) is a promising multi-mode combustion strategy to improve engine efficiency and reduce emissions
  - Spark-induced flame propagation for better phasing control
  - Compression-induced auto-ignition for reduced combustion duration
- Modeling challenges
  - Models needed for both flame propagation and auto-ignition
  - Need for large detailed chemistry in both low-T and high-T regions
  - Need for flame-wall interaction model
  - Sensitive to boundary conditions, e.g., wall temperatures
  - Sensitive to fuel (compared with premixed flame modeling)
- Approaches:
  - RANS: low-fidelity, suitable for design optimization
  - LES: predictive modeling, reasonable computational cost
  - DNS: new physical insights, validating RANS/LES models

SACI combustion in a DISI engine

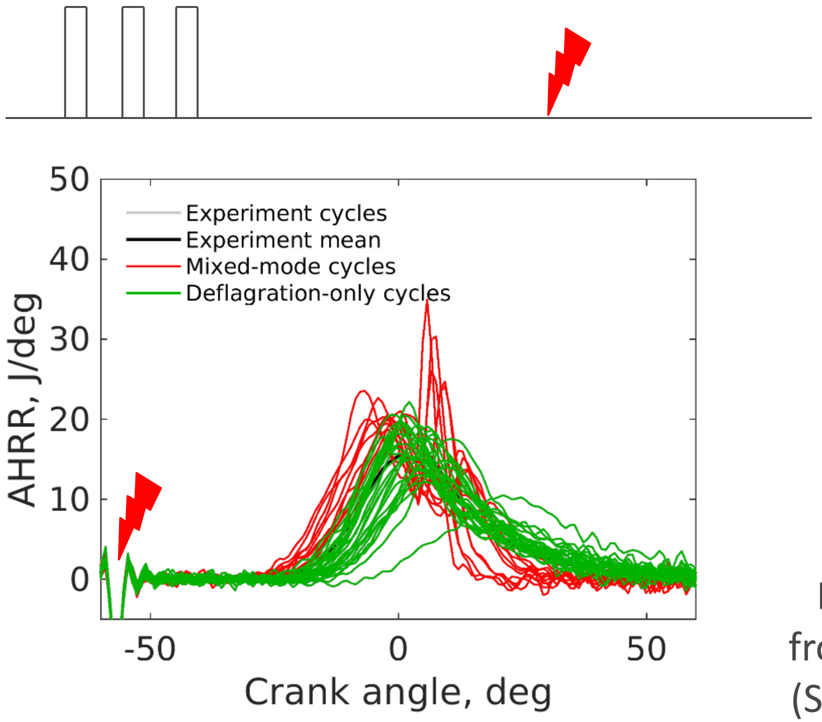




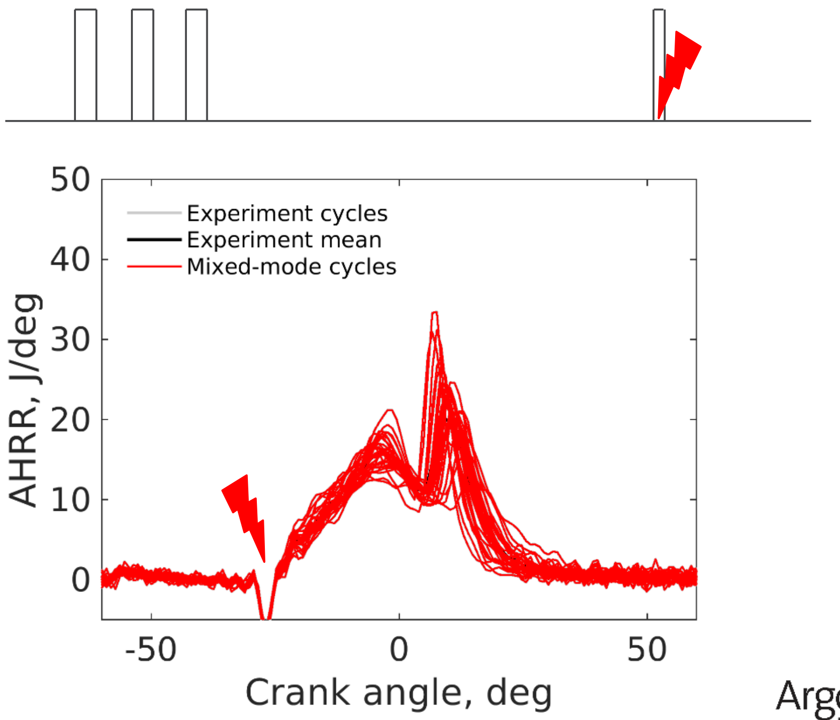
LEAN SACI OPERATIONS: WELL MIXED VS. PARTIAL FUEL STRATIFICATION ASSISTED

- When operating SACI in lean mixtures, conventional well-mixed operation requires advanced spark timing, and exhibits large cycle-to-cycle variability (CCV)
- Partial fuel stratification (PFS) can improve the combustion stability of lean operation by late-injecting small amount of fuel just before spark timing

Well-mixed SACI (WM-SACI)



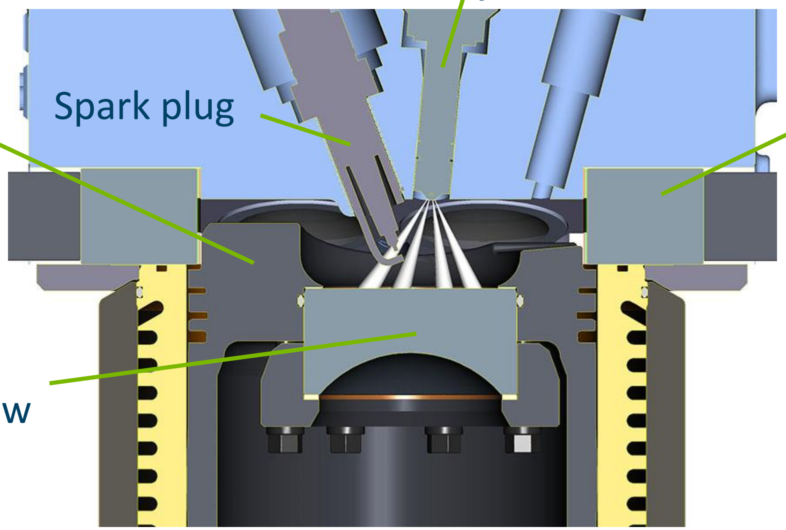
PFS-assisted SACI (PFS-SACI)



Experimental data from Magnus Sjöberg (Sandia National Lab)

ENGINE SPECIFICATION AND OPERATING CONDITIONS

Sandia Metal/Optical DISI Engine



Engine Specification

Parameter	Value
Bore	86.0 mm
Stroke	95.1 mm
Displacement	0.552 liters
Connecting Rod Length	166.7 mm
Piston Pin Offset	-1.55 mm
Compression Ratio	12:1

Operating Conditions

Parameter	WM-SACI	PFS-SACI
Engine Speed	1000 rpm	1000 rpm
Fuel/Air Equivalence Ratio	0.55	0.5
IMEP (Nominal, Net)	421 kPa	545 kPa
COV	2.2%	1.4%
Intake Temperature	100 °C	100 °C
Coolant Temperature	90/75 °C	90 °C
Intake Pressure	87.0 kPa	110.95 kPa
Exhaust Pressure	100.1 kPa	100.1 kPa
Injection Pressure	170 bar	166 bar
Injected Mass	17.8 mg	Early: 20.34 mg Pilot: 0.84 mg
Injection Timing, CA ATDC	-318, -303, -288	Early: -308, -288, -268 Pilot: -28
Injection Duration (each)	444 µs	Early: 437 µs Pilot: 210 µs
Spark Timing, CA ATDC	-57	-27
Fuel	E30	E30

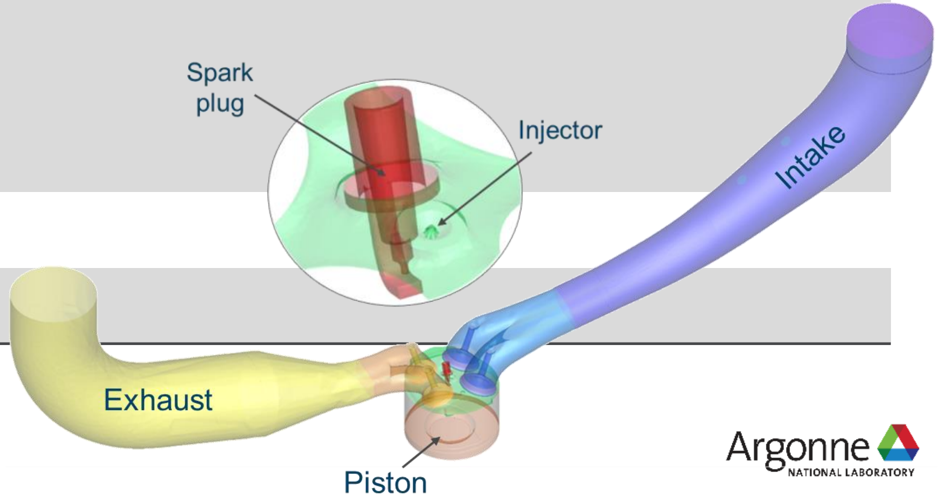
E30: RON105, MON91

MODELING APPROACHES

CFD code	CONVERGE 2.4
Turbulence	• Dynamic structure LES model
Spray	• KH-RT breakup • NTC collision model (model constant validated against ECN Spray G) • Frossling evaporation model

Combustion	• Hybrid G-equation/WSR model
	  • Flame propagation: G-equation with tabulated flame speeds
	  • Auto-ignition: Well-stirred reactor (WSR) multi-zone model

Spark ignition	• Spherical energy source with mesh refinement (0.125-0.25 mm)
Mesh	• Base: 4 mm; In-cylinder base: 1 mm; Near spark: 0.25 mm; Wall embedding: 0.5 mm; Spray embedding: 0.25 mm • AMR based on V&T: 0.5 mm • Peak cell count: 1.6 M
Fuel	• E30 (ANN-based TPRF-ethanol surrogate)
Chemistry	• 164-species skeletal mechanism



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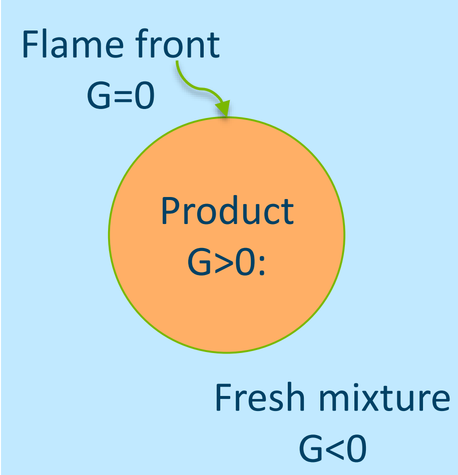
MODELING FLAME PROPAGATION AND AUTOIGNITION

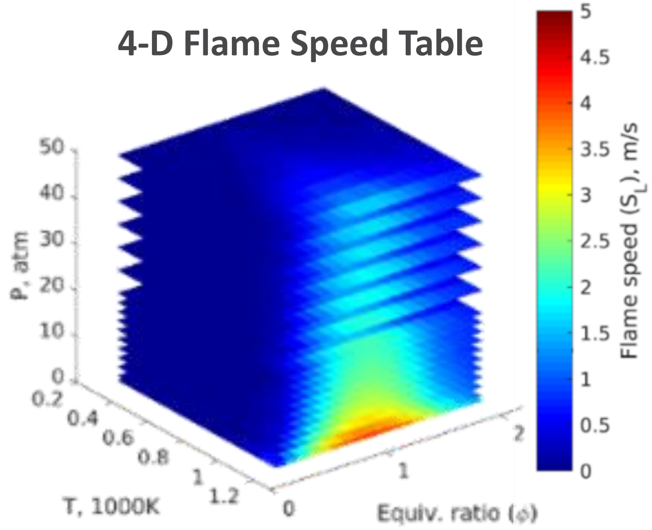
Track turbulence flame propagation using the G-equation model

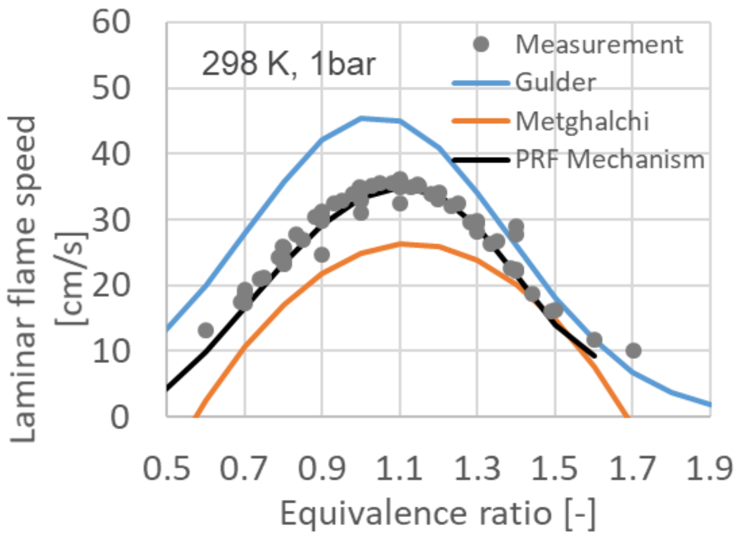
- Eliminate the need of resolving the thin flame structures
- Model turbulence-chemistry interaction (TCI) using Peter's turbulent flame speed correlation:

$$S_T = f(\boxed{S_L}, u'/S_L, Da) \qquad Da = Reaction\ rate/Mixing\ rate$$

- Tabulate laminar flame speed (S_L) as function of p, ϕ, T_0, and local residual gas fraction (RGF) using detailed chemistry







Predict end-gas auto-ignition using a hybrid approach

- With G identifying the end gas, well-stirred reactor (WSR) model is employed to model end-gas auto-ignition, and post-flame behaviors

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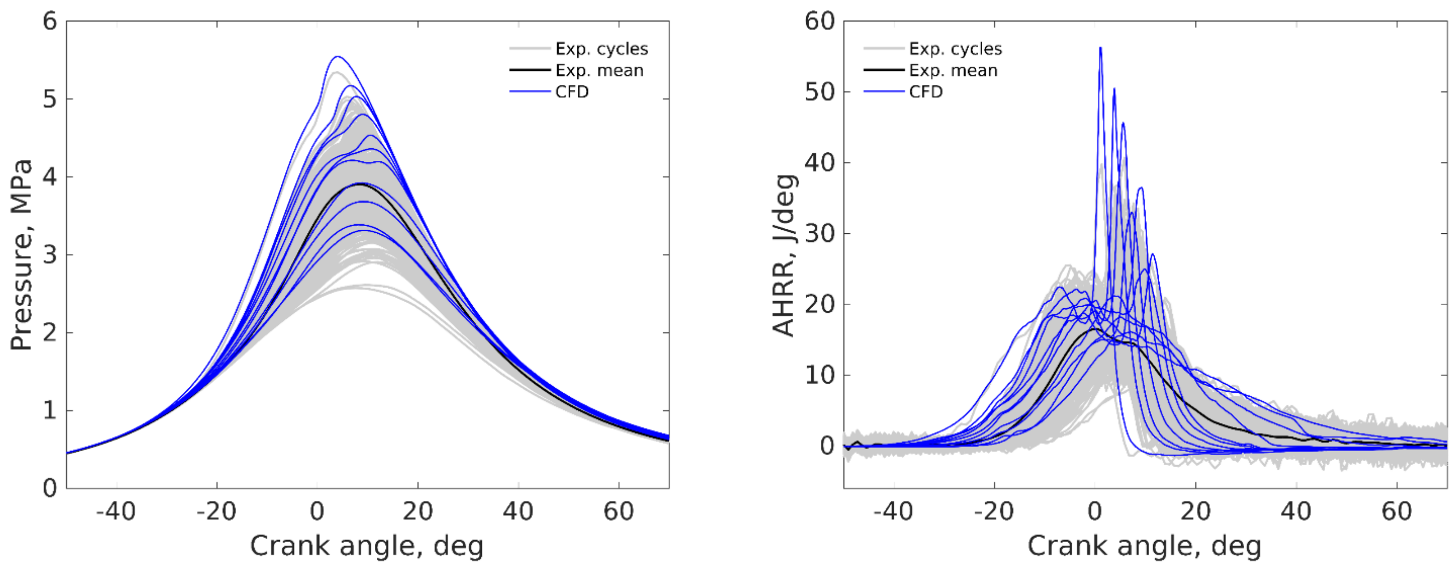
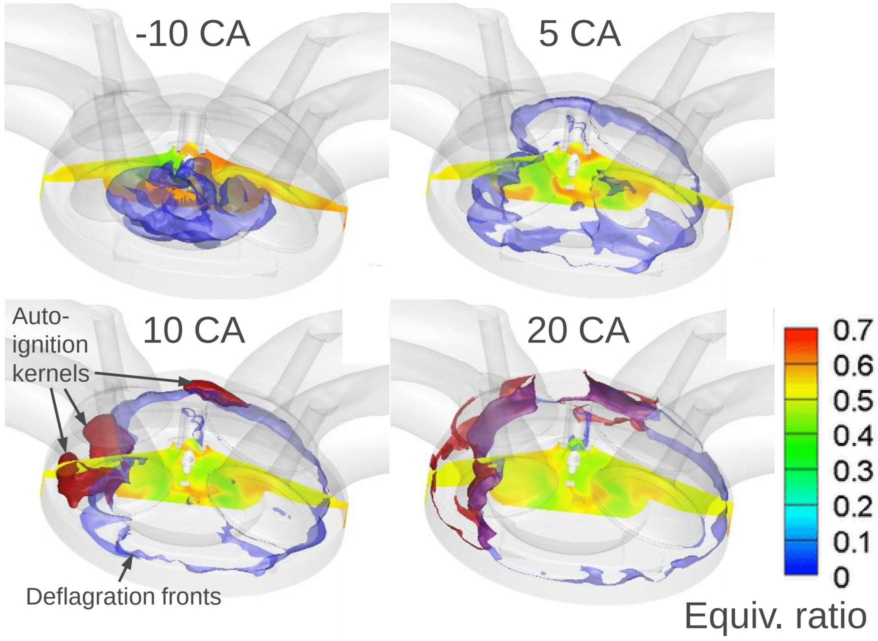
LES OF WELL-MIXED SACI: FLAME DYNAMICS

Pressure and heat release rate traces



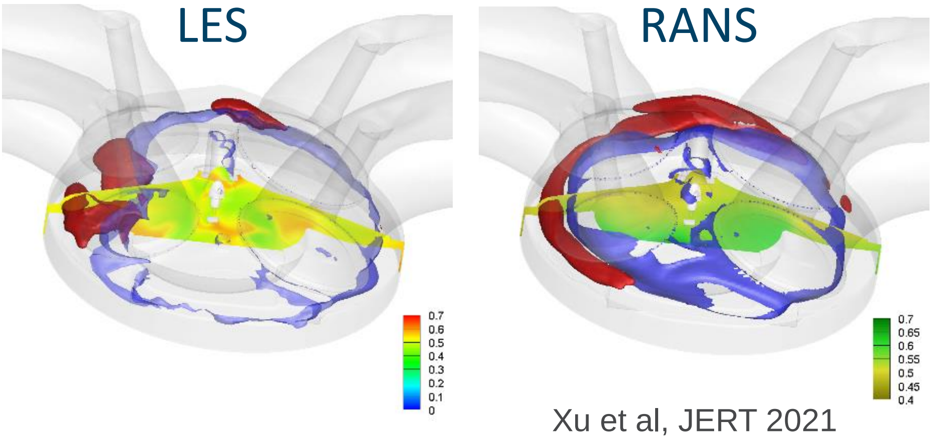
SACI flame dynamics



- 10 consecutive CFD cycles vs. 500 experimental cycles
- Pressure and heat release traces from simulation agree well with experimental data
- LES reveals detailed flame and autoignition dynamics in SACI combustion

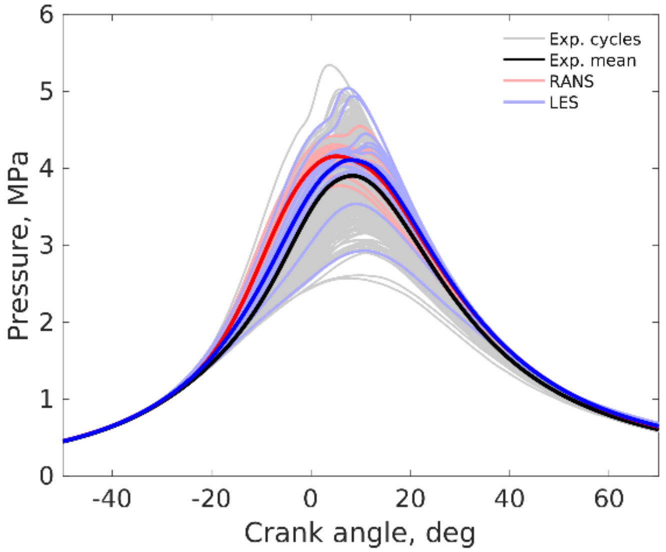
WELL-MIXED SACI: LES VS RANS

- LES is able to capture both deflagrative (1st AHRR peak) and auto-ignitive (2nd AHRR peak) combustion phasing, as well as CCV, while RANS fails
- Computational cost of the LES model is only slightly higher than RANS

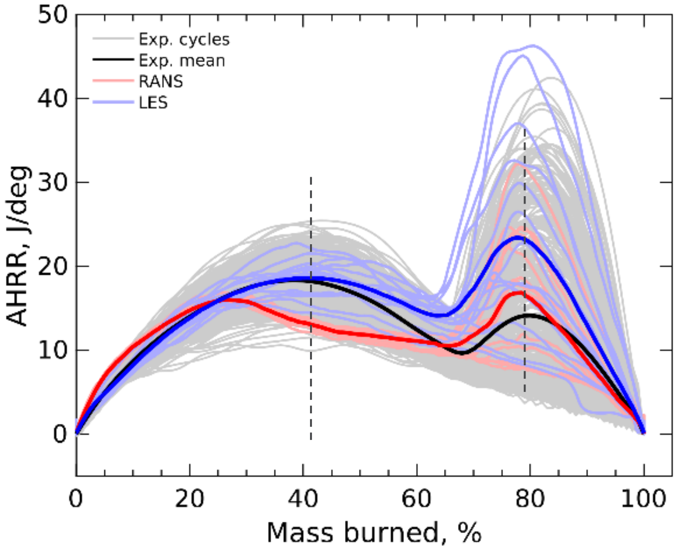


Quantity	Experiment	LES	RANS
P_{max}, MPa	3.93	4.14	4.17
COV of P_{max}, %	10.54	11.72	4.33
$IMEP_g$, kPa	446	513	497
COV of $IMEP_g$, %	3.82	2.42	0.90
CA10	-8.0	-11.6	-15.6
CA50	3.54	3.50	0.68
CA90	22.3	18.5	20.4

Pressure vs CA

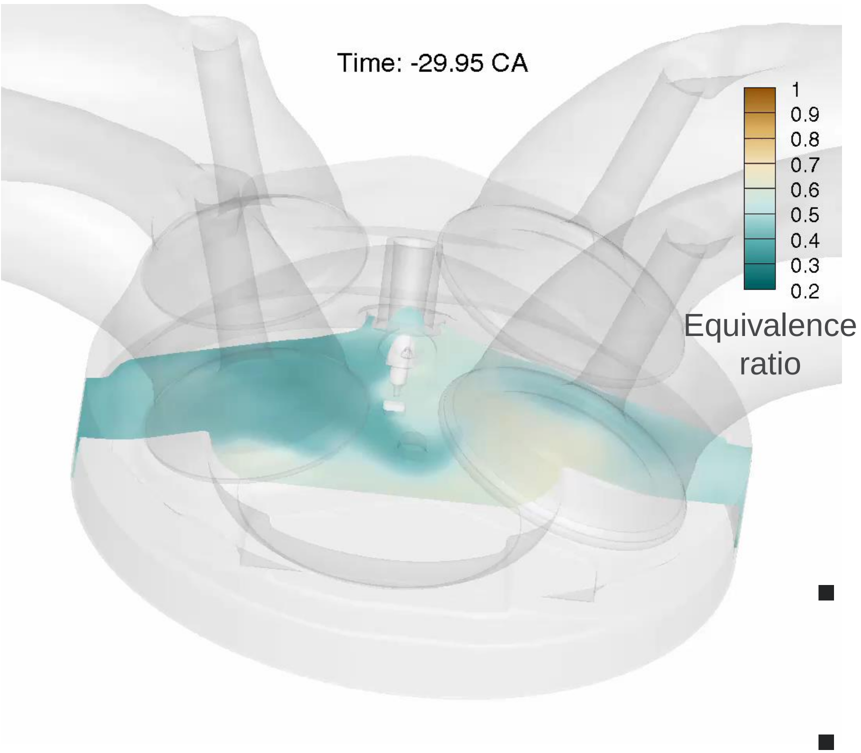


AHRR vs MFB



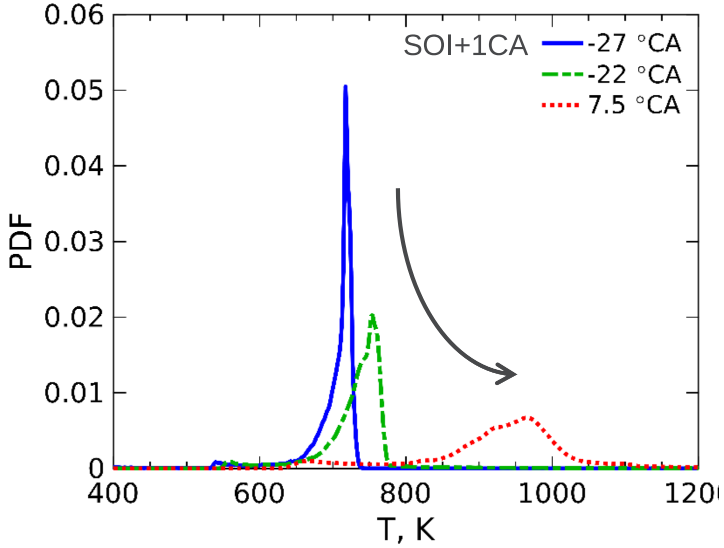
LES OF PFS-ASSISTED SACI: STRUCTURE AND THERMAL AND MIXTURE STRATIFICATION

LES of PFS-assisted SACI

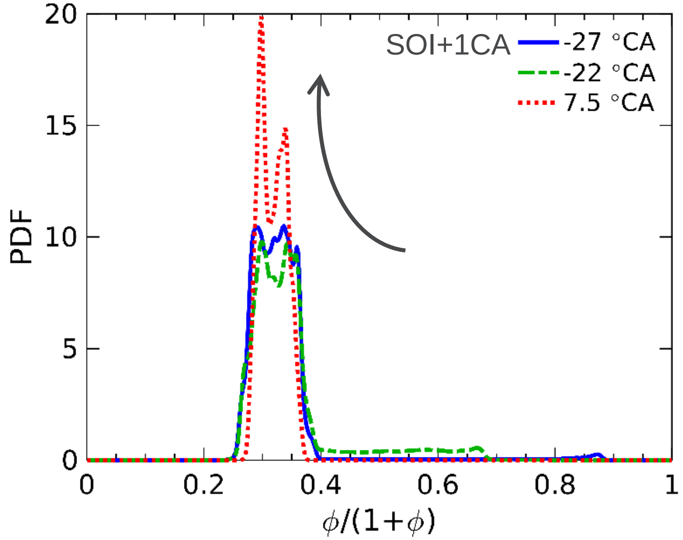


Isosurfaces: Purple: stoichiometric
Blue: flames; Red: auto-ignition

Thermal stratification



Mixture stratification



- Presence of different combustion modes: premixed flame propagation in stratified mixture and end-gas auto-ignition
- Evolution of temperature and equivalence ratio PDFs highlights the unique mixing process in PFS and its potential effects on combustion
  - Increased thermal stratification (wall heat transfer), but reduced mixture stratification (continuing mixing) with time after an initial jump

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PFS-SACI: FLAME KERNEL INITIATION AND DEVELOPMENT

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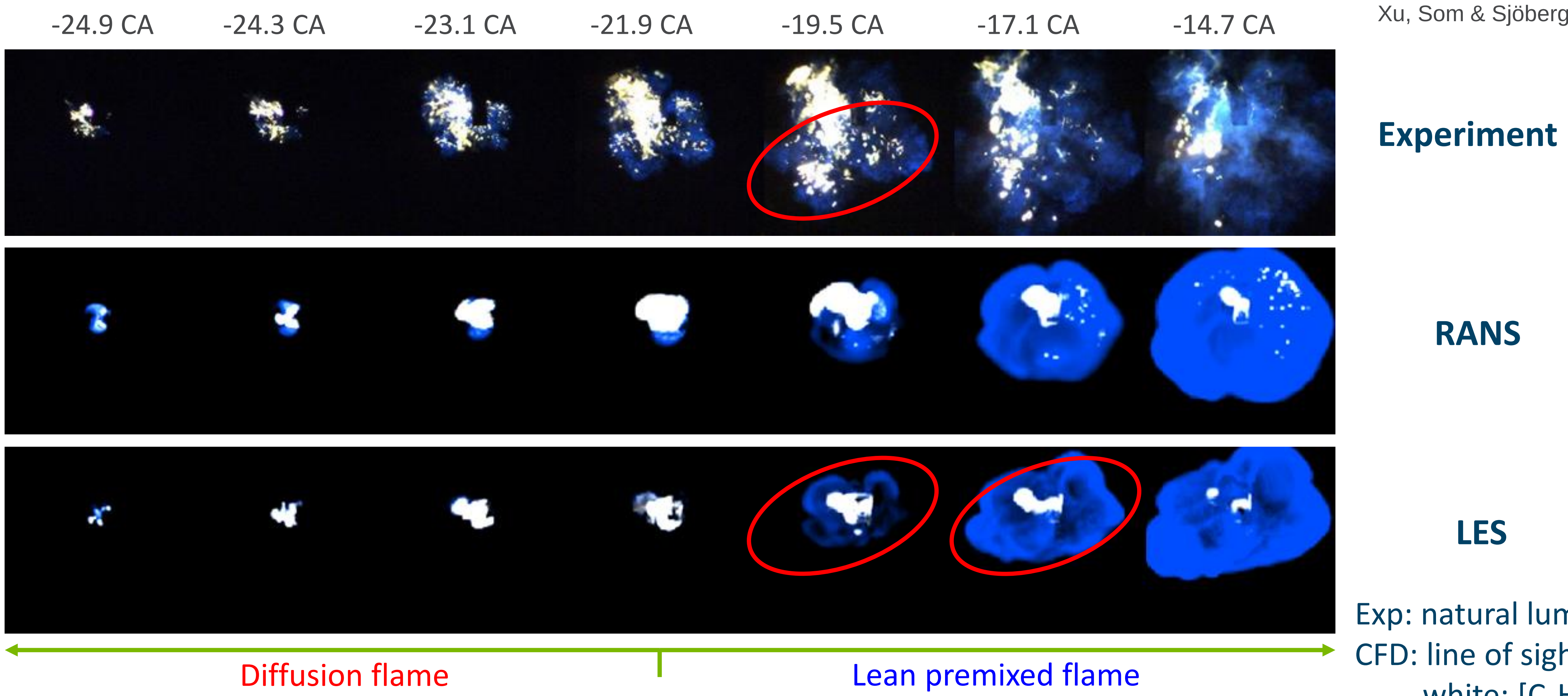
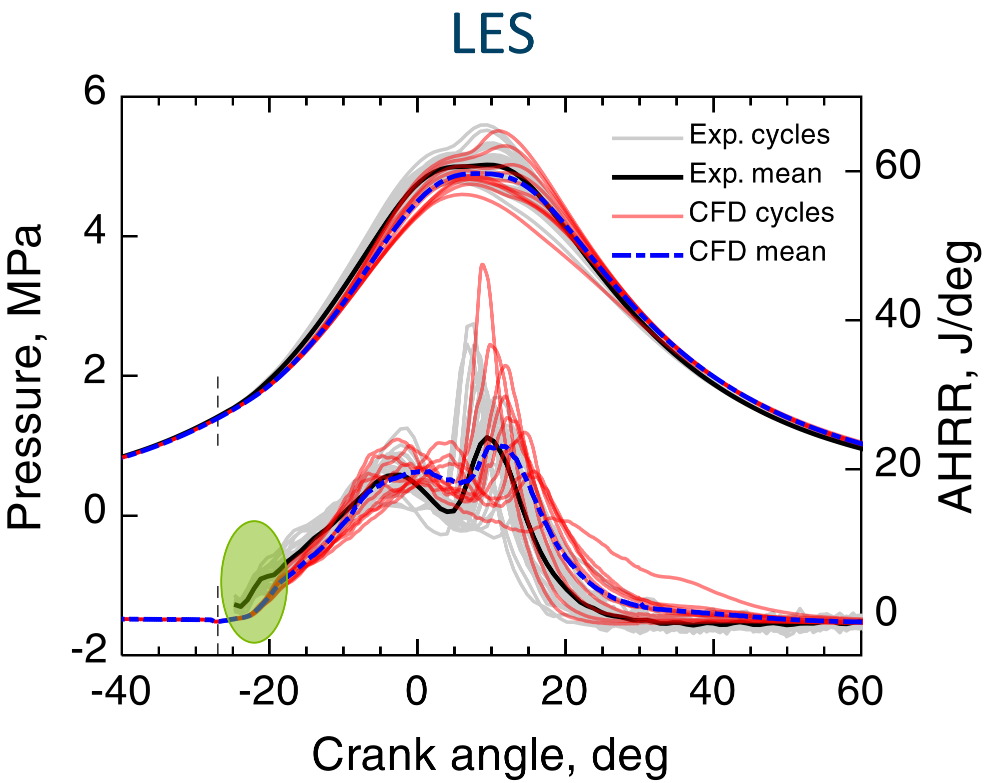
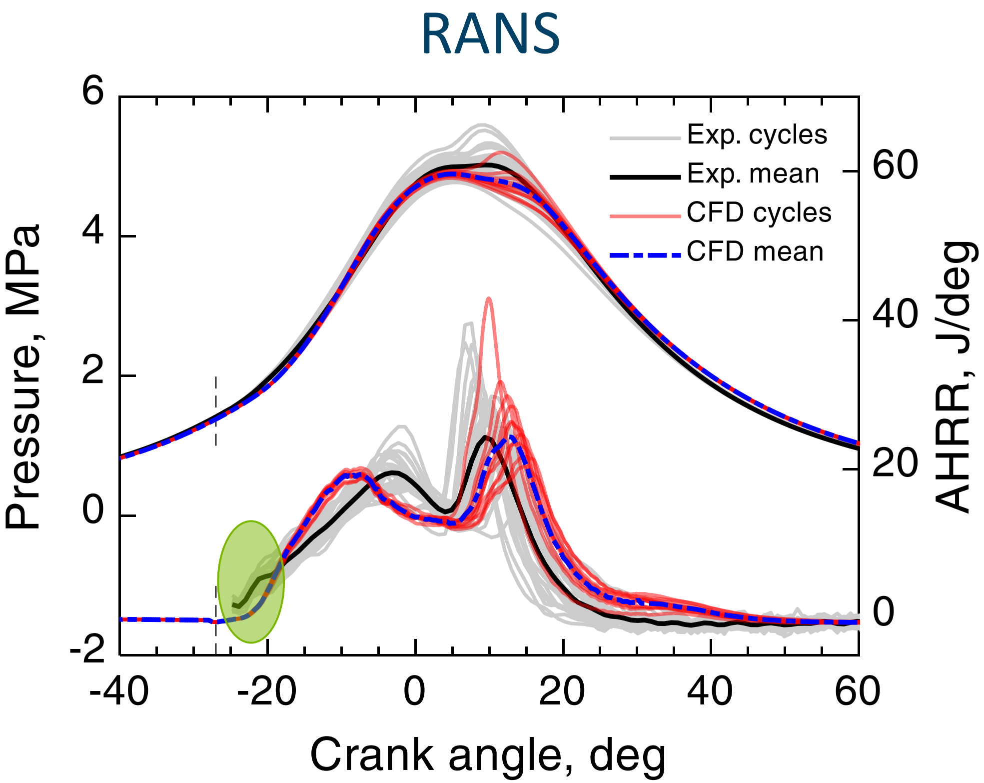


Exp: natural luminescence
CFD: line of sight
white: $[C_2H_2]$
blue: $[OH][CH_2O]$

- Transition from diffusion flame to lean premixed flame is well captured by CFD
- While RANS predicts the near-spherical flame development, LES shows more wrinkled and stretched flame fronts (similar to experiments)

PFS-ASSISTED SACI: LES VS RANS IN CRANK ANGLE SPACE





- LES predicts pressure and heat release rate (AHRR) traces very well, in terms of both mean and CCV
- RANS does not accurately capture first AHRR and underpredicts CCV
- Slightly lower AHRR at the start of combustion, probably due to insufficient ignition/combustion modeling

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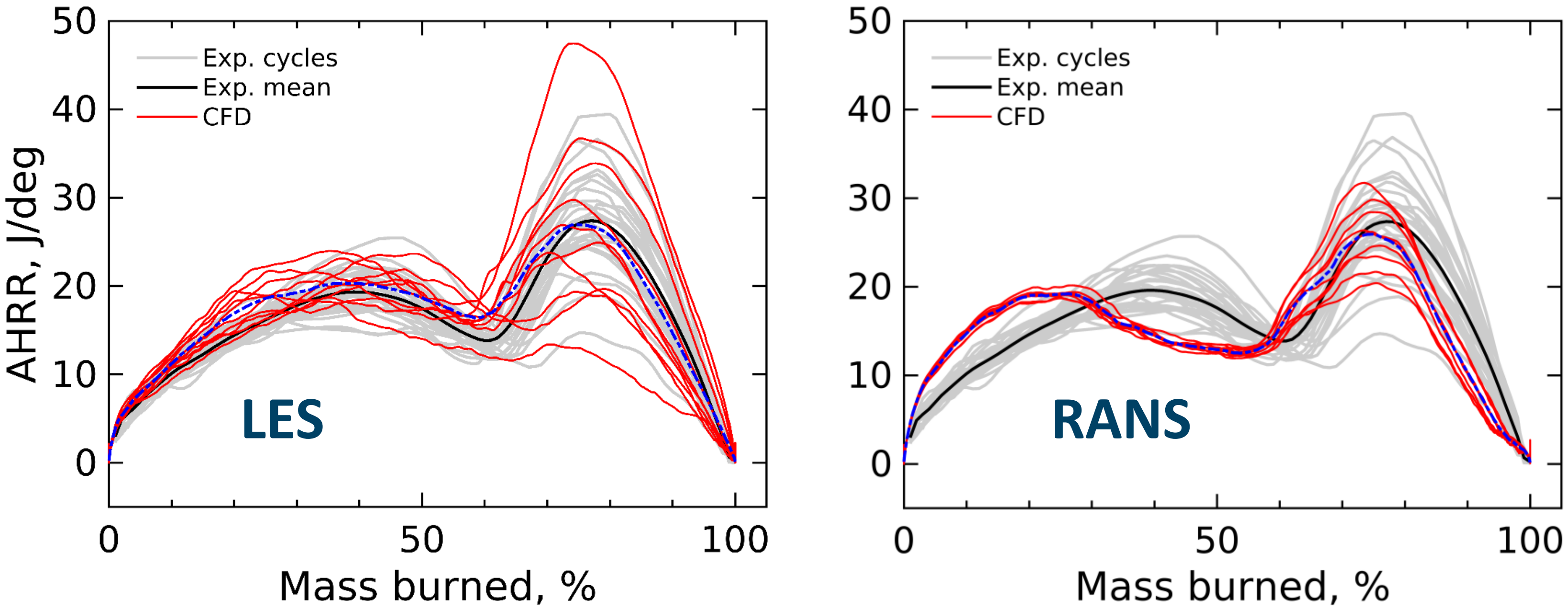
PFS-ASSISTED SACI: LES VS RANS IN MASS BURNED SPACE

- LES significantly improves the prediction of both mean and variation
  - Improved prediction of combustion phasing attributed to both deflagration and autoignition in the mass burned space
  - CCV predicted by LES matches what is observed in experiments
  - Consistent with the results from well-mixed charge operation
- Runtime: 1.5-2 days/cycle on 108 cores (36 hrs for RANS and 42 hrs for LES on average)



Blue dashed lines: CFD mean

Quantity	Experiment	RANS	LES
P_{max}, bar	50.6	48.9	49.5
ΔP_{max}, bar	8.2	1.1	9.1
P'_{max}, bar	2.0	0.29	2.6
$IMEP_g$, bar	5.63	6.12	6.13
$IMEP_n$, bar	5.75	6.17	6.18
COV, %	1.29	0.58	1.48

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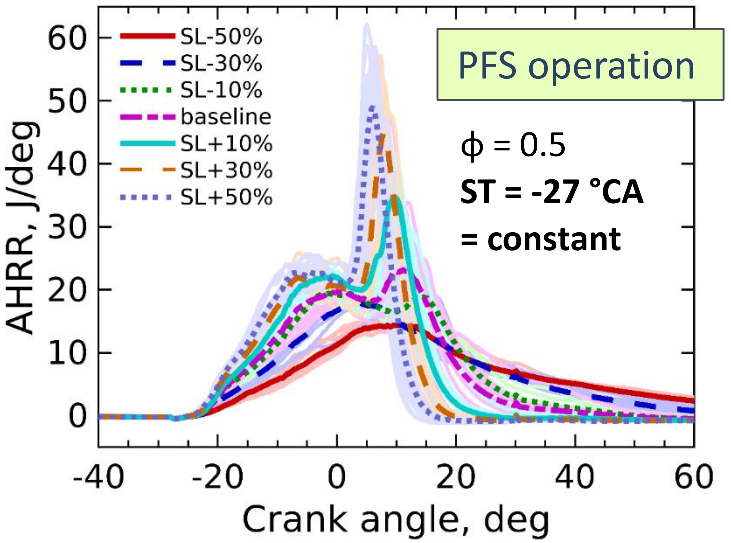
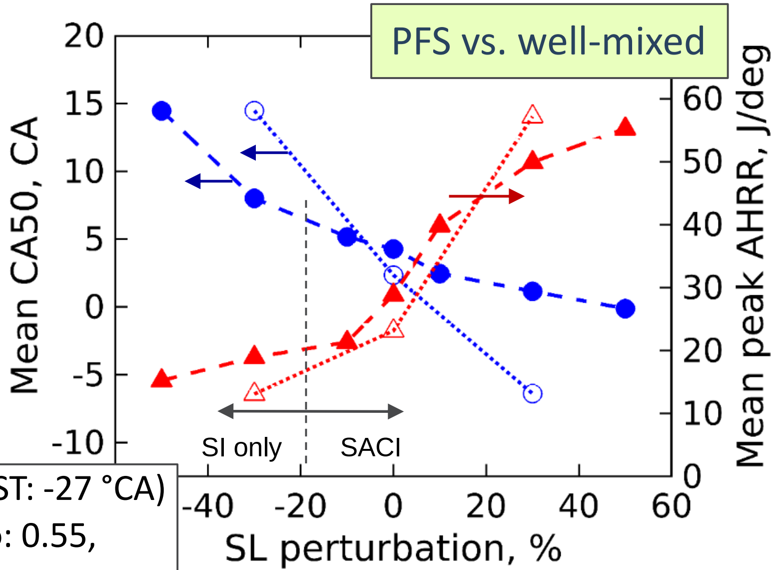
FUEL PROPERTY SENSITIVITY OF WM-SACI AND PFS-SACI

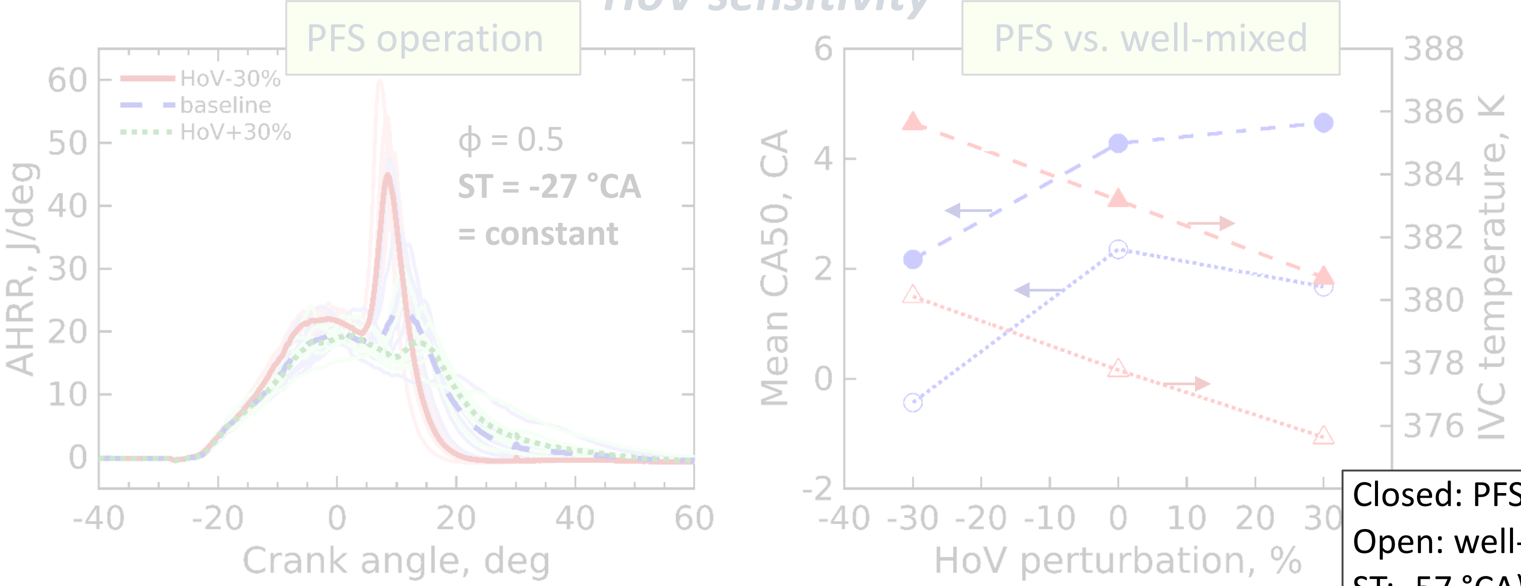
- High-fidelity LES-based CFD model enables systematic and efficient sensitivity analysis of fuel properties (e.g., HoV and S_L)
- **Heat of vaporization (HoV)** plays an important role by modifying the unburned gas temperature and thus combustion phasing; HoV sensitivity of the PFS operation is comparable with the well-mixed charge operation
- **Laminar flame speed (S_L)** directly controls the initial ramp-up of heat release rate in deflagration and thus affecting subsequent auto-ignition; S_L sensitivity of the PFS operation is smaller than the well-mixed charge operation

S_L sensitivity





HoV sensitivity



Closed: PFS (ϕ: 0.5, ST: -27 °CA)
Open: well-mixed (ϕ: 0.55, ST: -57 °CA)

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NEED OF FURTHER ASSESSMENT OF THE HYBRID COMBUSTION MODEL FOR PFS-ASSISTED SACI OPERATIONS

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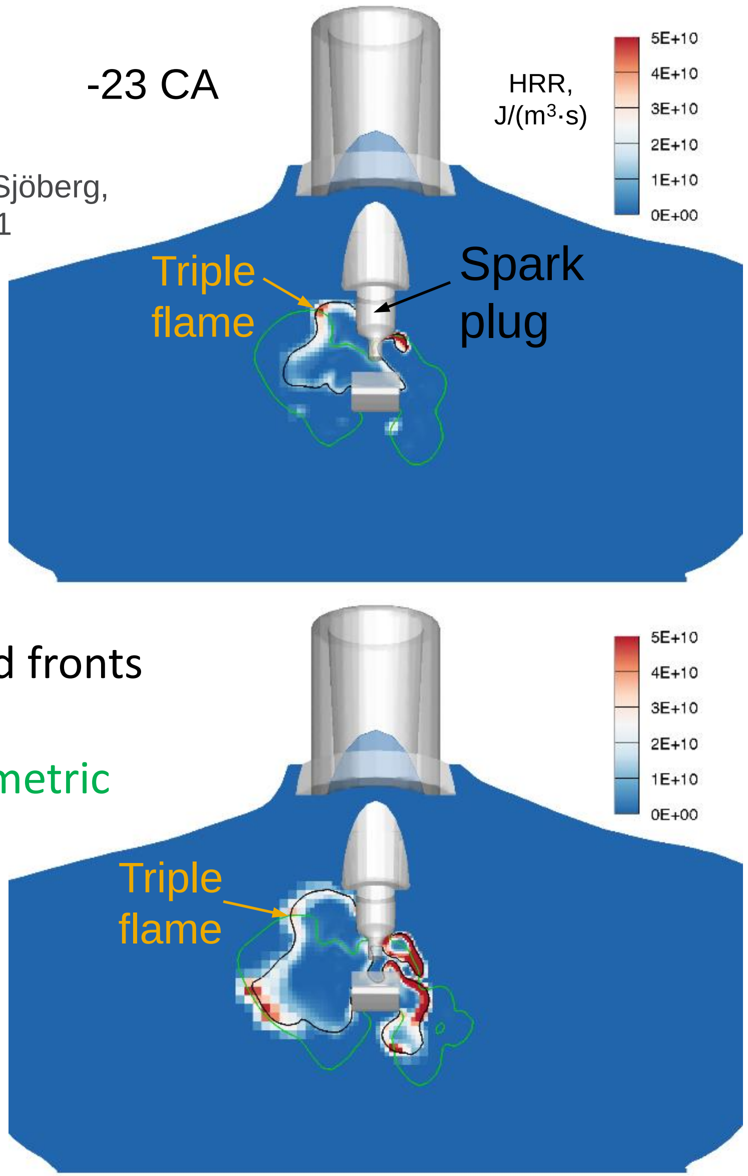
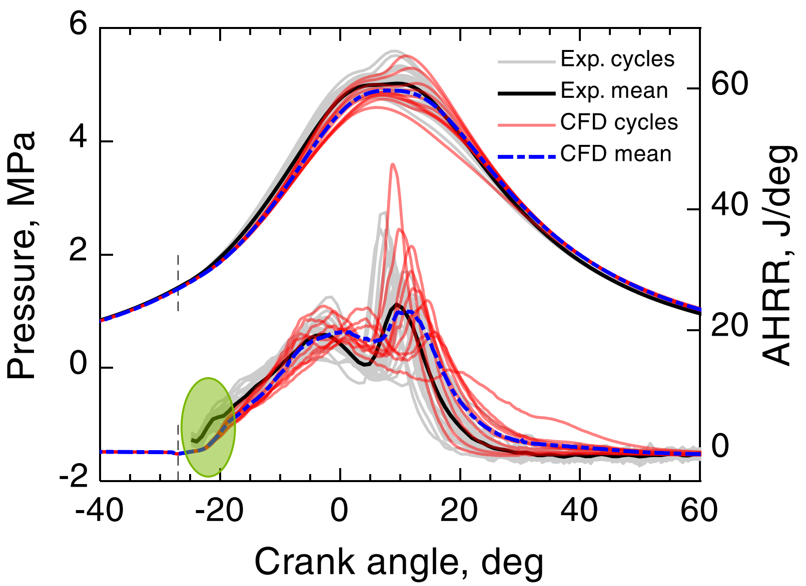


Black: premixed fronts

Green: stoichiometric



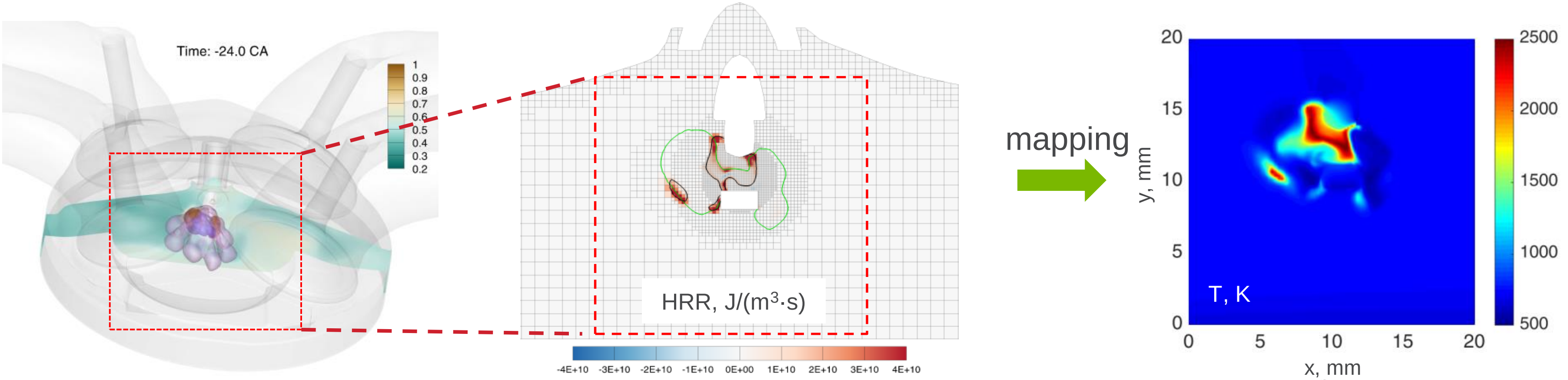
- Triple flames in PFS-SACI?
  - LES predicts mixed non-premixed (diffusion) and premixed combustion modes, suggesting triple flames exist. But
  - Does the diffusion flame really exist?
  - Is the current hybrid combustion model sufficient to capture different combustion modes?
- Underprediction of AHRR at the start of combustion
  - What are the causes?

2D DNS OF PFS WITH REALISTIC MIXTURE DISTRIBUTION AND PISTON MOTION

- 2D DNS is further employed to better understand the combustion modes right after pilot injection (spray-induced flow field, strong mixture stratification, etc.) for PFS-assisted SACI operation, and thus to evaluate the applicability of the LES hybrid G-equation/WSR combustion model (developed by the authors as part of the Co-Optima program)

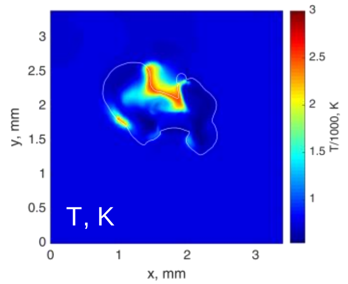
- DNS using Nek5000[1], a highly scalable spectral element CFD code developed at Argonne National Lab
  - A TPEF-E surrogate fuel for E30 with 90-species reduced mechanism
  - Laminar flame thickness for initial condition: $\delta_f = 70\ \mu\text{m}$
  - DNS resolution in Nek5000: $\Delta x = 4.7\mu\text{m} \approx \delta_f/15$, LES resolution in CONVERGE: $\Delta x_{\min} = 125\mu\text{m} \approx 1.8\delta_f$
  - Compression accounted for by imposing experimental pressure traces through artificial mass injection
  - Initial conditions $(p, T, \boldsymbol{u}, \boldsymbol{Y})$ directly from LES of PFS SACI at -24 °CA: $p \approx 16$ bar, $\phi_{back} \approx 0.48$, $T_0 \approx 750$ K (sub-grid turbulence neglected)
  - To achieve affordable DNS, computational domain and velocity are scaled with Damköhler number unchanged

[1] *2019 AMR presentation, ACE126, Muhsin Ameen*

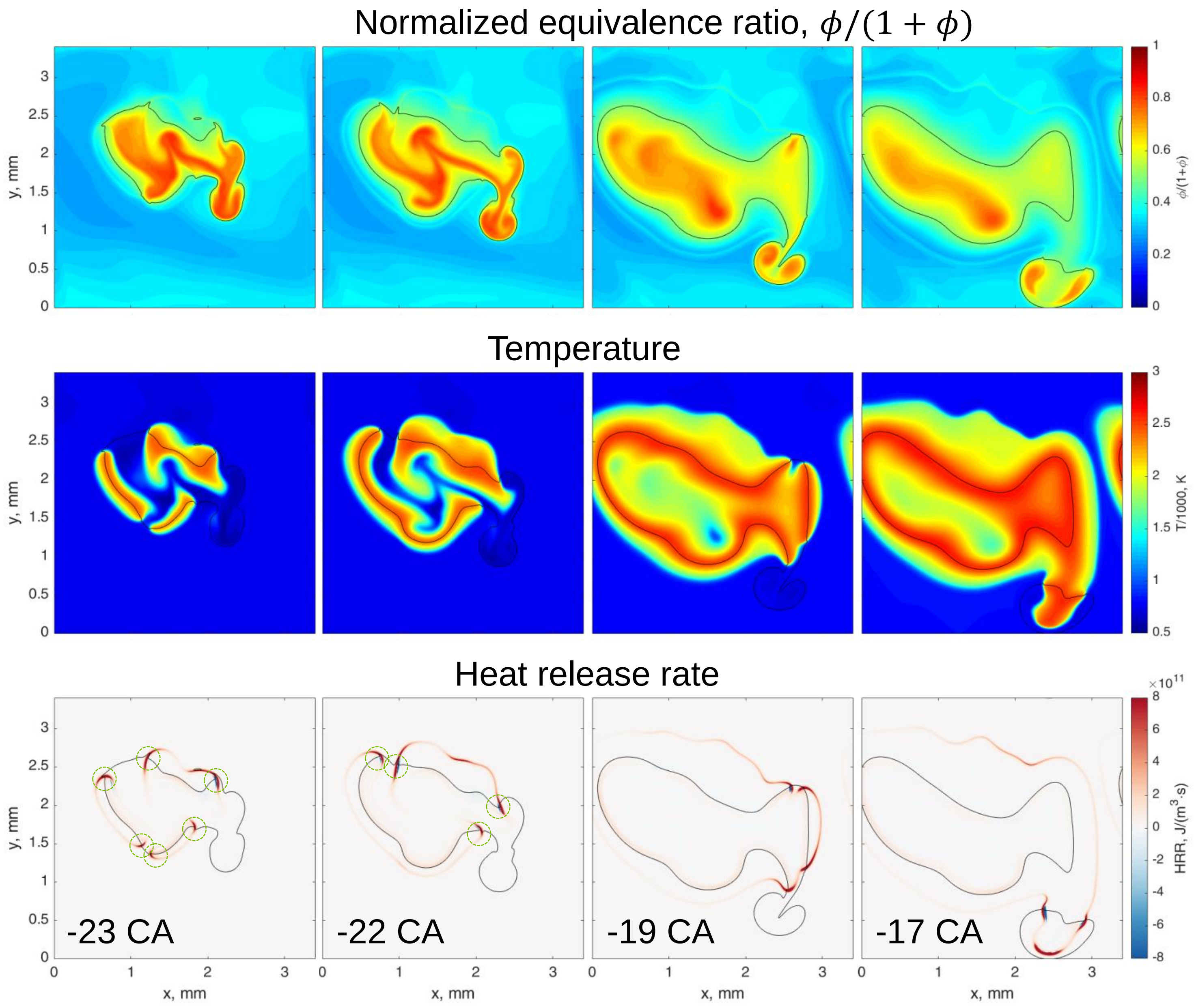


scaling

x6



FLAME STRUCTURE DURING FLAME KERNEL GROWTH

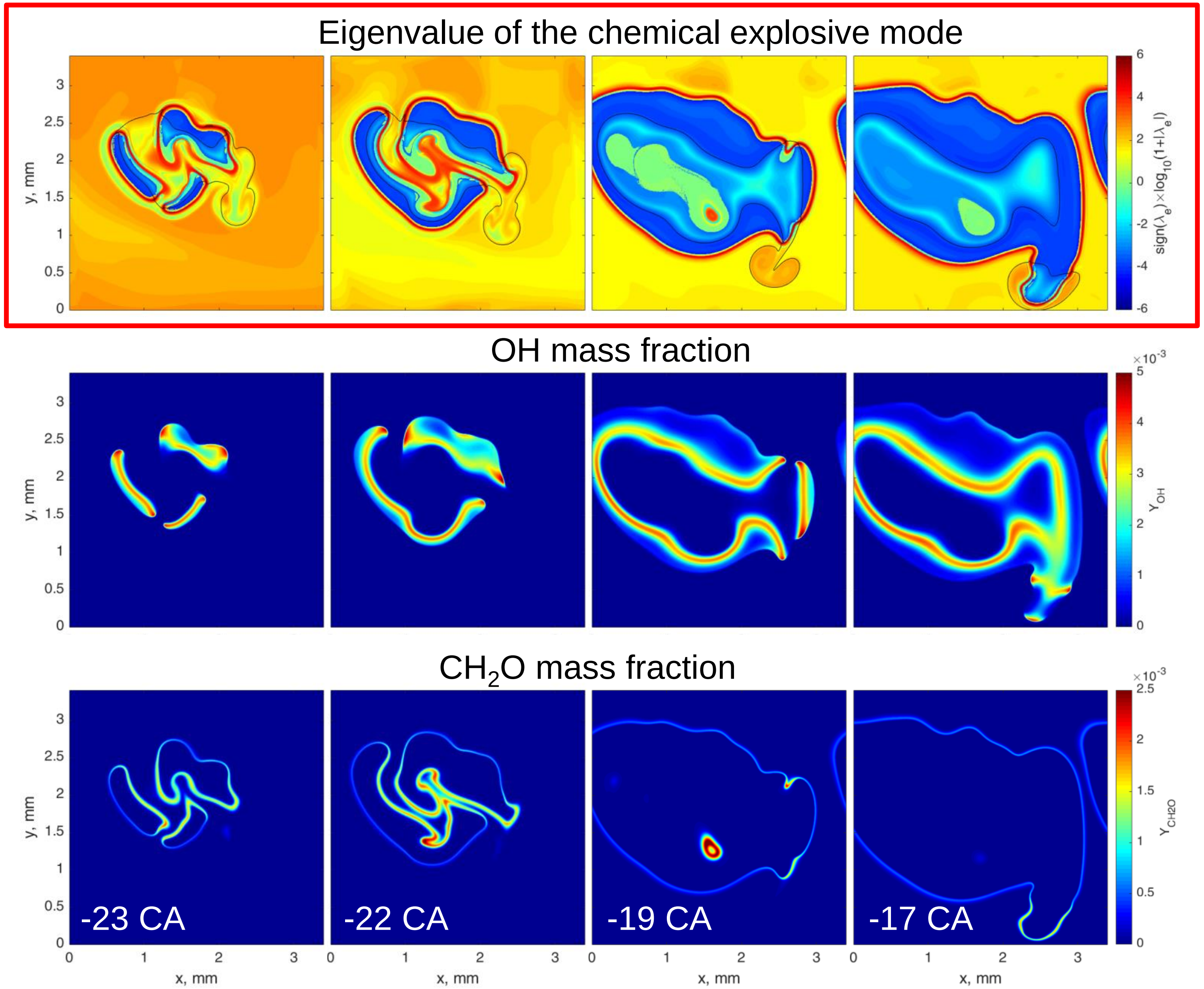


Black line: $\phi = 1$

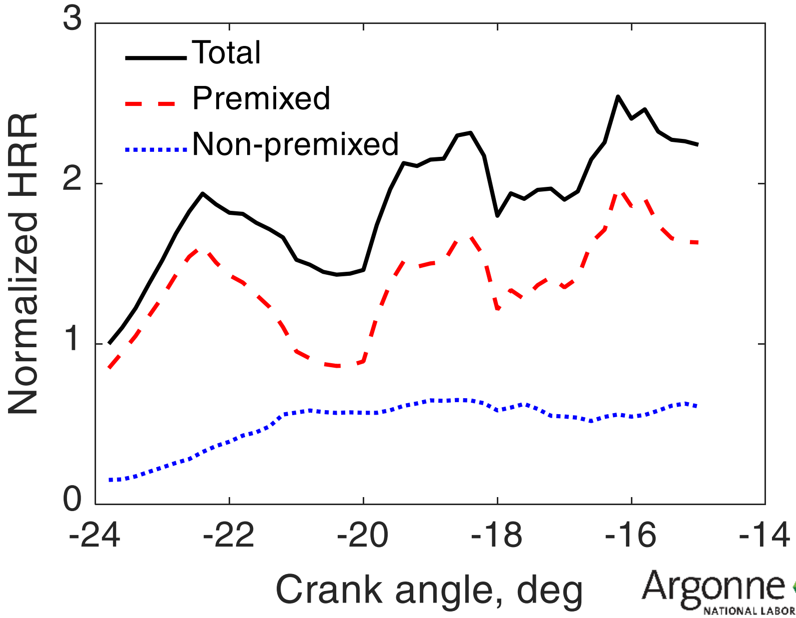
Flame structure

- Mixture is highly stratified
- Flame islands are centered at stoichiometric mixtures
- Heat release rate (HRR) layers are observed on both lean and rich sides
- Weak HRR layers are observed along the stoichiometric line
- HRR structure suggests presence of triple flames (green circles)

FLAME STRUCTURE DURING FLAME KERNEL GROWTH: CEMA



- Lean and rich premixed flames confirmed by chemical explosive mode analysis (CEMA): $\lambda_e = 0$
- Regions centered at $\lambda_e = 0$ with two times flame thickness is identified as premixed mixtures
- Premixed combustion is dominant; contribution to total HRR from non-premixed flames is non-negligible



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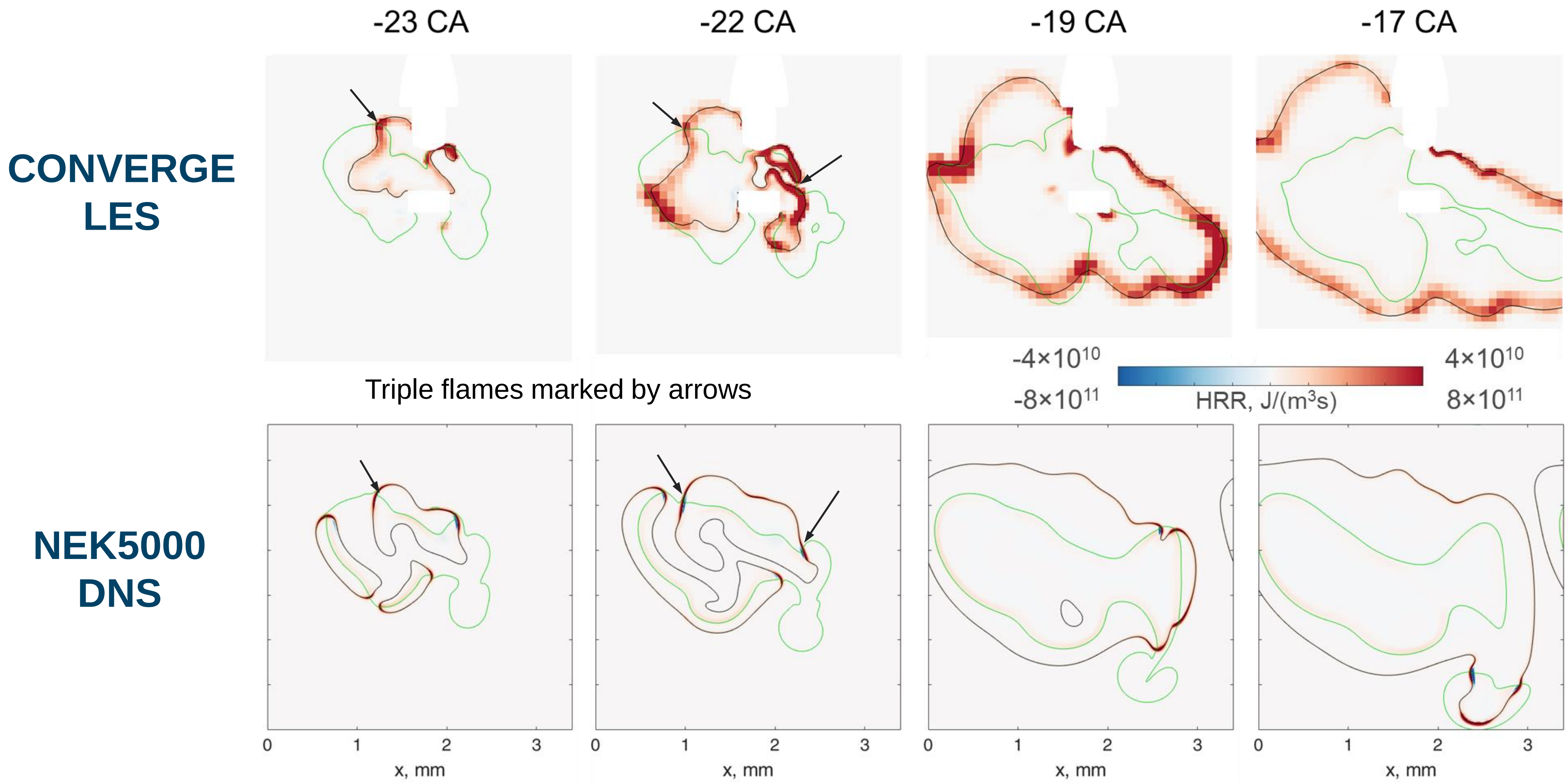
EFFECT OF PFS ON INITIAL FLAME DEVELOPMENT

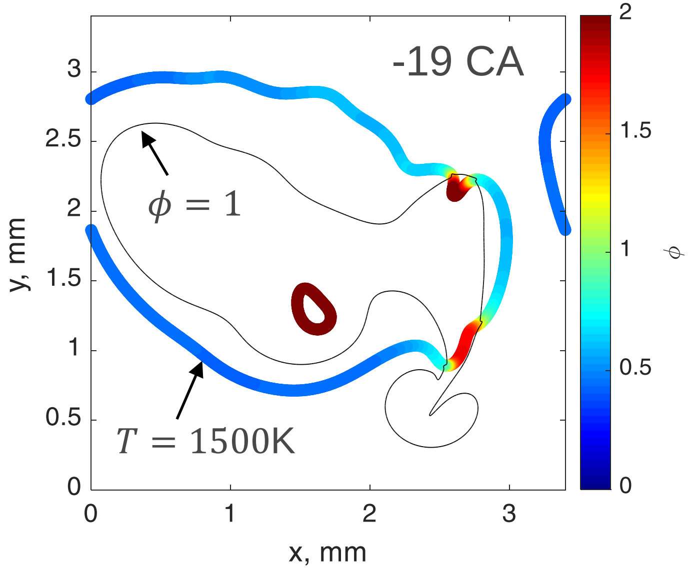
Black: premixed fronts
Green: stoichiometric



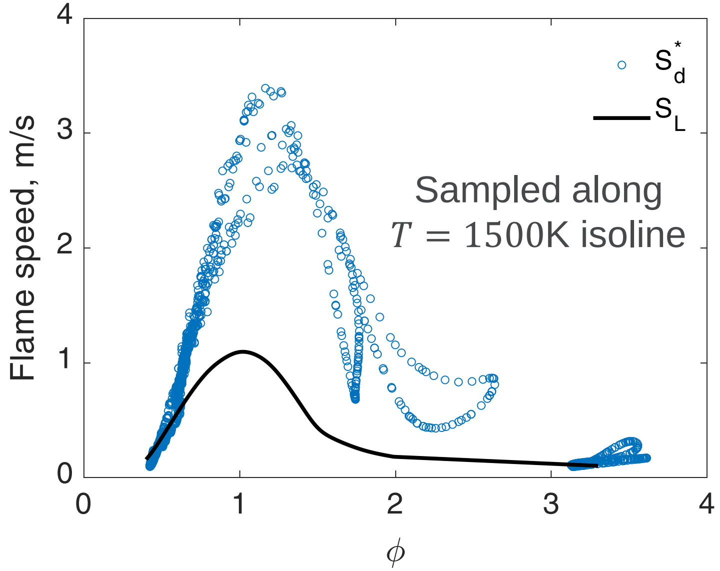
- Same triple flame features are predicted by DNS and the hybrid G-equation/WSR LES model, demonstrating the applicability of the hybrid model

ASSESSMENT OF G-EQUATION MODEL IN PFS: DISPLACEMENT SPEED

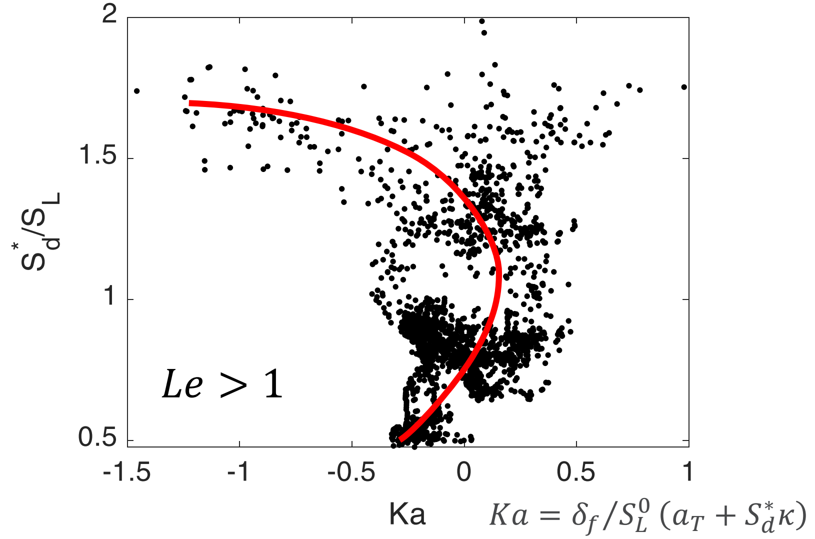
Equivalence ratio along premixed flame fronts (colored line)



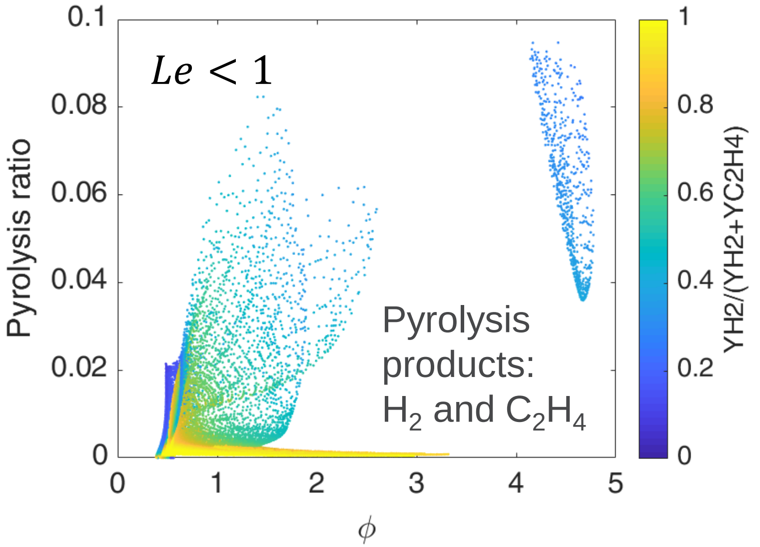
Local displacement speeds



Lean: $\phi < 0.7$



Rich: $1 < \phi < 2$



- During the initial stage of flame kernel growth in stratified mixtures, local displacement speed is found much larger than the unstretched counterpart in 1D laminar flames, except for very lean mixtures
- Possible reasons: (1) Lewis number effects with flame stretch; (2) Pyrolysis effects (higher flame speeds of H_2 and C_2H_4)
- This suggests that in PFS, these two effects need to be accounted for in the flame speed data, which is a key input in the G-equation model

SUMMARY AND CONCLUSIONS

- A large eddy simulation (LES) based CFD modeling framework was developed and successfully applied to multi-cycle SACI engine simulations with and without partial fuel stratification (PFS)
- The LES model, leverages a hybrid G-equation/WSR combustion model, accurately predicts the pressure and HRR traces in both well-mixed SACI and PFS-assisted SACI
- The LES model shows significant accuracy gains compared with RANS models, with only a slight increase in computational cost
- The LES model identifies a key difference between WM-SACI and PFS-SACI in fuel property impacts: PFS-SACI is found more tolerable to SL perturbation than WM-SACI
- DNS with a simplified 2D geometry but realistic thermodynamic conditions provide new insights to the initial flame growth in PFS operation:
  - Triple flames are observed during the initial stage, with nonpremixed flames contributing non-negligibly to the total heat release
  - Local displacement speeds are much larger than the unstretched flame speed counterpart, suggesting the important roles of thermodiffusive instability and fuel pyrolysis
- Future work: improve the G-equation model using the DNS insights in PFS-SACI

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Chao Xu, Muhsin Ameen, Pinaki Pal, Sibendu Som, Direct numerical simulation of partial fuel stratification assisted lean premixed combustion for assessment of hybrid G-equation/well-stirred reactor model, *ASME 2021 Internal Combustion Engine Division Fall Technical Conference*, submitted.

Chao Xu, Magnus Sjöberg, Sibendu Som, Large eddy simulation of lean mixed-mode combustion assisted by partial fuel stratification in a spark-ignition engine, *Journal of Energy Resources Technology*, 143:7 (2021) 072304.

Chao Xu, Pinaki Pal, Xiao Ren, Magnus Sjöberg, Noah Van Dam, Yunchao Wu, Tianfeng Lu, Matthew McNenly, Sibendu Som, Numerical investigation of fuel property effects on mixed-mode combustion in a spark-ignition engine, *Journal of Energy Resources Technology*, 143:4 (2021) 042306.

Chao Xu, Zongyu Yue, Sibendu Som, A hybrid flamelet model for predicting mixed-mode combustion in a spark-ignition engine, Spring Technical Meeting Central States Section of The Combustion Institute, 2020.

Thank you!

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