Co-Optimization of
Fuels & Engines

Multi-Mode: From In-Cylinder Combustion Diagnostics to Drive-Cycle Fuel Economy

Magnus Sjöberg, Namho Kim, SNL
Sibendu Som, Chao Xu, ANL
Dan Flowers, LLNL

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2020 DOE Vehicle Technologies Office
Annual Merit Review

better fuels | better vehicles | sooner

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Overview: Light-Duty DISI Multi-Mode

Advanced Engine Development & Toolkit Development

Timeline Phase 1 Phase 2

Task	FY16	FY17	FY18	FY19	FY20	FY21
E.1.1.3: SNL	Start		End	Re-Start		End
E.1.1.4: SNL	Start		End	Re-Start		End
G.2.1: ANL	Start		Start	Re-Start		End
G.5.7: LLNL				Start		End

Task	FY19	FY20
E.1.1.3: SNL Optical Light-duty DISI Engine: Fuel Effects on In-Cylinder Processes of Lean Well-mixed and Stratified Operation. Sjöberg, Kim, Vuilleumier, Reuss, Singh.	$320k	$300k
E.1.1.4: SNL, Metal Light-duty DISI Engine: Fuel Effects on Lean Mixed-Mode Combustion. Sjöberg, Kim, Vuilleumier, Reuss, Johnson, Singh.	$320k	$300k
G.2.1: ANL, Fuel Property Sensitivity Analysis for a Multi-Mode DISI Engine Using Simulations. Som, Xu.	$175k	$130k
G.5.7: LLNL, Multi-mode co-optimization via data consolidation and analysis. Flowers, Lapointe, McNenly.	$164k	$225k

Barriers [a]

- Lack of robust high-dilution stoichiometric and lean-burn technology and controls.
- Determine factors limiting low temperature combustion (LTC) and develop methods to extend limits.
- Understanding impact of likely future fuels on LTC and whether LTC can be more fully enabled by fuel specifications different from gasoline.

Partners

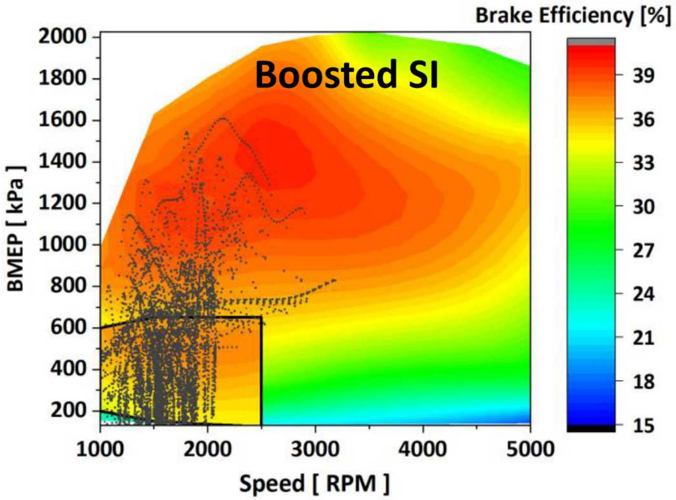
- Co-optima partners include nine national labs, one industry, 20+ universities, external advisory board, and stakeholders (80+ organizations).
- 15 Industry partners in the AEC MOU.
- Task specific partners:
- General Motors – Hardware.
- Toyota – Funds-in knock project.
- LLNL (Pitz *et al.*) – Kinetics
- Convergent Science Inc. – Software.
- + Many more – details in later slides

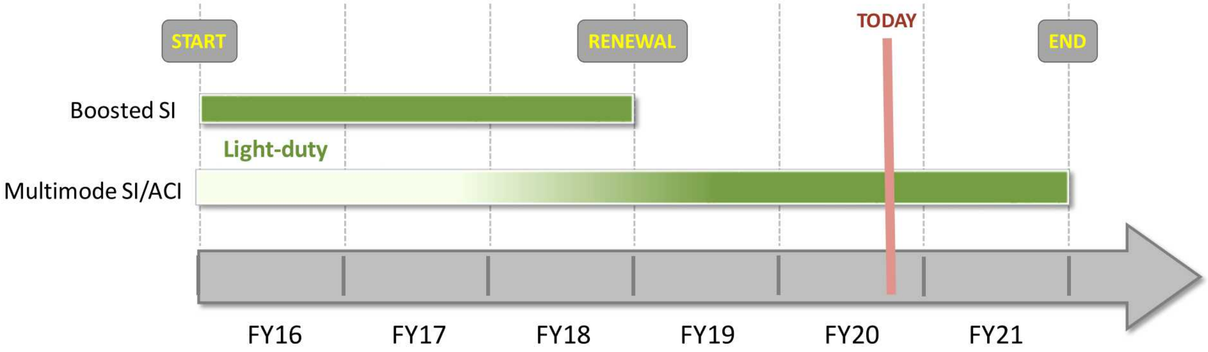
[a] Barriers 2018 U.S. DRIVE ACEC Tech Team Roadmap.

Relevance

- Broader Co-Optima effort; pre-competitive, early-stage research aims to develop better understanding how changes to fuel properties can enable advanced combustion, see Wagner FT037.
- These particular engine development and computational toolkit research tasks support:
- Light-duty Multimode (MM) engine operation for near-term Co-Optima fuel-economy gain targets.
- MM uses advanced combustion at lower loads in combination with boosted SI at high loads.
  - Lean mixed-mode combustion (SACI).
    Deflagration and autoignition.
    Octane-appetite assessment.
  - Lean stratified-charge SI operation
    Deflagration-based combustion.
    Focus on emissions mitigation.
- Other advanced combustion concepts are integrated via data consolidation and analysis.

Figure Source | J. Szybist, ORNL





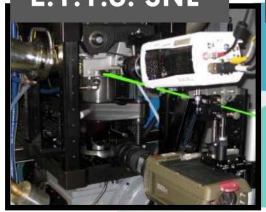
Milestones

Month / Year	Description of Milestone or Go/No-Go Decision	Status
March 2019, SNL E.1.1.3	Determine differences in in-cylinder soot distribution for stratified operation using fuels that show inconsistency between PMI and engine-out PM.	**Complete**
March 2019, ANL G.2.1	Sandia DISI Engine Simulations (Sensitivity Analysis for Multi-Mode Operation). Perform global sensitivity analysis for lean operation and quantify the effect of fuel properties on engine efficiency.	**Complete - Local SA performed instead of GSA owing to the availability of resources**
December 2019, ANL G.2.1	Validate CFD model that can be applied to both mixed-mode operations with and without partial fuel stratification	**Complete**
March 2020, SNL E.1.1.3	For mixed-mode combustion (SACI), acquire and transfer optical validation data to CFD modelers at ANL.	**Complete**

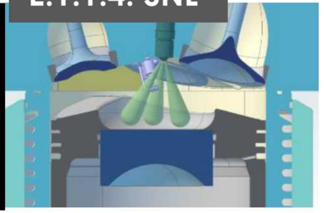
Overall Technical Approach:
4 tasks / 3 labs + many collaborations

Utilize Co-Optima core fuels, promising blendstocks and custom blends as needed

E.1.1.3: SNL

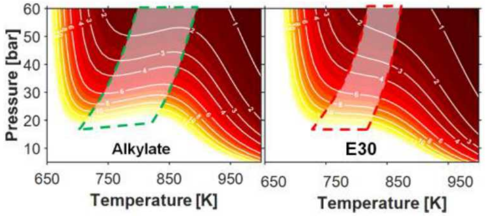


E.1.1.4: SNL



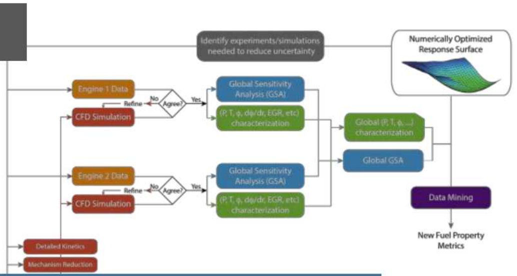
Combine DISI metal- and optical-engine experiments and modeling.

Use Fundamental Knowledge Base



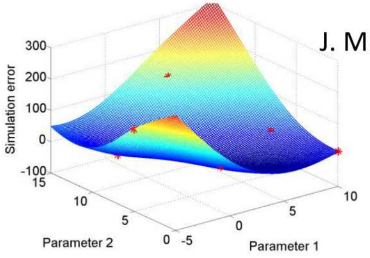
Multi-mode SI / ACI

G.5.7: LLNL



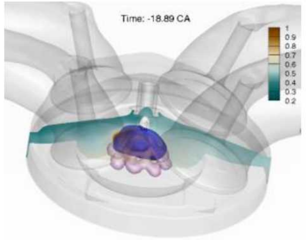
Consolidate and analyze data to identify multi-mode approaches with high co-optimization potential.

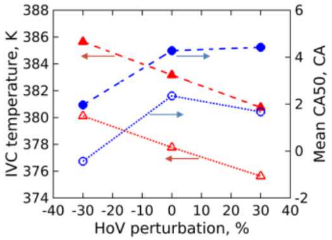
Collaborative Kinetics/ Toolkit tasks



J. Mueller, LBL

G.2.1: ANL

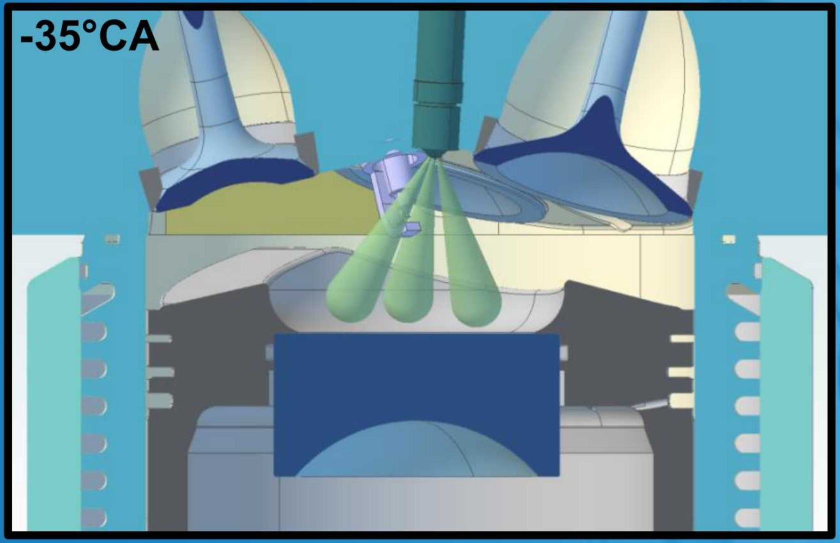




Enhance understanding and accelerate development through linked modeling efforts.

Approach – SNL DISI

- Drop-down single-cylinder engine.
  Bore: 86 mm, Stroke: 95 mm, CR:12, 0.55L.
- Piston bowl and closely located spark and injector ⇒
  Highly relevant for stratified SI.
  But use early injections for well-mixed operation.



- Identical geometry for all-metal testing and optical diagnostics.
- Mie or DBI - Liquid Spray, Flame imaging - Deflagration and soot, DBI - soot mass, RIM - Wall Wetting, IR - Fuel Vapor, PIV - Flows.

- Combine metal- and optical-engine experiments to develop a broad understanding of the impact of fuel properties on DISI combustion processes.

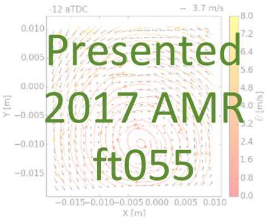
- Utilize Co-Optima Core fuels, AKI87 E10, promising blendstocks in mid-level RON98 surrogate blends, as well as PRF and TRF reference blends.
- First, conduct performance testing with all-metal engine over wide ranges of conditions; well-mixed to stratified.
  - Assess octane appetite of lean mixed-mode combustion (SACI).
  - Relate exhaust smoke emissions to Particulate Matter Index (PMI) and other sooting metrics.
- Second, apply optical diagnostics to:
  - Determine dominating soot-production pathways.
  - Probe spray development.
  - Clarify shortcomings of PMI.

- Third, extend scope of fuel studies through the use of validated GT-Power, CHEMKIN and drive-cycle models like ALPHA and Autonomie.

Approach / Workflow: ANL - CFD

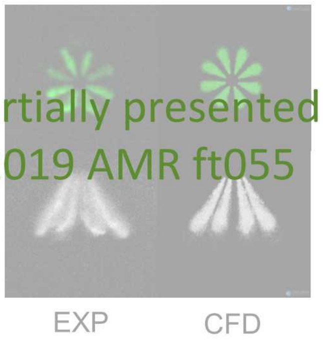
- **Turbulence model:** Combination of higher throughput RANS and higher fidelity LES enabling fuel property sensitivity analysis
- **Spray:** State-of-art Lagrangian models allowing for fuel-stratification studies
- **Turbulence-chemistry interaction:** Hybrid model (G-equation + Well-stirred Reactor or Tabulated flamelet model) – improving mixed-mode prediction with affordable computational efficiency

Motored Flow



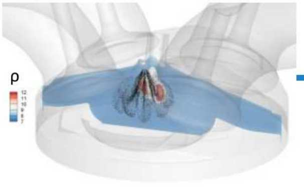
Presented 2017 AMR ft055

Spray Validation

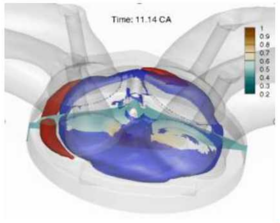


Partially presented 2019 AMR ft055

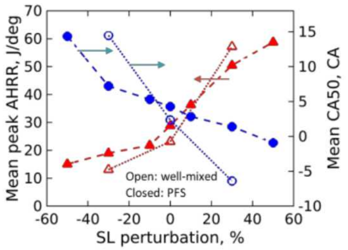
Motored with Fuel Injection

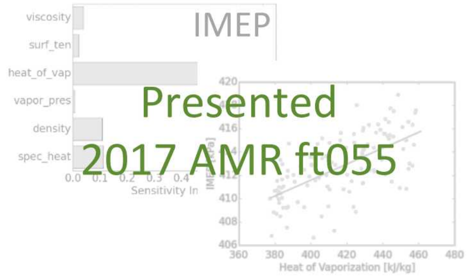


Combustion



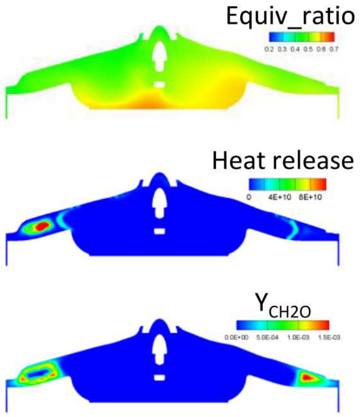
Sensitivity Analysis

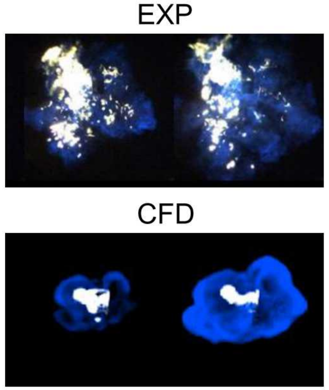




Presented 2017 AMR ft055

Probing underlying physics





Approach / Workflow: LLNL Data Consolidation

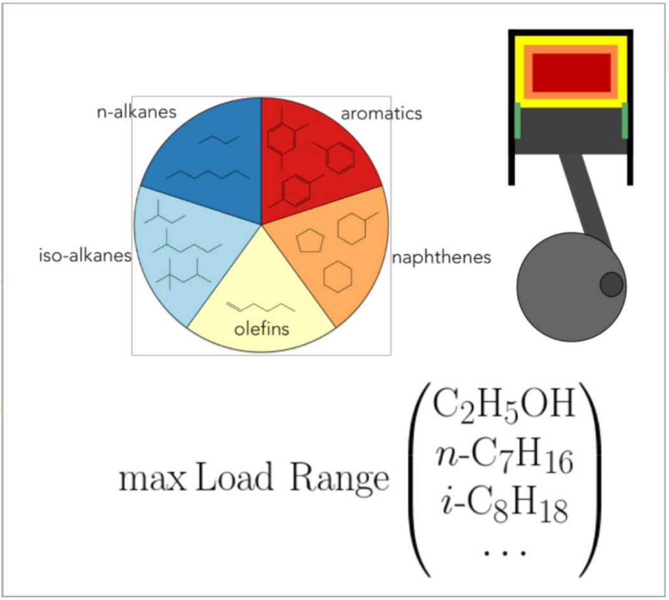
Accelerate hypothesis testing using accurate fuel chemistry models for broad blend explorations in a tight feedback loop with experiments:

Current applications:

- Maximize each PIONA class at a fixed RON and MON to test the Central Fuel Hypothesis for BOB blending (2018 AMR).
- Maximize the load range and number of feasible operating conditions for DISI multi-mode performance (2019 & 2020 AMR).

START

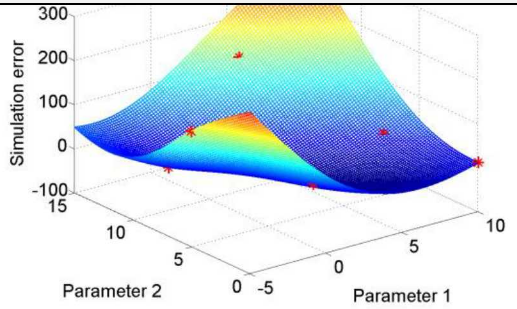
$$Q\begin{pmatrix} RPM \\ CR \\ C_2H_5OH \\ n\text{-}C_7H_{16} \\ i\text{-}C_8H_{18} \\ \cdots \end{pmatrix}$$

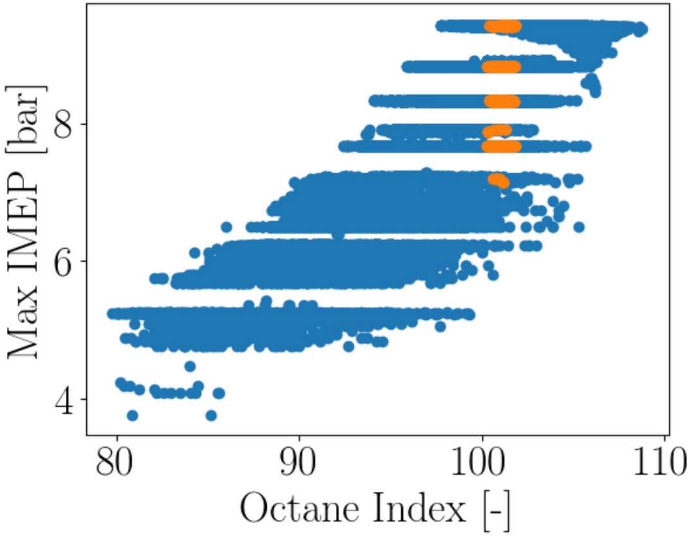


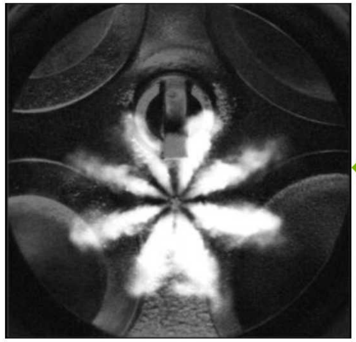
$$\max \text{Load Range} \begin{pmatrix} C_2H_5OH \\ n\text{-}C_7H_{16} \\ i\text{-}C_8H_{18} \\ \cdots \end{pmatrix}$$

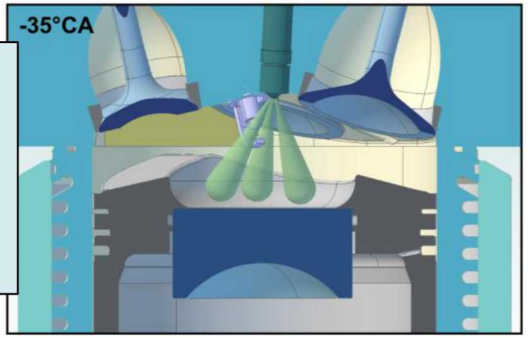
Surrogate Model Optimization

see J. Mueller's talk FT076









Use this high throughput process to augment available multi-mode experiments and compare fuel-engine impacts

Technical Accomplishments Summary

ACCOMPLISHMENTS (1/15)

DISI @ SNL

- Continued assessment of relevance of PMI and other sooting metrics for 9 fuels across 3 well-mixed and 2 stratified operating strategies.
  - Examined fuel effects of spray for PMI shortcomings.
  - Explored effective ways to incorporate YSI as a sooting metric.
- Used RIM and spray imaging to assess spray dynamics responsible for piston-top fuel-film formation.
- Refined and used a methodology to determine the octane appetite of mixed-mode combustion using GT-Power and CHEMKIN.
- Developed and used a GT-Power – ALPHA methodology to quantify fuel-economy benefits of lean operation.
- Assessed stoichiometric and lean operation with ϕ-sensitive CB#1* fuel, as well as other key fuel blends.
- Led team efforts within Co-Optima and IEA's Low-Temperature Combustion task.
- Numerous technical publications.

*Developed by Lopez-Pintor and Dec at SNL.

CFD @ ANL

- Developed a LES-based CFD model for lean mixed-mode combustion (SACI) assisted by partial fuel stratification and demonstrated model accuracy in capturing spray and flame structures, and key combustion dynamics.
- Developed a computational-efficient hybrid G-equation/ tabulated chemistry model to accelerate SACI combustion modeling and fuel sensitivity analysis
- Leveraged the high-fidelity LES-based CFD model to investigate fuel property sensitivities, including heat of vaporization and laminar flame speed, for PFS-assisted SACI
- Several technical publications.

Data Consolidation @ LLNL

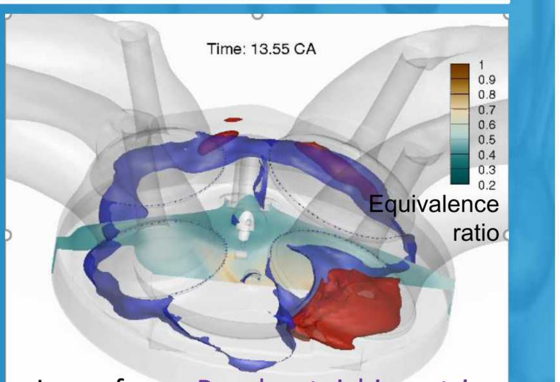
- Validated virtual fuel search and neural network octane prediction used in multimode workflow with a 4-component surrogate tested in the SACI engine.
- Screened 80k new fuel blends in the virtual SACI model over a refined set of conditions.
- Found evidence that there may be another fuel property in addition to Octane Index affecting SACI performance.

ANL Accomplishments: Enabling Predictive Simulations of Mixed-Mode Combustion (SACI) with Partial Fuel Stratification (PFS)

Predictive computational fluid dynamic (CFD) model for mixed-mode combustion (SACI) assisted by partial fuel stratification (PFS)

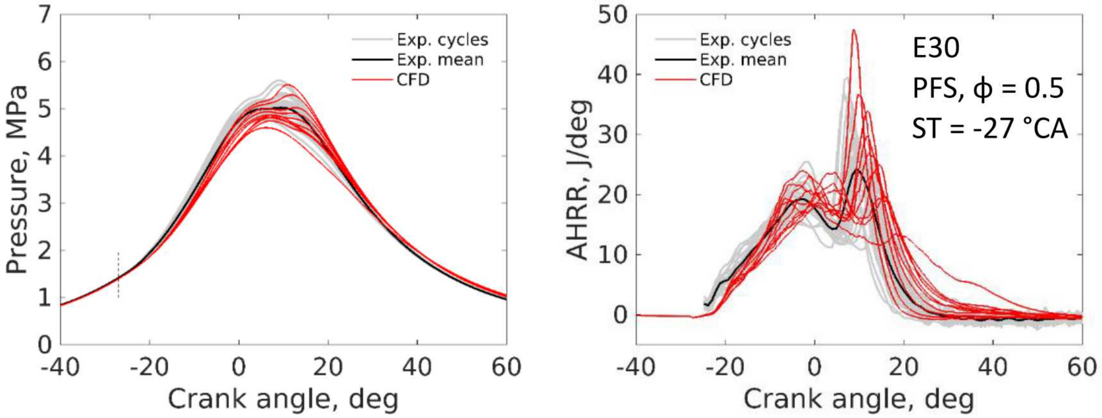
- A large eddy simulation (LES) based engine CFD model was developed for PFS-assisted SACI combustion (FY19: RANS-based model for well-mixed charge SACI) and successfully validated against experimental data.
- The new CFD model accurately predicts pressure and heat release rate traces, and captures key features in spray and flame dynamics.

- ***High fidelity was demonstrated for the developed CFD tools for PFS-assisted multi-mode engine operation.***

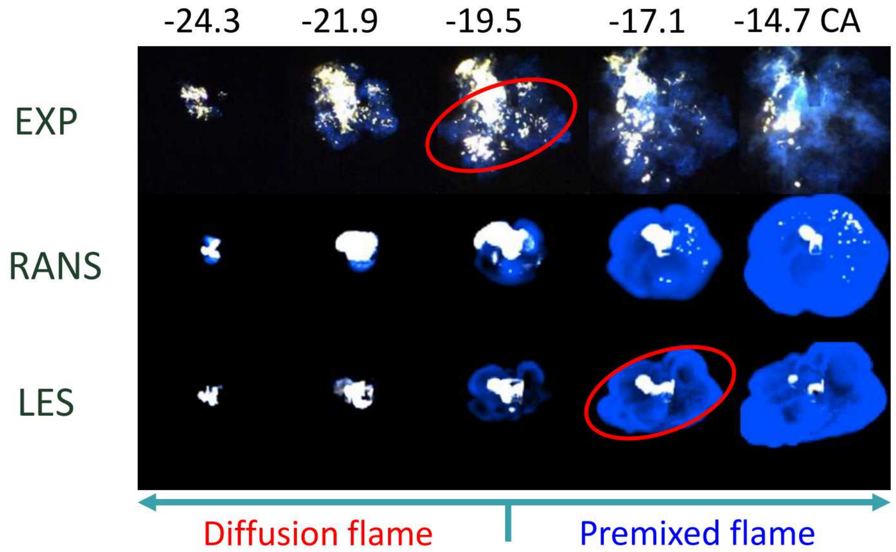


Isosurfaces: Purple: stoichiometric
Blue: flames; Red: auto-ignition

- LES-based CFD model captures both mean and cycle-to-cycle variations in pressure and heat release rate.



- Model captures key flame features in PFS-assisted SACI.

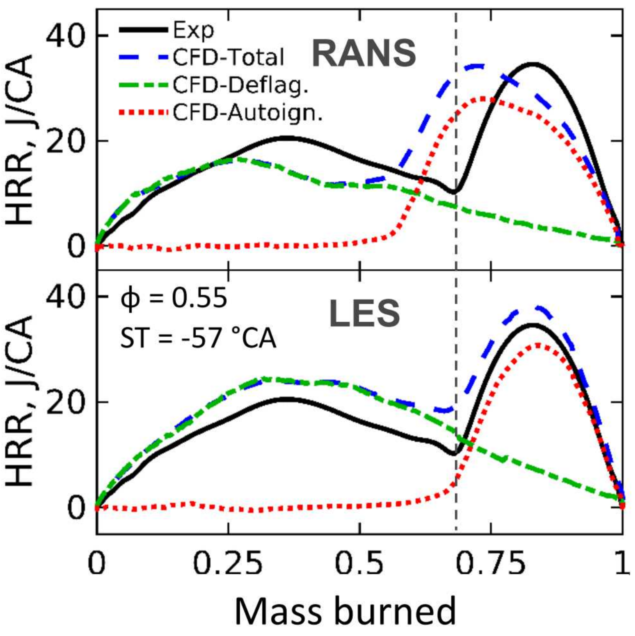


ANL Accomplishments: Improving Model Accuracy and Computational Efficiency for Lean SACI Engine Operation

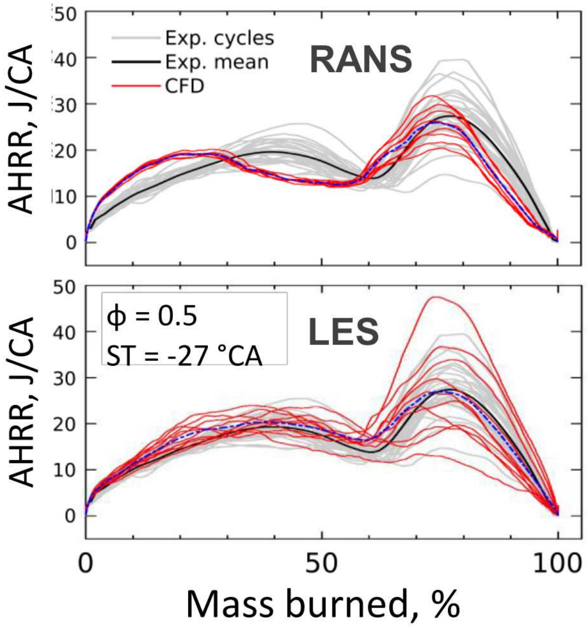
- **Model Accuracy:** LES-based models significantly improve the prediction of mean and CCV for both well-mixed charge and PFS operations compared with the widely-used RANS-based models. This is mainly attributed to the improved prediction of deflagration and autoignition combustion phasing in the mass burned space.
- **Computational Efficiency:** A new hybrid G-equation/tabulated chemistry model (G-eqn+TC) was developed to accelerate SACI modeling with a speedup factor of ~2 compared with existing hybrid G-equation/multi-zone (G-eqn+MZ) model.

Effects of turbulence modeling approaches

Well-mixed (WM) charge

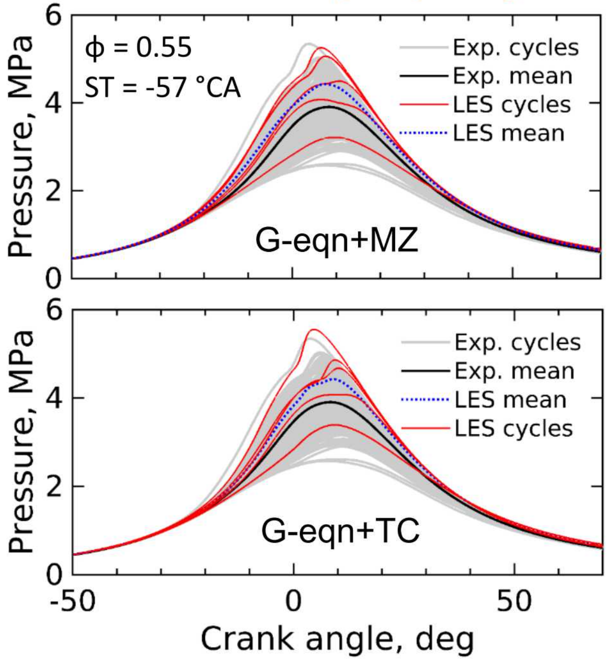


PFS



Effects of combustion models

Well-mixed (WM) charge

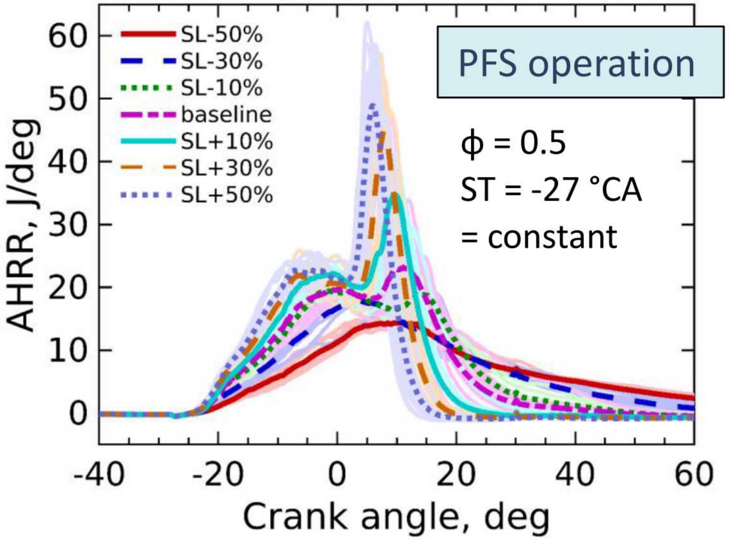


ANL Accomplishments: Understanding Fuel Property Sensitivity of PFS-Assisted SACI Combustion

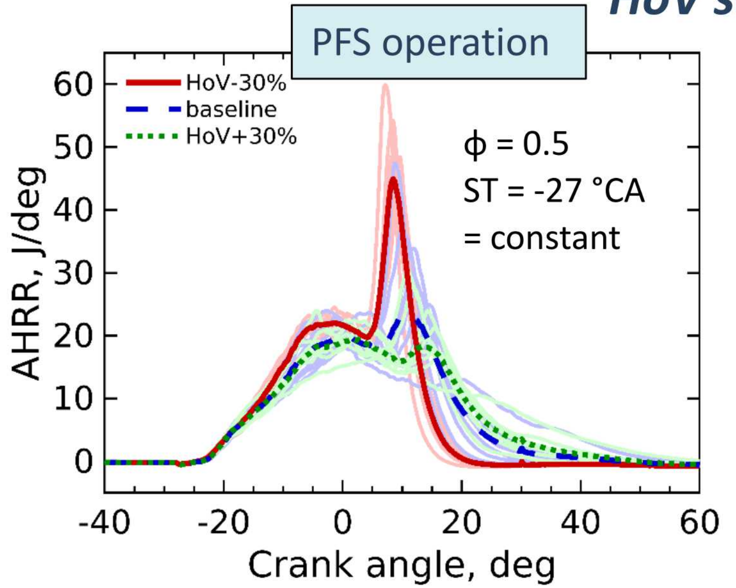
High-fidelity LES-based CFD model enables systematic and efficient fuel property sensitivity analysis

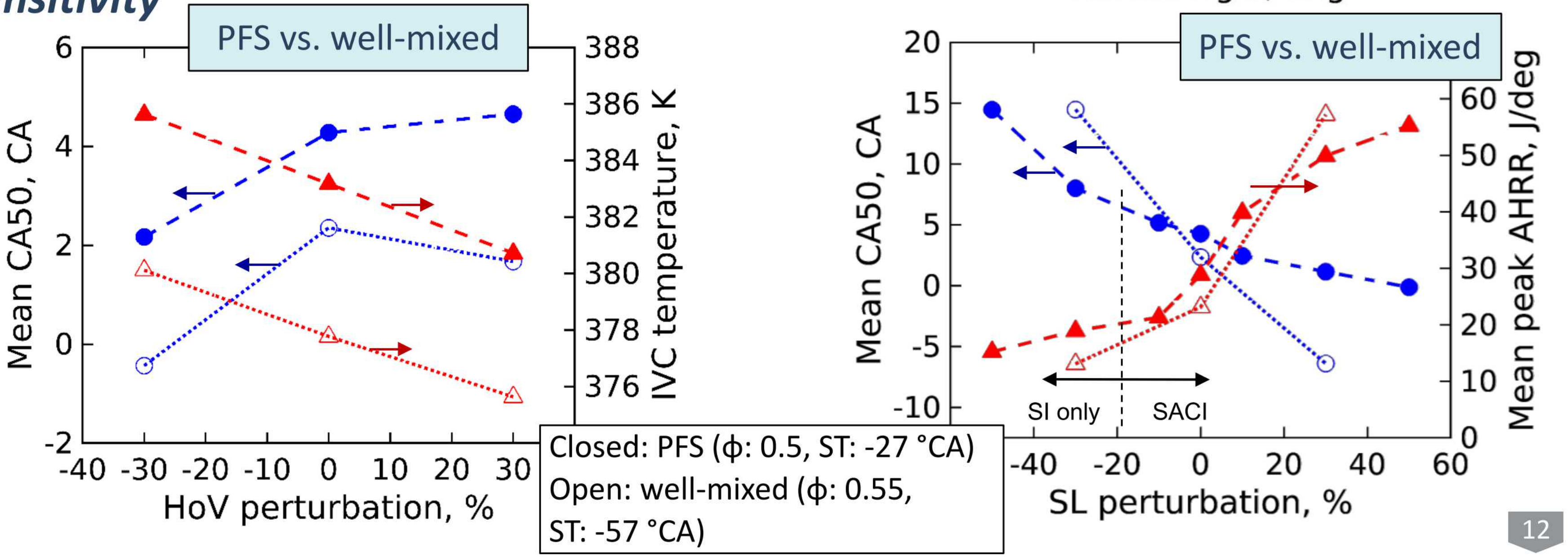
- Heat of vaporization (HoV) plays an important role by modifying the unburned gas temperature and thus combustion phasing; **HoV sensitivity of the PFS operation is comparable with the well-mixed charge operation**
- Laminar flame speed (S_L) directly controls the initial ramp-up of heat release rate 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

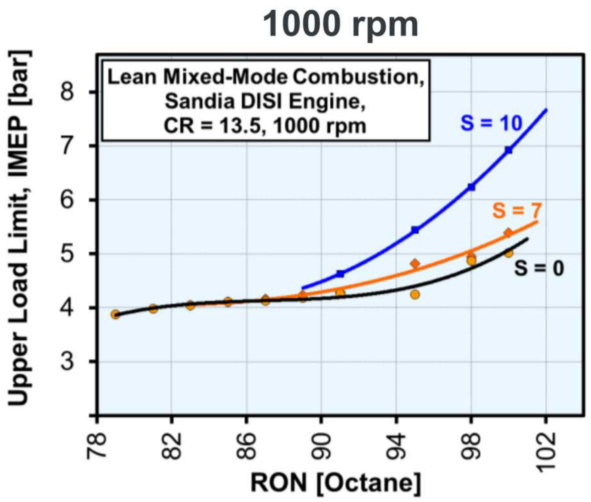


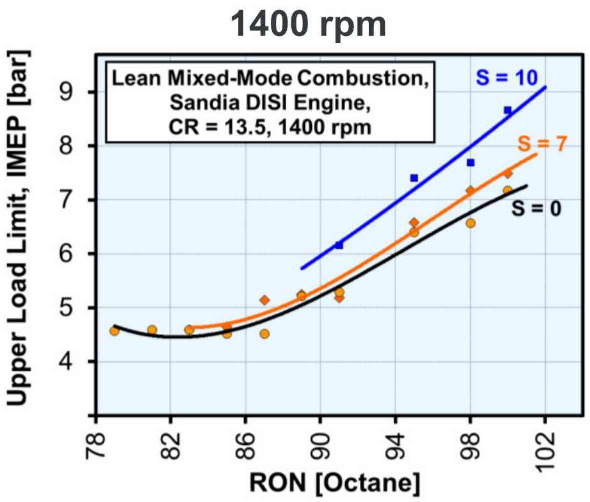


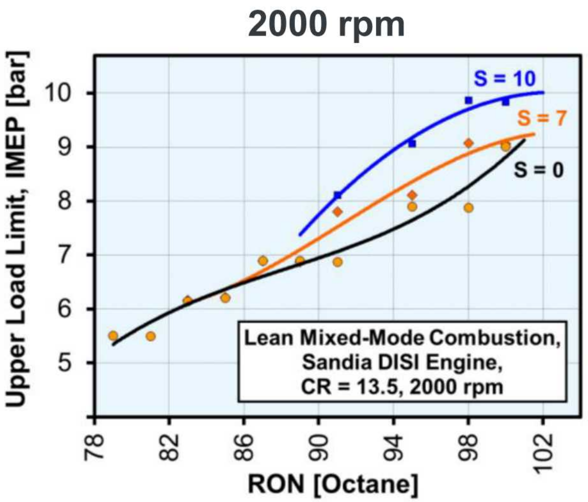
Closed: PFS (ϕ: 0.5, ST: -27 °CA)
Open: well-mixed (ϕ: 0.55, ST: -57 °CA)

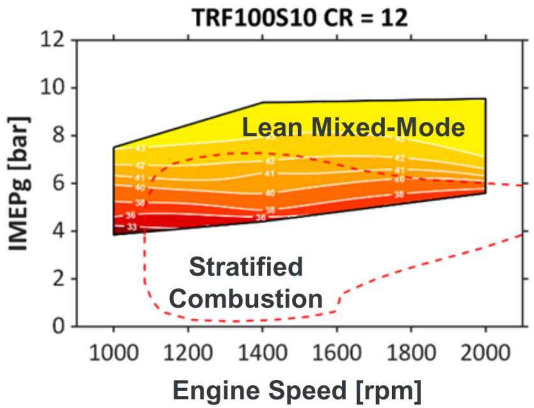
SNL Accomplishments: Increased RON and S Enable Higher Loads with Lean Mixed-Mode Combustion (SACI)

ACCOMPLISHMENTS (5/15)

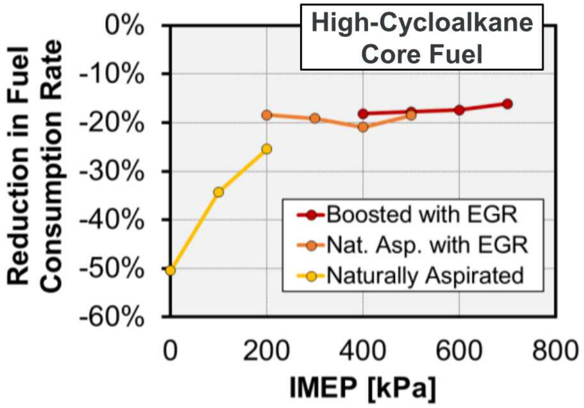


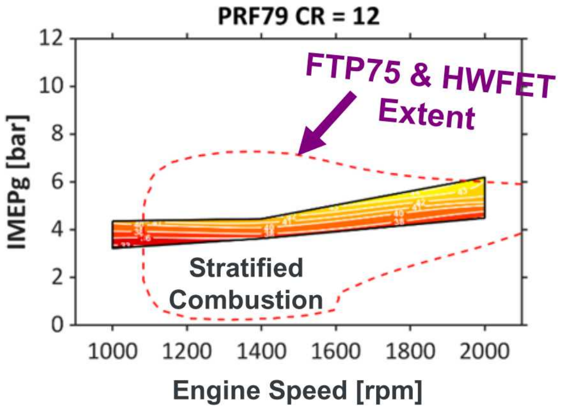






- Used validated GT-Power in combination with CHEMKIN to span large parameter space.
- Increasing RON ⇒ higher loads.
- Increasing octane sensitivity (S) ⇒ higher loads, especially at low speed.



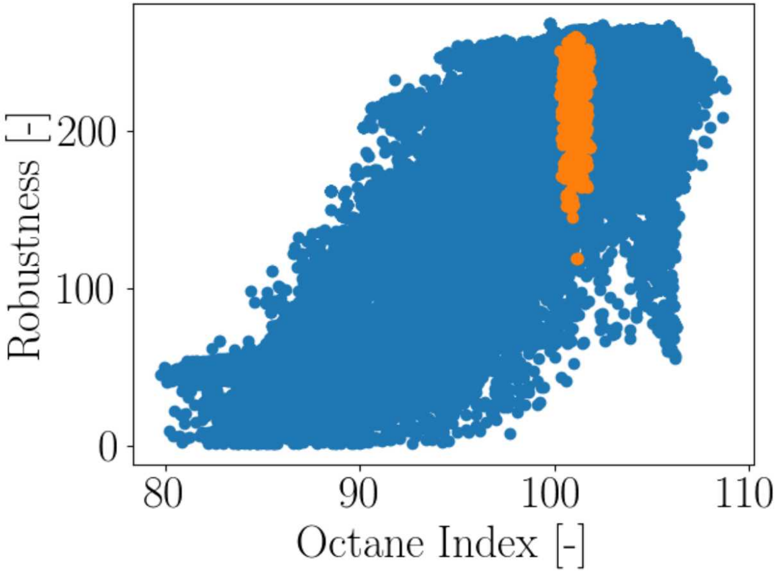


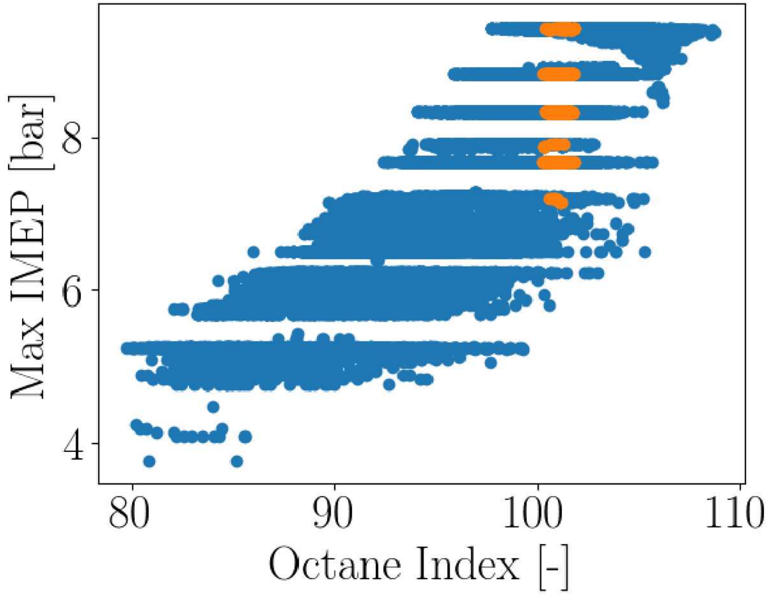
- Here, lower load range is not limited by fuel type.
  - Controlled by pre-selected lowest ϕ_m = 0.35 and lowest P_{in} = 100 kPa.
- Stratified-charge (SC) SI operation can be used for reaching lower loads with superior efficiency.
  - To be considered for drive-cycle modeling.

LLNL Accomplishments:
Fuel Search for Mixed-Mode Combustion (1)

ACCOMPLISHMENTS (6/15)

- Optimization strategy finds fuels which maximize the number of operating points (robustness) and the max IMEP.
- Parallel Zero-RK reactor model allows to test **tens of thousands of fuels/day** using detailed Co-Optima gasoline surrogate mechanism**.**
- Increased the number of operating conditions considered:
  - Sweep over ignition phasing, intake pressure, IVC temperature, and equivalence ratio at a fixed RPM (1400) and compression ratio (12).
  - FY19 search: 96 operating points.
  - FY20 search: 312 operating points.
- Simulated 80,000 fuels from three-component TRF to nine-component surrogates.
- Octane numbers predicted by a neural network.
- High RON and high-S fuels achieve the highest IMEP and highest robustness.
- There is significant scatter at a fixed RON and S; maximum IMEP varies from 7.2 to 9.4 bar for RON = 95±0.5, MON = 86±0.5.





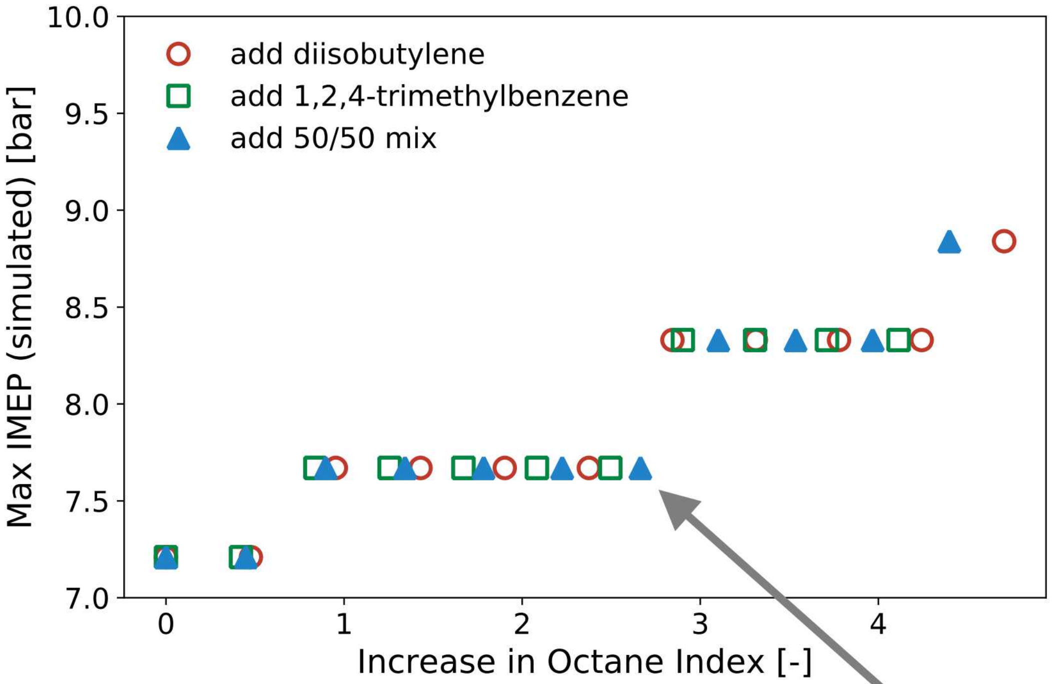
LLNL Accomplishments:
Fuel Search for Mixed-Mode Combustion (2)

- Want to test if the multi-mode performance scatter predicted by the simulations is observed in engine experiments.
- Three blends within the narrow 95/86 RON/MON range were identified for engine tests:
  - Low-performing LLNL-MM-2, max IMEP of 7.2 bar.
  - High-performing LLNL-MM-3 and LLNL-MM-4, similar max IMEP of 9.4 bar.
- Octane numbers measured at Southwest Research Institute illustrate some discrepancies between predicted and actual values:
  - LLNL-MM-3 and LLNL-MM-4 have similar octane index (OI = 103.8 - 103.9)
  - LLNL-MM-2 has lower RON and S.
  - Suggests lower predicted load of LLNL-MM-2 could be due to its lower octane index.

Blends (vol. fraction)	LLNL-MM-2	LLNL-MM-3	LLNL-MM-4
n-pentane	0.17289	0.11178	0
iso-pentane	0.10636	0.08862	0.1058
n-heptane	0.04584	0.10232	0.13238
di-isobutylene	0.13873	0.25354	0.36168
iso-octane	0.32786	0	0.21691
trimethylbenzene	0.20835	0.06328	0
1-hexene	0	0.06124	0.08419
toluene	0	0.23946	0.09903
cyclopentane	0	0.07976	0
max IMEP	7.205	9.421	9.419
robustness	166	218	223
pred. RON	94.6	95.2	95.3
pred. S	9.1	9.2	9.7
actual RON	94.5	96.2	96.7
actual S	7.2	11.6	10.6
actual OI (K = -0.67)	99.3	103.8	103.9

LLNL Accomplishments:
Fuel Search for Mixed-Mode Combustion (3)

- Discrepancies in the octane index (K = -0.67) between LLNL-MM-2 and LLNL-MM-3 and LLNL-MM-4 can be reduced through small composition changes:
  - Decrease fraction of n-heptane by ~2% and increase fraction of di-isobutylene and/or trimethylbenzene.
  - Gaussian Process Regression model for local composition changes predicted RON increases by about 2 octane numbers.
  - Predicted maximum IMEP increases to 7.67 bar.
- SACI simulations suggest the max IMEP will still be significantly lower than that of LLNL-MM-3 or LLNL-MM-4 even if RON and S values are closer.
- Octane number tests and engine experiments necessary to confirm the simulation trends.



-2.4% n-heptane (by mole)

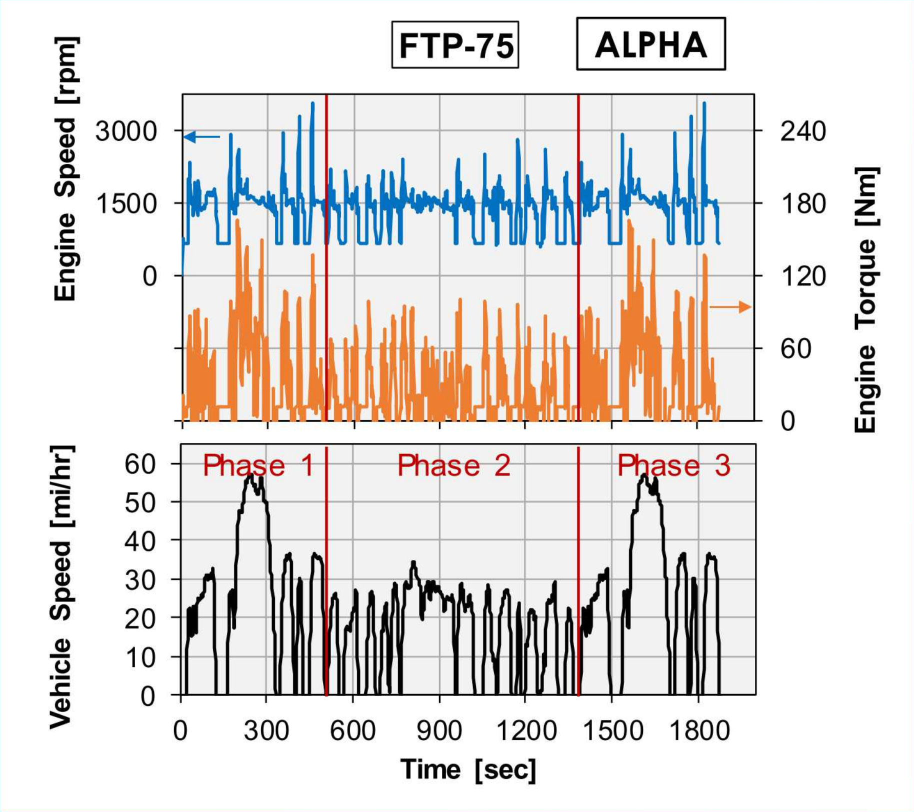
+1.2% diisobutylene

+1.2% 1,2,4-trimethylbenzene

ΔOI = 2.7

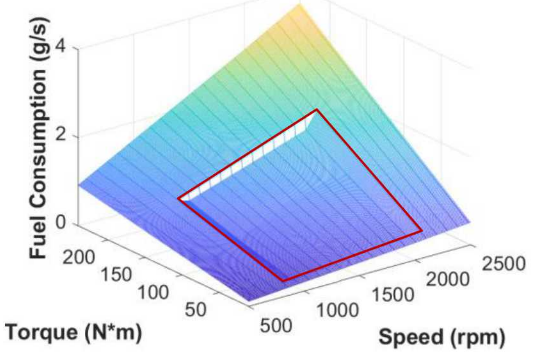
SNL Accomplishments:
GT-Power + CHEMKIN + ALPHA Framework

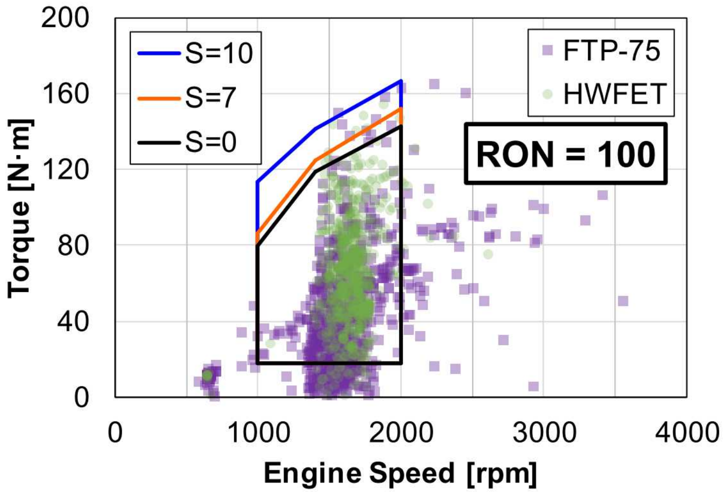
- Use EPA's ALPHA vehicle simulation tool to estimate fuel economy - FTP-75 & HWFET.
- Vehicle type: Standard passenger car
- 1620 kg, 8-speed transmission.
- Utilized GT-Power fuel-consumption rate maps.



- Each map being specific to the combination of CR, combustion mode and ACI load coverage.
- Here, highly simplified assessment, assuming $\lambda = 2$ operation down to 1 bar BMEP.
- Upper load limit dependent on RON & S.

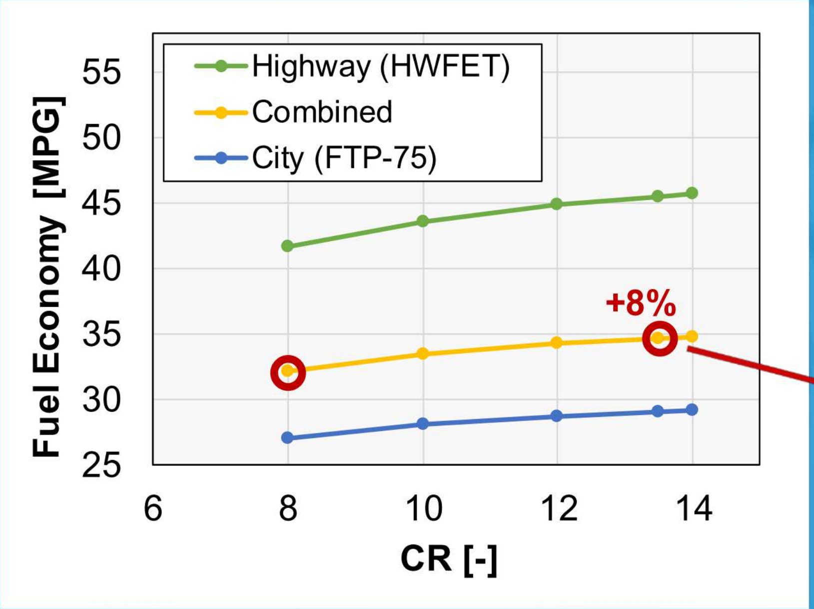
Fuel-consumption rate map (Stoichiometric + lean $\lambda = 2$)



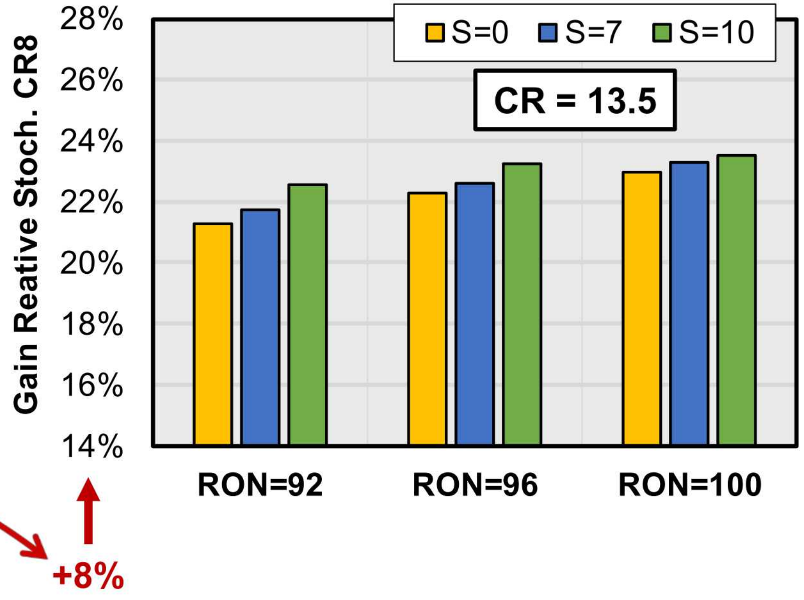


SNL Accomplishments:
GT-Power + CHEMKIN + ALPHA Framework (2)

- Predicted FE Gains for stoichiometric-only operation are slightly lower than predicted by the Merit Function.
- Merit Function assumes downsizing.
- Here, engine size remains 2.2L for all CRs.
- Lean multimode operation provides additional gains of 11 – 14%.

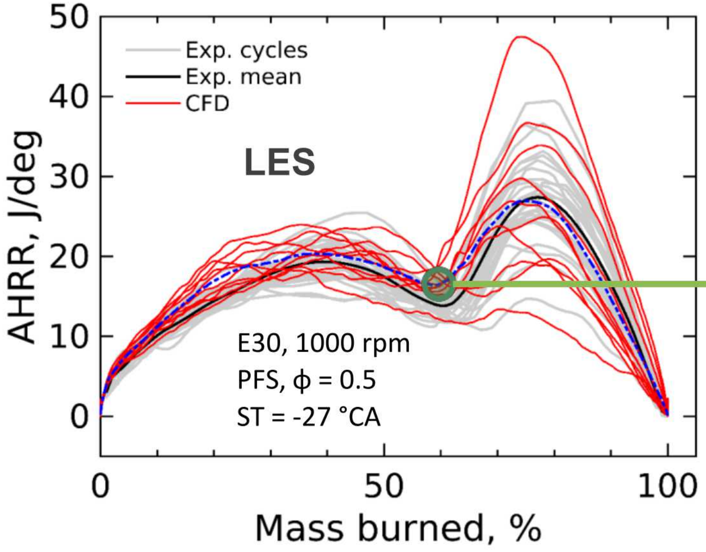


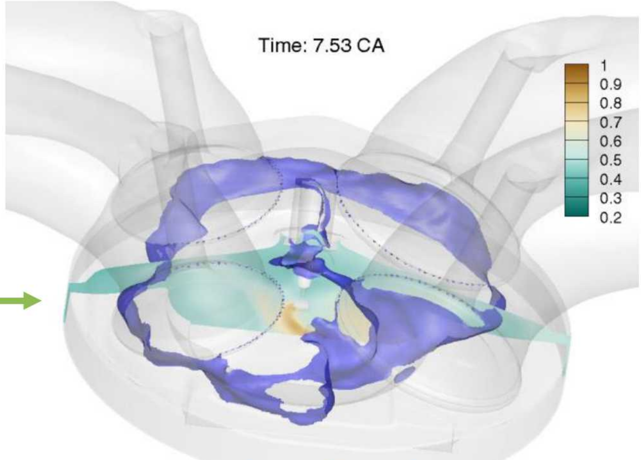
- Higher RON and S are advantageous.
- More than 20% FE Gain is possible.
- Provides motivation for high-RON / high-CR in combination with lean combustion.
  - Here, multiple simplifications and assumptions.
  - Various penalties will detract from practical FE Gains.
  - Stoichiometric knock limits, non-ideal CA50 for mixed-mode combustion, mode switching etc.
  - Refinements will be implemented using Autonomie.



ANL Accomplishments: Utilizing ϕ-sensitivity in PFS-assisted SACI - a CFD-based Assessment

- **Multi-dimensional CFD simulations can shed light on in-cylinder stratification and inform reduced-order modeling that incorporates ϕ-sensitivity effects**
  - End-gas can be rigorously identified and separated from the burned product in CFD
  - Analysis of CFD data reveals the presence of non-negligible mixture stratification ($\Delta\phi \approx 0.2$) and temperature stratification ($\Delta T \approx 500$ K) in the end-gas for lean PFS-assisted SACI

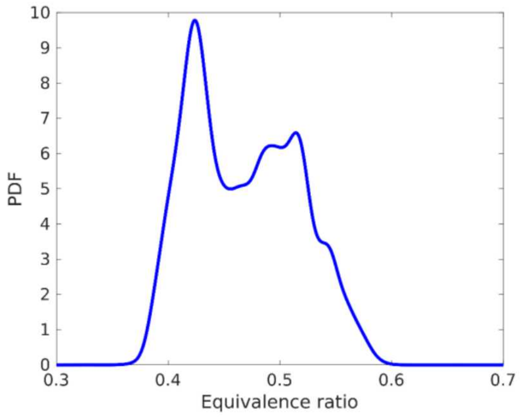




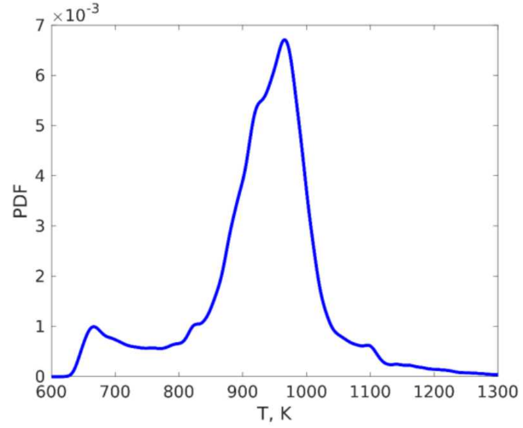
Isosurfaces: flame fronts

Cross-section: equivalence ratio

ϕ - stratification

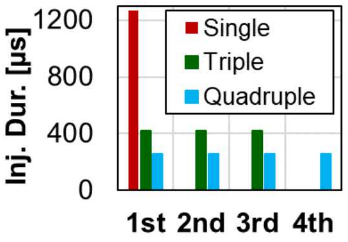


T - stratification

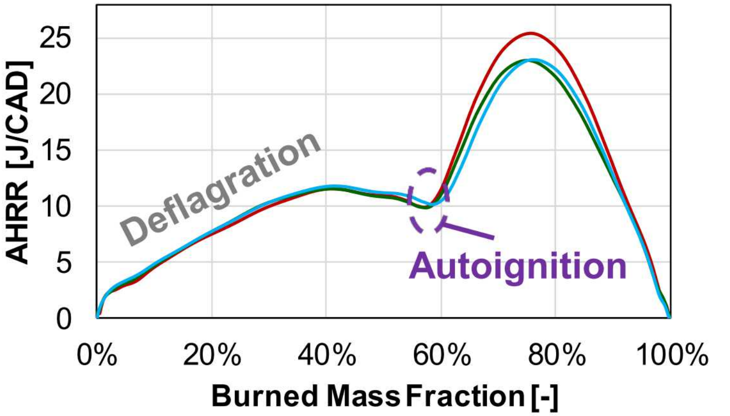


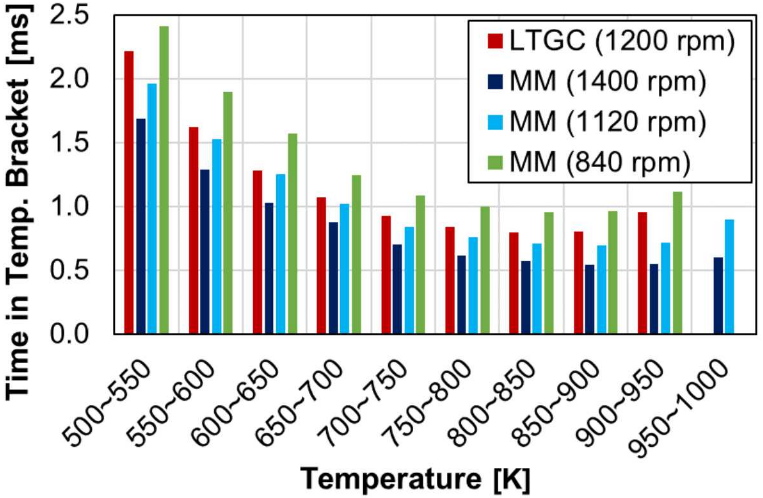
SNL Accomplishments:
Initial DISI Trial with ϕ–sensitive Multimode Fuel

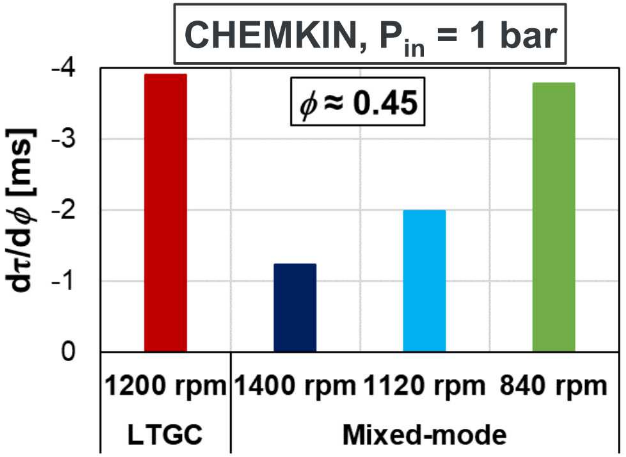
- Partial fuel stratification (PFS) can be used to smooth heat-release rates in autoigniting mixtures. Fuels with higher ϕ-sensitivity can enhance this effect.
- In DISI engine, performed initial tests with CB#1 fuel* developed by Lopez-Pintor and Dec.
  - RON = 93.3, S = 10.7, 12.4% vol. iso-butanol, ϕ-sensitivity higher than RD5-87. (See FT089)
- For an SACI approach, need to stratify end-gas without affecting the early deflagration.
  - Not trivial. Explored options like SOIs, dwell between injections, and number of injections.
- In this example, deflagration is not affected in the range of 1-4 early injections.
- Only moderate reduction of peak AHRR observed experimentally ⇒ CHEMKIN was used to assess if engine operation is conducive to exploiting ϕ–sensitivity.
- Analysis reveals that the fast end-gas compression to autoignition by deflagration leaves little time for ϕ–sensitive reactions in SACI mode, as compared to only piston-compression in LTGC engine.
- CHEMKIN predicts that engine speed needs to be reduced to around 840 rpm for CB#1 to show full potential in SACI mode.



1400 rpm
T_{in} = 90°C
$\phi_{end\text{-}gas}$ = 0.40
Intake injs.







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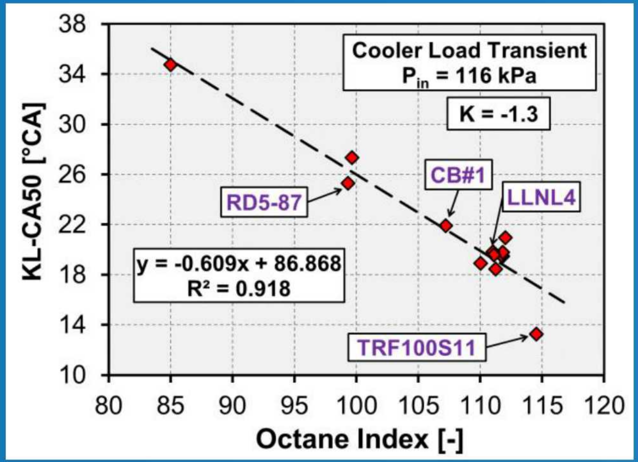
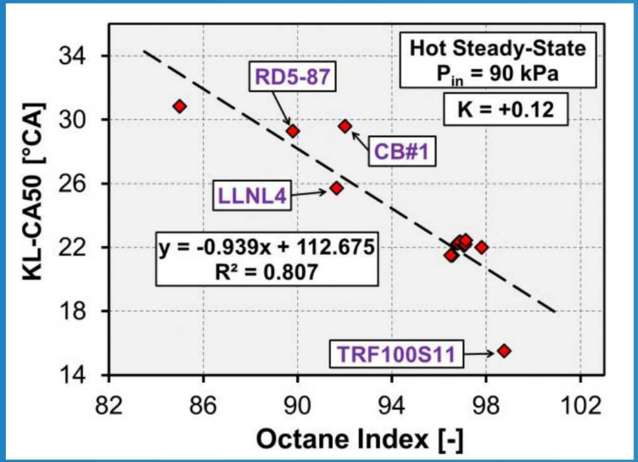
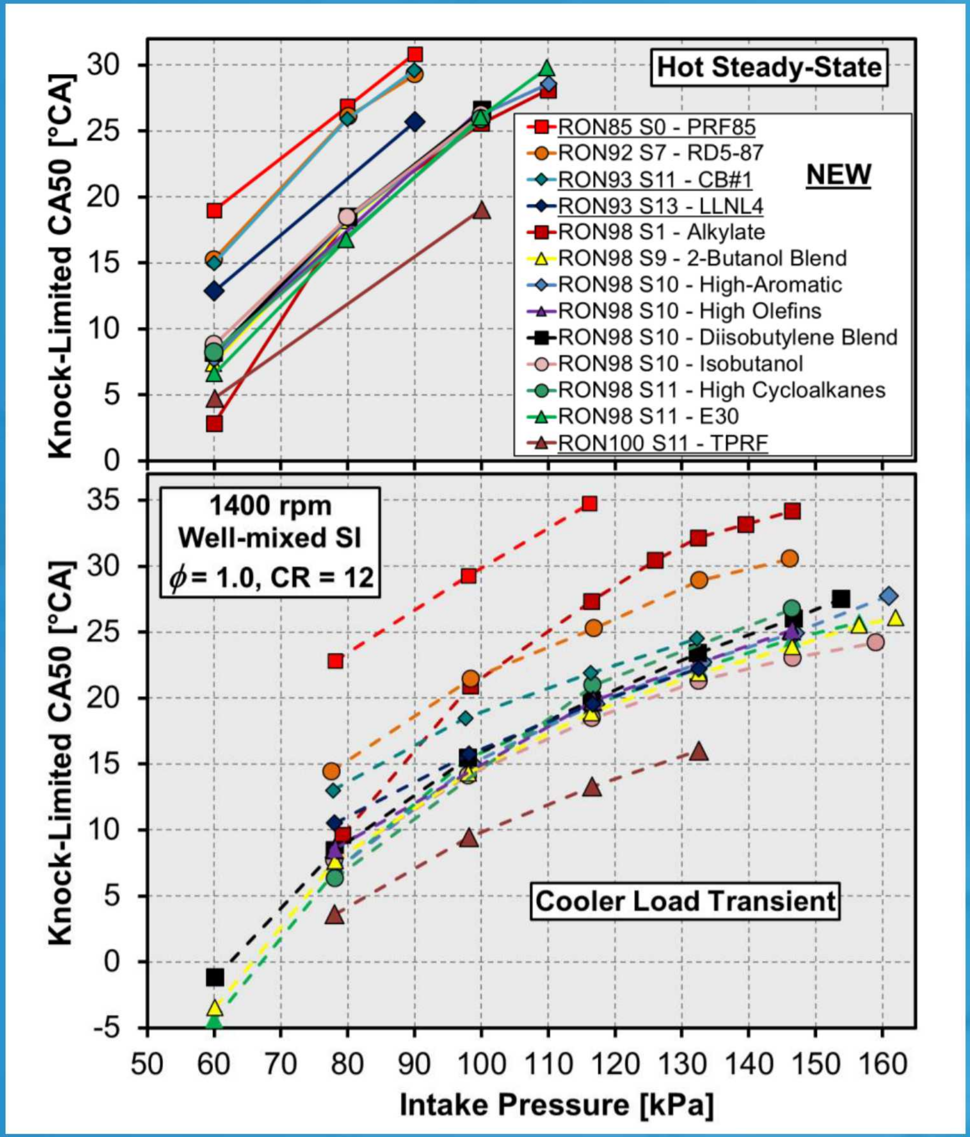
* Named Blend #4 in SAE 2019-01-0961 and evaluated experimentally as CB#1 in SAE 2020-01-1136.

SNL Accomplishments: Stoichiometric Knock Limits for (Novel) Multimode Fuels – an Assessment of OI Framework

- TRF100S11 and PRF85 were blended and tested to acquire validation data for GT-Power / CHEMKIN models used to assess octane appetite for lean SACI.
- Fuel search at LLNL identified a promising 4-comp. blend for mixed-mode comb.
- Knock limits were assessed for both hot steady-state and cooler transient operation.
- Compared to Octane Index, CB#1 is slightly more reactive for hot steady-state.
  - Consistent with design intent for LTGC operation. (Despite differences in their OIs, RD5-87 and CB#1 have similar KL-CA50 at P_{in} = 90 kPa, in agreement with LTGC data* at P_{in} = 100 kPa.)
- CB#1 complies with OI for cooler boosted conditions.
- TRF100S11 is generally less reactive than expected based on OI.
  - Contains 69% toluene, known to be resistant to autoignition and cause OI deviations.







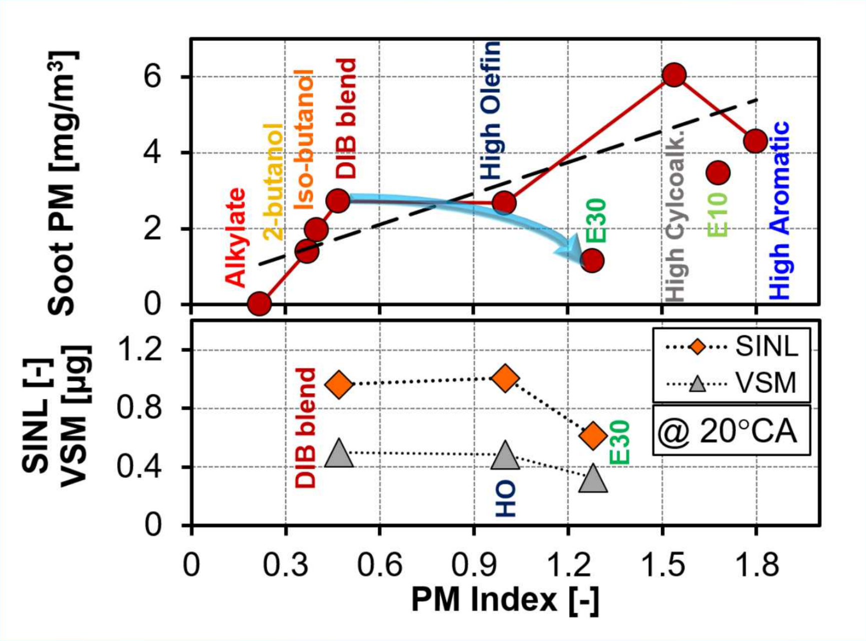
* SAE 2020-01-1136.

SNL Accomplishments:
PMI Shortcomings for Boosted Stratified Charge Operation

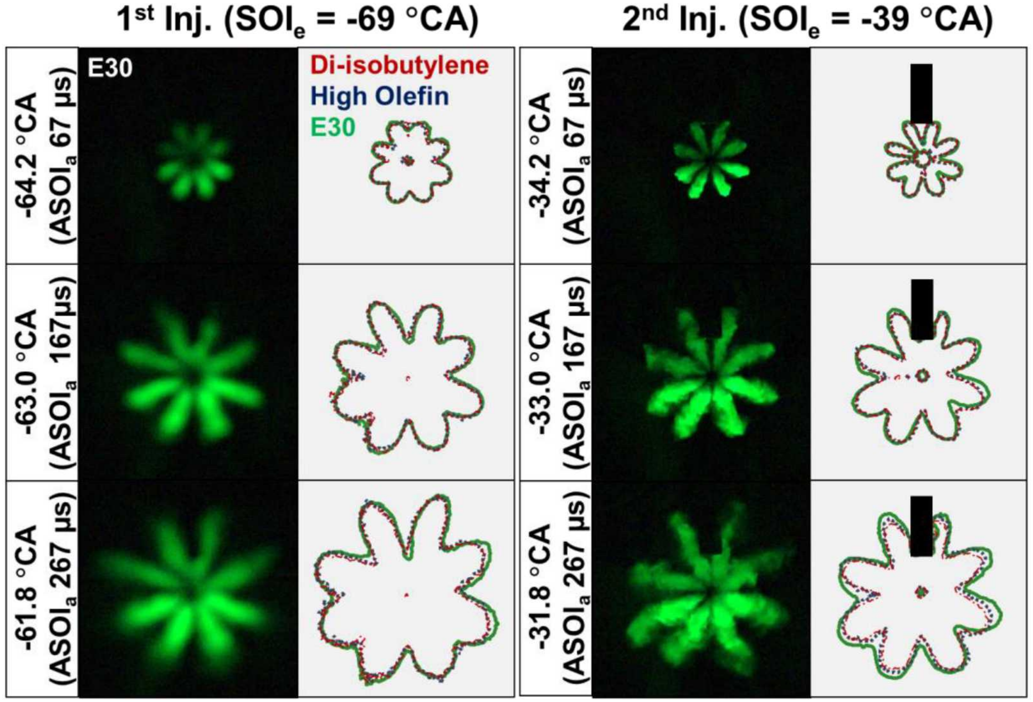
- Future fuels need to enable clean engine operation ⇒ Assess fuel sooting metrics for advanced comb.
- FY19 results highlighted shortcomings of commonly used PMI.

$$PMI = \sum_{i=1}^{n} I_{[443K]} = \sum_{i=1}^{n} \left(\frac{DBE_i + 1}{VP\,(443K)_i} \times Wt_i \right)$$

- E30 produces less soot, DIB blend with toluene more, than expected based on PMI.

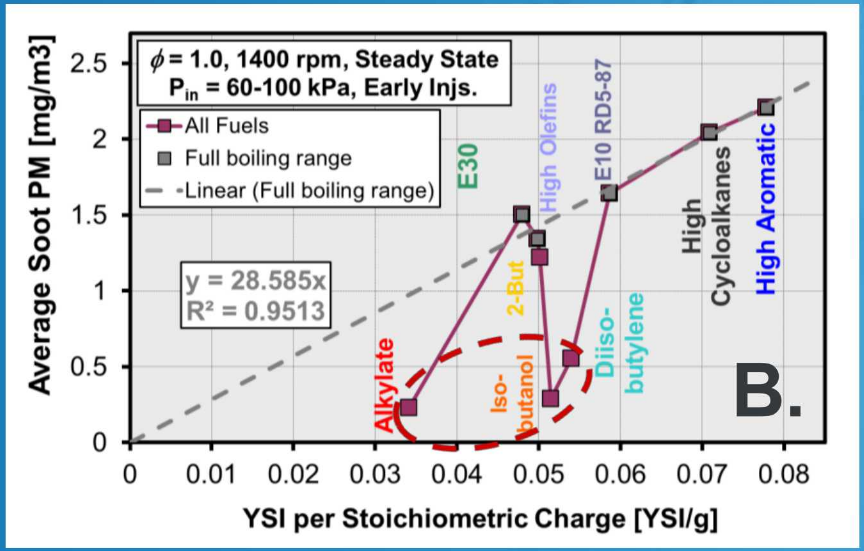


- Other conditions have shown direct effects of fuel on spray development.
- Spray diagnostics in FY20 indicate nearly identical spray morphologies for the three fuels examined.
- Conclusion remains that PMI shortcomings stem from PMI not accounting for O in fuel + incorrect importance of vapor pressure for SC operation.

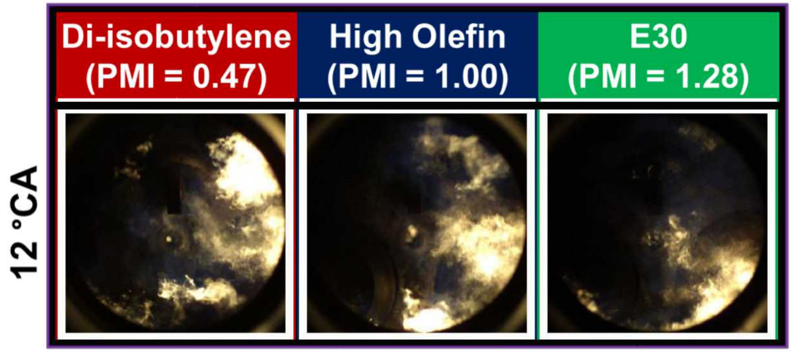


SNL Accomplishments: The Use of YSI for: A) Lean Boosted SC B) Stoichiometric Operation

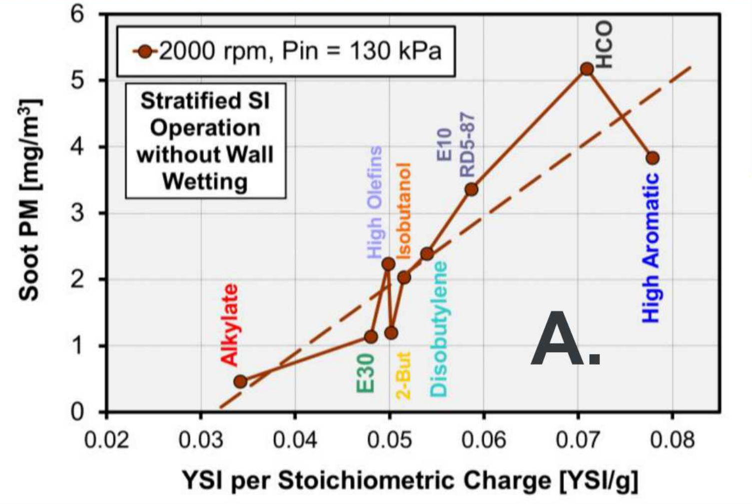
- Collaboration with LLNL, Yale, NREL and PSU.
- YSI values cannot be used directly. (See back-up.)
- YSI per mass of stoichiometric charge works OK for full-boiling range fuels.
  - Indicates that wall wetting is similar.
  - Soot PM under predicted for 3 (of 4) volatile fuels.
  - Suggest very little wall wetting.
- New sooting metrics need to factor in volatility.
  - *E.g.* Data-Derived Sooting Index at NREL (St. John *et al.*)



- Flame and RIM diagnostics show:
  - Minimal wall wetting. Bulk-gas soot dominates.



- Exploring the use of YSI to explain these trends.
- YSI per mass of stoichiometric charge does a reasonable job bringing E30 closer to trend-line.



Responses to Previous Year Reviewers' Comments

(Positive comments with suggestions for future work, which we are considering.)

Overall Approach:

A reviewer noted "The reviewer found the experimental capabilities, which are linked to outstanding simulation capabilities, to be outstanding.", but also suggested "Much can be learned from steady-state studies; but to implement the outcomes from this work, the reviewer said that perhaps the approach can expand to include consideration of mode switching." Another reviewer noted "The barrier does refer to controls, and there is not much activity on that end." Yet another reviewer commented "Overall, it was not clear to the reviewer how, or if, the different tasks and approaches fit together within a cohesive effort, or how they are responsive to overcoming the technical barriers. For the optical engine work, the focus on the particulate matter index (PMI) and particulates does not seem well connected to the mixed-mode project focus. Also, the reviewer said that emissions and any associated aftertreatment requirements must also factor into the analysis since this may change the overall optimal fuel properties." Response: We appreciate all the positive remarks. However, both regarding the approach and future work there were numerous somewhat critical comments that we do not sufficiently incorporate load transients, mode switching and exhaust aftertreatment. Transient control and mode switching are certainly important for overcoming barriers to real-world implementation of advanced lean combustion. To address this deficiency, future experimental work in these tasks will include some efforts on mode switching between stoichiometric SI, lean mixed-mode combustion (SACI), and lean stratified-charge (SC) operation. This should also better tie the different sub-tasks together for multimode operation. However, this limited effort will not go all the way to demonstration of an emissions-compliant multi-cylinder engine. It should be recognized that the primary interest of the Co-Optima multimode project is to identify which fuel properties are governing load range, combustion control, noise generation and emissions formation. Following this, appropriate ranges for these fuel properties should be determined while establishing the role of bioblendstocks for achieving these fuel properties. The primary outcomes of this project are the guidance regarding fuel properties and the scientific basis for a certain fuels "appetite" and as well phenomenological explanation for the observed challenges/barriers. Overcoming these barriers and experimentally demonstrating a calibrated multimode engine are well beyond the scope and budget for the current multimode tasks in Co-Optima. Specifically regarding compliance with NO_x and PM emissions - these are tasks that require substantial efforts to optimize hardware such as fuel-injection system, intake ports and combustion-chamber geometry, and well as coupling with advanced aftertreatment systems. Such hardware-intensive efforts can be considered, but are not currently in scope. Nevertheless, we are monitoring emissions level and how those are affected by fuel properties (including PMI and other sooting metrics) and these results will contribute to an assessments of pathways towards emissions compliance led by ORNL. Furthermore, in future work we will examine how fuel properties can help towards reduced NO_x formation for lean operation.

Accomplishments:

Several reviewers praised the amount of accomplishments with comments like "The reviewer found the technical progress on this project to be outstanding." but one reviewer also noted that "The modeling work and data project outputs are a little vague on impact." Response: We appreciate the positive feedback. While the CFD work for FY19 largely focuses on model validation, for FY19 and FY20, we will be leveraging the developed CFD models to probe physics, to understand fuel property effects on SACI engine performances including engine efficiency, stability and emissions, and to inform reduced-order models. Specifically, impact of the CFD modeling work on this Co-Optima multi-mode project is two-fold. First, establishing a well-validated CFD modeling framework for lean SACI operation is essential since it enables direct visualization of various in-cylinder processes (spray, flow, combustion, emission, etc.) and isolated investigation of individual fuel properties, both of which are challenging in experiments, thus improving the understanding of fuel-engine interactions in SACI. For example, the detailed information from CFD on in-cylinder temperature and mixture stratification provides key insights to knock mitigation strategies and such new fuel properties as ϕ-sensitivity. Second, high-fidelity CFD generates enormous amount of data, which can be leveraged to inform reduced-order models. For example, within this collaboration, the CFD data will be provided to the SNL team and the LLNL team to enhance multi-zone engine models using novel machine learning techniques.

Collaboration and Coordination:

A reviewer noted "The reviewer remarked that coordination among the collaborators appears to be outstanding."

Proposed Future Research:

A reviewer remarked "…that the effort to coordinate Laboratories and project for future research is very positive. Several other reviewers noted sentiments like "…examine what technical barriers exist in moving this project from concept and low TRL toward a multi-cylinder engine". Response: See above.

Relevance—Does this project support the overall DOE objectives?

Very positive feedback on this question, for example one reviewer remarked "…this is exactly the type of project DOE needs to be doing." Response: We appreciate the positive feedback.

Collaboration and Coordination with Other Institutions
Leveraging Co-Optima Collaborations

- **Strong industry engagement including industry-led external advisory board and stakeholder phone calls.**
- **Collaboration across nine national laboratories, two DOE offices, and twenty+ universities.**
- **DOE's PACE effort provides further opportunities for collaboration between National Labs.**
- **15 Industry partners in the AEC MOU. University partners as well.**

PACE
PARTNERSHIP
TO ADVANCE
COMBUSTION
ENGINES

SNL - DISI
E.1.1.3, E.1.1.4

- General Motors – hardware / discussions.
- CFD work with Som and Xu at ANL.
- Funds-in knock project with Toyota.
  - Effects of EGR and fuel type on knock.
- Pitz & Wagnon at LLNL.
  - Surrogate-gasoline mechanisms.
- McNenly & Lapointe at LLNL.
  - Optimal fuel search for SACI.
- Dec and Lopez-Pintor at SNL.
  - CHEMKIN analysis of custom LTGC blend.
- Ding & Böhm at TU Darmstadt.
  - RIM techniques for wall wetting.
- Xu He at Beijing Institute of Technology.
  - RIM and flame-speed studies.
- Pickett *et al.* at SNL for spray insights.
- McEnally at Yale on fuel sooting metrics.

ANL - CFD
G.2.1

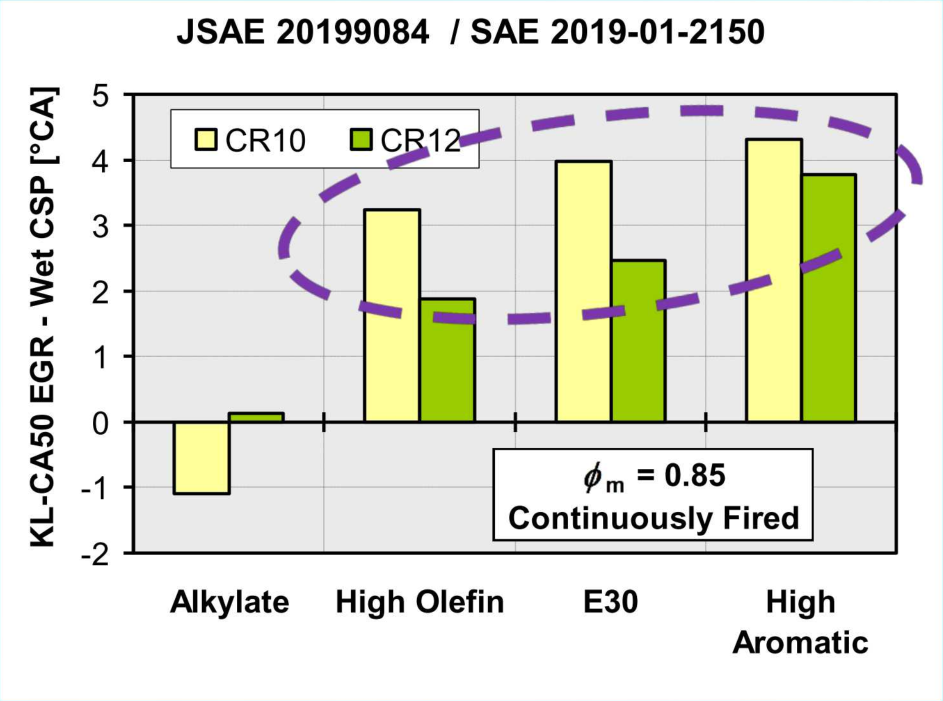
- Direct collaborations with Sjöberg at SNL for DISI engine experimental data and reduced-order modeling.
- Whitesides & McNenly at LLNL for fuel surrogate model and data-informed multi-zone modeling.
- UConn (Prof. Lu) for chemical mechanism.
- Convergent Science Inc. for software.
- Yue at Tianjin University for knock modeling.

LLNL – Data Consolidation
G.5.7

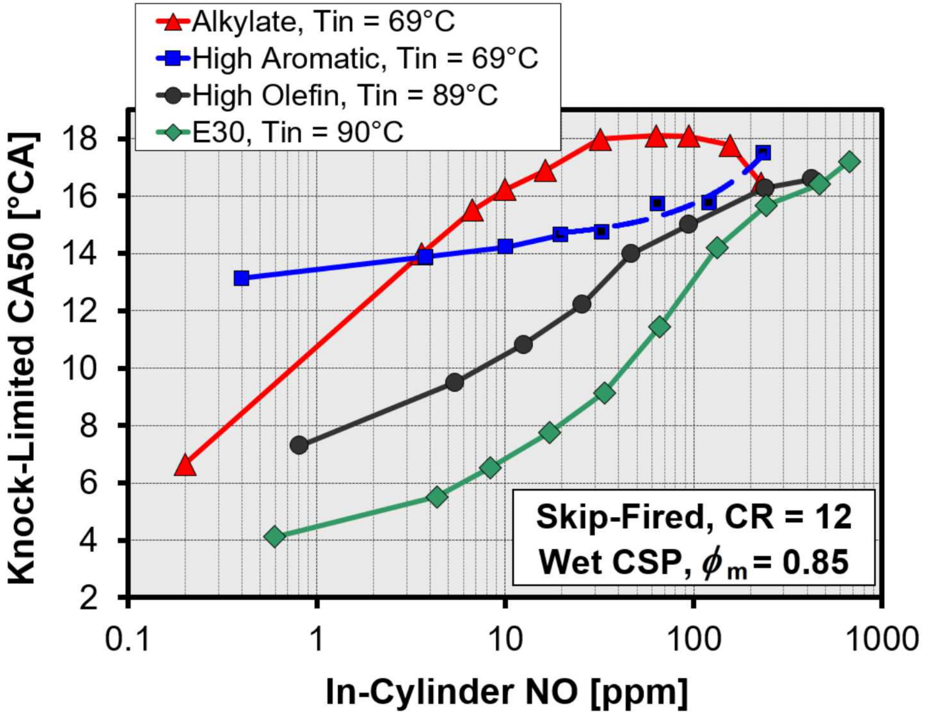
- Collaboration with multi-mode experimental and simulation efforts at ORNL, SNL, ANL.
- Direct collaboration with J. Mueller (LBNL) on statistical surrogate modeling.
- Data evaluation with J. Szybist ORNL and M. Sjöberg SNL.

Collaborations (SNL)

- Funds-in knock project with Toyota.
- Open literature dissemination.
- Research scope include comparing efficacy of EGR taken before and after the 3-way catalyst.
- For fuels with high octane sensitivity, EGR with trace species is less effective than clean EGR.



- NO-seeding experiments reveal that the effects of NO on autoignition play a key role for these observed differences.
- The insights complement Co-Optima studies of lean mixed-mode combustion.
- NO in trapped residuals can affect fuels differently.



Remaining Challenges and Barriers

SNL Multimode Engine Operation:

- Unclear how well steady-state results translate to transient operation in drive-cycles.
- Unclear if increased heat of vaporization (HoV) benefits lean operation like it does for knock-limited stoichiometric operation.
- Exhaust emissions compliance is challenging for lean SI operation.

ANL CFD:

- Computationally efficient knock modeling strategies for lean SACI operation remain to be developed.
- Predictive modeling of NO_x and soot emissions remains challenging.

LLNL Data Consolidation:

- Integration of mass data from CFD into reduced-order and/or system-level evaluation tools remains to be explored.
- Fuel-Engine experiments and high-fidelity simulations can not generate enough data to discover hidden fuel properties using unsupervised learning (data mining).
- Creating a framework to fairly compare the benefits of different mixed-mode strategies and fuel combinations.

Proposed Future Research*

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

SNL Multimode Engine Operation:

- Expand experimental efforts to include load transients and mode switching.
- Investigate effect of HoV on load range and NO_x emissions.
- Refine assessment of fuel effects on drive-cycle fuel economy.
  - Use Autonomie and account for penalties associated with mode switching and exhaust compliance.
- Test performance of selected fuels identified in LLNL search of SACI fuels.
- Examine optically fuel/load combinations that have PM or stability issues.
- Identify fuel properties that support robust implementation and clean exhaust.
- Collaborate on the development of new fuel sooting metrics for advanced combustion modes.

ANL CFD:

- Expand CFD modeling efforts for lean SACI operation to wider ranges of fuel types, loads, and speeds.
- Evaluate fuel composition and RON&MON effects in CFD through collaboration with LLNL fuel search.
- Develop accurate and computationally-efficient knock modeling capability for lean stratified SACI operation.
- Quantify fuel property effects on engine efficiency with knock constraint and on NO_x and soot emissions.
- Investigate potential ways of mitigating in-cylinder NO_x formation using CFD.

LLNL Data Consolidation:

- Generate multi-mode engine maps with most promising fuels using validated multi-zone model trained on experiments and detailed CFD.

Summary *

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

Relevance

- Longer-term co-development of fuels for advanced SI and SI-ACI multi-mode combustion.

Approach

- Multi-lab team, approach spanning optical engine, CFD and data-integration expertise.

Technical Accomplishments

- Refined and used a methodology to determine the octane appetite of mixed-mode combustion (SACI) using GT-Power and CHEMKIN.
- Developed and used a GT-Power – ALPHA methodology to quantify fuel-economy benefits of lean operation.
- Examined role of fuel effects on spray for PMI shortcomings.
- Developed a computational-efficient LES-based CFD model for lean SACI assisted by partial fuel stratification (PFS).
- Used the high-fidelity LES-based CFD model to investigate fuel property sensitivities, including HoV and laminar flame speed, for PFS-assisted SACI.

Technical Accomplishments cont.

- Found evidence that there may be another fuel property in addition to Octane Index affecting SACI performance.

Collaboration and Coordination

- Strong collaboration between established PIs with post-docs, and with close ties to key partners.

Proposed Future Research*

- Expand experimental efforts to include load transients and mode switching. Refine assessment of fuel effects on drive-cycle fuel economy.
- Investigate potential ways of mitigating in-cylinder NO_x formation using experiments and CFD.
- Expand CFD modeling efforts for lean SACI operation to wider ranges of fuel types, loads, and speeds.
- Generate multi-mode engine maps with most promising fuels using validated multi-zone model trained on experiments and detailed CFD.

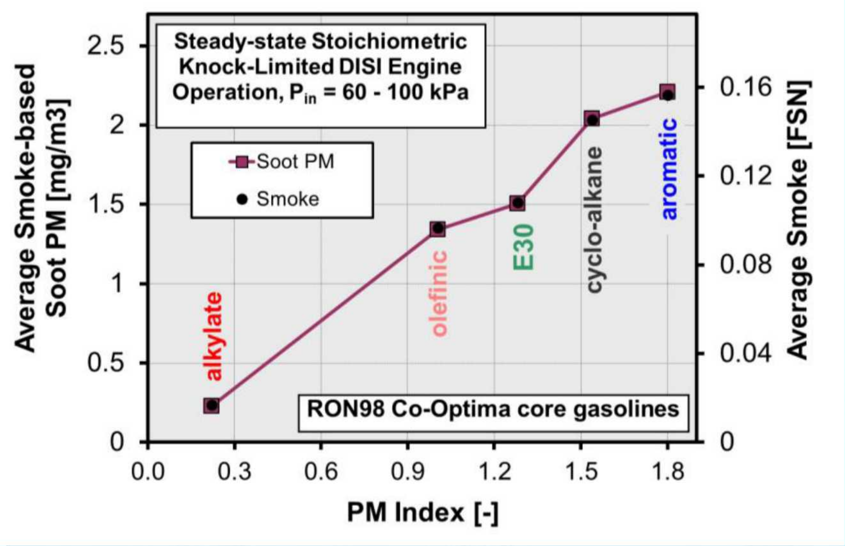
Technical Back-Up Slides

SNL Backup Slides #1:
The Use of PMI and YSI for Stoichiometric Operation

- Example with Co-Optima Core Fuels for steady-state stoichiometric operation.

1. PMI works well.
2. YSI cannot be used directly. E30 data point is way off.
   - YSI measured for 1000 ppm fuel concentration.
   - Low molecular weight of E30, and low AFR_{st}.
3. YSI per mass of stoichiometric charge works OK.
   - Not as good as PMI.
   - Missing information on volatility differences between fuels.

1.



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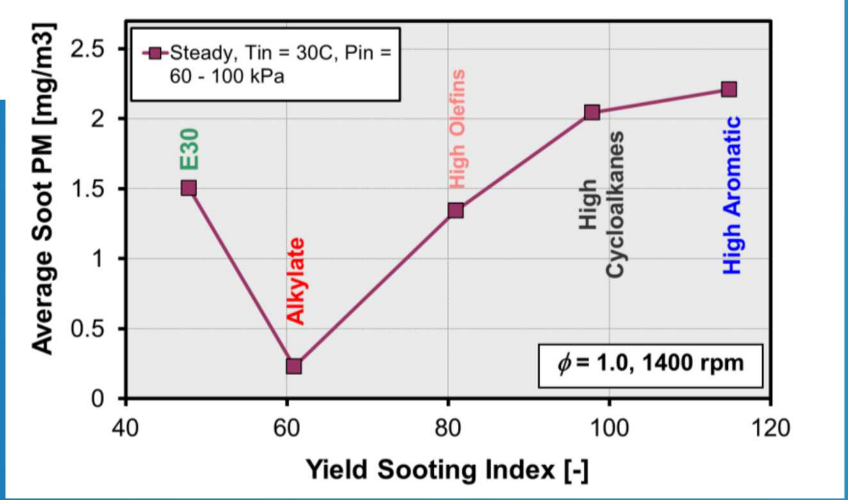

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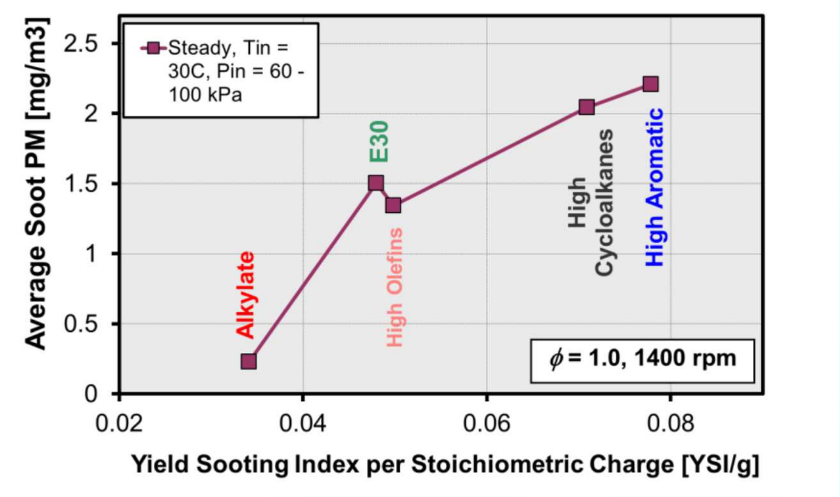

SNL Backup Slide #2:
Fuel Properties Table

- TRF98S10 and PRF85 were blended and tested to acquire validation data for GT-Power / CHEMKIN models used to assess octane appetite for lean SACI.
- A promising 4-component blend for mixed-mode combustion was identified by the fuel search at LLNL.
- CB#1 was designed by Lopez-Pintor and Dec to provide increased ϕ-sensitivity for naturally aspirated operation in LTGC ACI mode.
- The listed fuel properties stem from both published and not-yet-published measurements, simulations and estimates. It is likely to include some errors and inconsistencies.

		Co-Optima Core Fuels					Tier III Blendstocks + NREL BOB			Recent Multimode Test Fuels			
	E10 RD5-87	**Alkylate**	**E30**	**High Aromatic**	**High Olefin**	**High Cycloalkane**	**Isobutanol Blend**	**2-Butanol Blend**	**Diisobutylene Blend**	**#CB1**	**TRF100S11**	**LLNL 4-Comp MM**	**PRF85**
RON	90.6	98.0	97.9	98.1	98.3	97.8	98.1	98.2	98.3	93.3	100.1	93.3	85.0
MON	83.9	96.7	87.1	87.6	87.9	86.9	88.0	89.1	88.5	82.6	89.0	79.6	85.0
Octane Sensitivity	6.7	1.3	10.8	10.5	10.4	11.0	10.1	9.1	9.8	10.7	11.1	13.7	0.0
AKI	87.3	97.3	92.5	92.8	93.1	92.3	93.1	93.7	93.4	88.0	94.55	86.5	85.0
Oxygenates [vol.%]	10.6	0.0	30.6	0.0	0.0	0.0	24.1	28.4	0.0	12.4	0	0	0.0
Aromatics [vol.%]	22.8	0.7	13.8	39.8	13.4	33.2	19.0	17.9	20.1	30.9	68.7	45.7	0.0
Alkanes [vol.%]	48.7	98.1	40.5	46.2	56.4	40.6	53.1	50.1	56.3	38.4	31.3	4.3	100.0
Cycloalkanes [vol.%]	12.1	0.0	7.0	8.0	2.9	24.2	0.0	0.0	0.0	0.0	0	0	0.0
Olefins [vol.%]	5.9	0.1	5.6	4.5	26.5	1.6	3.8	3.6	23.6	18.3	0	50.0	0.0
T10 [°C] (most volatile for surrogates)	57	93	61	59	77	56	63	63	63	36	98	63	98
T50 [°C] (non-surrogates only)	98	100	74	108	104	87	-	-	-	-	-	-	-
T90 [°C] (least volatile for surrogates)	156	106	155	158	136	143	111	111	111	138	111	111	99
Net Heat of Combustion [MJ/kg]	41.9	44.5	38.2	43.0	44.1	43.2	40.6	40.1	43.2	41.9	41.6	42.4	44.4
Heat of Vaporization [kJ/kg]	412	309	565	412	337	393	412	415	337	417	386	382	311
AFR Stochiometric	14.1	15.1	12.9	14.5	14.8	14.5	13.8	13.6	14.7	14.1	13.9	14.1	15.1
HoV [kJ/kg stoichiometric charge]	27.3	19.2	40.7	26.6	21.4	25.3	27.9	28.5	21.5	27.6	25.9	25.2	19.3
Average Molecular Formula	C: 6.01 H: 11.84 O: 0.2	C: 7.76 H: 17.45	C: 4.49 H: 9.87 O: 0.5	C: 6.92 H: 12.41	C: 7.130 H: 14.23	C: 6.460 H: 11.71	C: 6.299 H: 12.744 O: 0.326	C: 6.122 H: 12.532 O: 0.378	C: 7.519 H: 14.420	C: 6.155 H: 11.56 O: 0.16	C: 7.12 H: 10.14	C: 6.56 H: 10.17	C: 7.84 H: 17.67
Particulate Matter Index	1.68	0.22	1.28	1.80	1.00	1.49	0.40	0.37	0.47	0.91	0.91	0.69	0.19
YSI, *estimated	>78*	61	48	115	81	98	71	67	89	85	142	107	57
Density@15°C [g/ml]	0.7480	0.6968	0.7527	0.7572	0.7229	0.7555	0.7517	0.7556	0.7318	0.7369	0.8128	0.7636	0.6932

LLNL Backup Slide #1:
Fuel Search for Multi-Mode Combustion

- Discrepancies in octane numbers between LLNL-MM-2 and LLNL-MM-3 and LLNL-MM-4 can be reduced through small composition changes:
  - Decrease fraction of n-heptane by 2% and increase fraction of di-isobutylene (LLNL-MM-2.1) or trimethylbenzene (LLNL-MM-2.2).
  - Predicted RON increases by more than 1.
  - Predicted maximum IMEP increases to 7.67 bar.
- Results suggest the max IMEP will still be significantly lower than that of LLNL-MM-3 or LLNL-MM-4 even if RON and sensitivity values are closer.
- Octane number tests and engine experiments necessary to confirm the simulation trends.

Blends	LLNL-MM-2	LLNL-MM-2.1	LLNL-MM-2.2
n-pentane	0.17289	0.17289	0.17289
iso-pentane	0.10636	0.10636	0.10636
n-heptane	0.04584	0.02584	0.02584
di-isobutylene	0.13873	0.15873	0.13873
iso-octane	0.32786	0.32786	0.32786
trimethylbenzene	0.20835	0.20835	0.22835
1-hexene	0	0	0
toluene	0	0	0
cyclopentane	0	0	0
max load	7.205	7.67	7.67
robustness	166	185	189
pred. RON	94.6	95.7	95.5
pred. S	9.1	9.3	9.2

Reviewer-Only Slides

Publications

SNL

- C.P. Ding, D. Vuilleumier, N. Kim, D.L. Reuss, M. Sjöberg, and B. Böhm, (2019), "Effect of engine conditions and injection timing on piston-top fuel films for stratified direct-injection spark-ignition operation using E30", International Journal of Engine Research, doi: 10.1177/1468087419869785.
- Q. Yang, Z. Liua, X. Hou, X. He, M. Sjöberg, D. Vuilleumier, C. Liu and F. Liu, "Measurements of laminar flame speeds and flame instability analysis of E30-air premixed flames at elevated temperatures and pressures", FUEL 259 (2020) doi: 10.1016/j.fuel.2019.116223
- Z. Hu, J. Zhang, M. Sjöberg, and W. Zeng, "The Use of Partial Fuel Stratification to Enable Stable Ultra-lean Deflagration-based SI Engine Operation with Controlled End-gas Autoignition of Gasoline and E85", International Journal of Engine Research (2019), doi: 10.1177/1468087419889702
- F. Liu, Z. Liu, Z. Sang, X. He, M. Sjöberg, D. Vuilleumier, C. Liu, X. Li, "Numerical study and cellular instability analysis of E30-air mixtures at elevated temperatures and pressures", Fuel 271, (2020), doi: 10.1016/j.fuel.2020.117458
- J.P. Szybist, S. Busch, R.L. McCormick, J.A. Pihl, D.A. Splitter, M. Ratcliff, C.P. Kolodziej, J.E. Storey, M. Moses-Debusk, D. Vuilleumier, M. Sjöberg, C.S. Sluder, T. Rockstroh, and P. Miles, "What Fuel Properties Enable Higher Thermal Efficiency in Spark-Ignited Engines?", in revision for PECS.

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- C. Xu, P. Pal, X. Ren, S. Som, M. Sjöberg, N. Van Dam, Y. Wu, T. Lu, M. McNenly, "Numerical Investigation of Fuel Property Effects on Mixed-Mode Combustion in a Spark-Ignition Engine", Proceedings of the ASME 2019 Internal Combustion Engine Division Fall Technical Conference, ICEF2019-7265.
- C. Xu, M. Sjöberg, S. Som, "A computational fluid dynamic study of mixed-mode combustion assisted by partial fuel stratification in a lean-burn spark-ignition engine", abstract submitted to ASME ICEF 2020, manuscript in preparation.
- Z. Yue, C. Xu, S. Som, C.S. Sluder, K.D. Edwards, R. Whitesides, M.J. Mcnenly, "A transported Livengood-Wu integral model for knock prediction in CFD simulation", abstract submitted to ASME ICEF 2020, manuscript in preparation.

LLNL

- Two of the above with ANL as the lead author.
- Lapointe, S. L., Whitesides, R. A., McNenly, M. J., "Sparse, Iterative Simulation Methods for One-Dimensional Laminar Flames," *Combust Flame*, *204*, 23-32 (2019).
- Song, C., Kang, D., Fridlyand, A., Goldsborough, S. S., Saggese, C., Wagnon, S., McNenly, M. J., Mehl, M., Pitz, W. J., Vuilleumier, D., "Autoignition behavior of gasoline/ethanol blends at engine-relevant conditions," *Combust Flame*, *216*, 369-384 (2020).

Presentations

SNL

- M. Sjöberg, D. Vuilleumier, N. Kim, C. Johnson and E. Singh “Fuel Effects on Mixed-Mode Combustion in a DISI Engine”, AEC Program Review Meeting at USCAR, Aug 2019.
- M. Sjöberg, N. Kim, C. Johnson & D. Vuilleumier, “Coupling GT-Power and ALPHA for Fuel-Economy Predictions of Vehicles that Use Mixed-mode Engines”, Co-Optima Stakeholder Conference Call, Sept 24, 2019
- M. Sjöberg and N. Kim, “Applicability of PMI as a sooting propensity metric for a DISI multimode engine”, Co-Optima Stakeholder Conference Call, March 24, 2020.
- M. Sjöberg, N. Kim, D. Vuilleumier, C. Johnson and E. Singh “Multimode update: Where Octane Index Works”, Co-Optima Stakeholder Conference Call, April 28, 2020.

ANL

- C. Xu, S. Som and M. Sjöberg, “RANS and LES Based Modeling of Mixed-Mode Combustion in a DISI Engine”, AEC Program Review Meeting at USCAR, Aug 2019.
- C. Xu, S. Som and M. Sjöberg, “Computational Model Captures Multi-Mode Combustion Features of Direct-Injection Spark-Ignition Engines”, Co-Optima Stakeholder Conference Call, Aug 27, 2019.
- C. Xu, Z. Yue, and S. Som, “Potential efficiency improvements with Co-Optimization of Fuels and Engines”, CONVERGE User Conference at New Orleans, LA, Sep 2019
- C. Xu, Z. Yue, and S. Som, “Efficient knock and auto-ignition modeling in boosted SI and mixed-mode combustion engines”, AEC Program Review Meeting at SNL, Feb 2020.

Critical Assumptions and Issues

Emissions compliance

- While research in this presentation focuses on combustion fundamentals and engine efficiency, it is understood that emissions compliance is vital for advanced combustion engine concepts to be used in the real world.
- Emissions compliance is challenging for lean operation since lean-NO_x aftertreatment is still relatively costly.
- However, progress is being made in this aftertreatment area, both within and outside Co-Optima.
- Furthermore, minimizing NO_x and PM while achieving highest possible thermal efficiency is one of the research objectives.

Overarching Co-Optima assumptions / issues

- There are engine architectures and strategies that provide higher thermodynamic efficiencies than available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed/load range.
- Fuel Property Hypothesis: If we understand the critical fuel properties correctly, then fuels with those properties will provide comparable performance regardless of the chemical composition.
- The barriers associated with bringing a new fuel into the market on a mass scale can be overcome if the benefits to society and industry are sufficiently high (fuel economy, consumer cost, market incentives, GHG benefits, etc.).

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