SAND2019-5497PE

Co-Optimization of Fuels & Engines

Multimode (MM): Autoignition in MM / Advanced Compression Ignition (ACI) Combustion, Part 1

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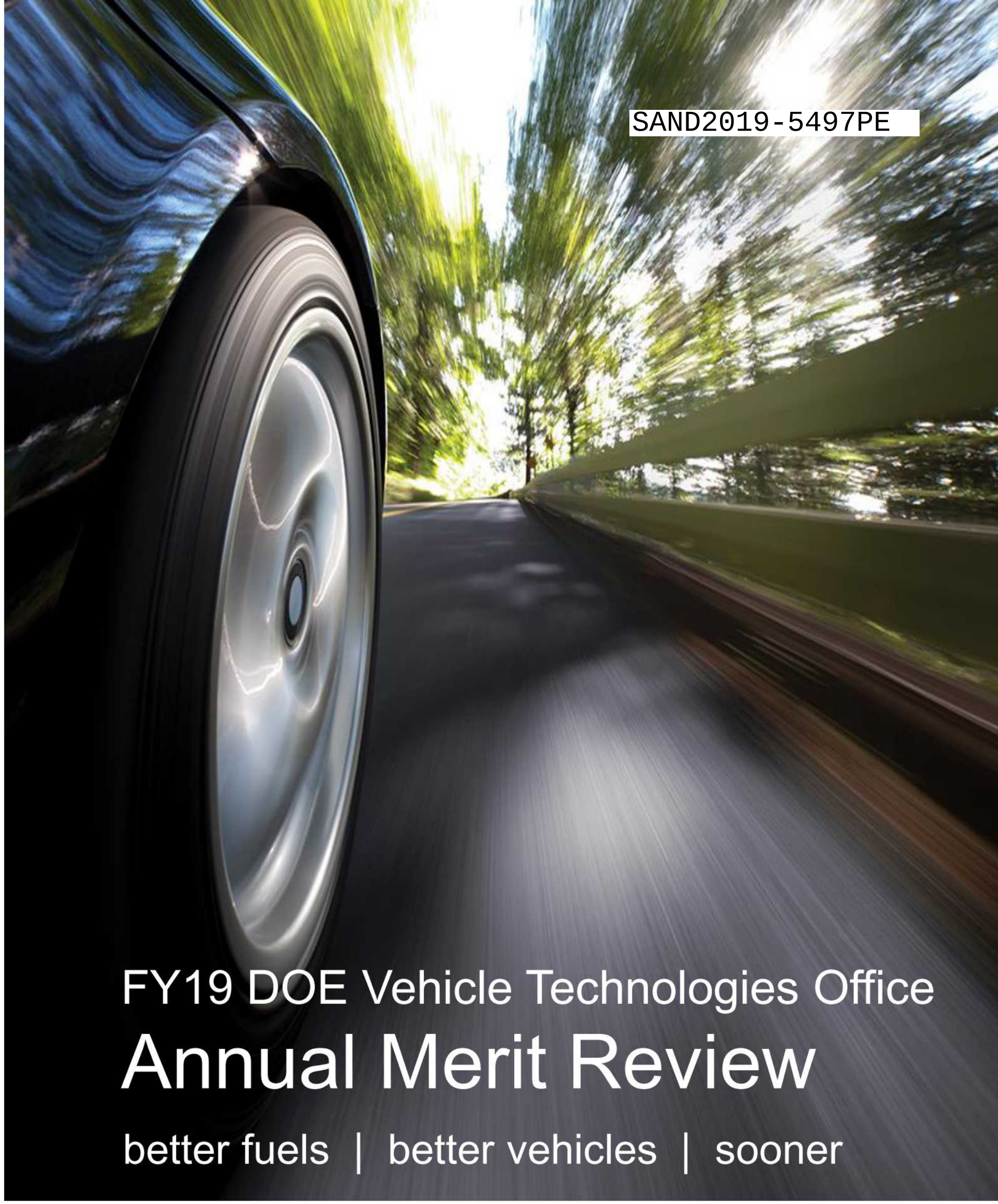
June 12, 2019

Project # FT070



U.S. DEPARTMENT OF ENERGY | Energy Efficiency &

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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

Budget

Task	FY18	FY19
E.1.1.3: SNL, Optical Diagnostics: Fuel Effects on Lean Well-mixed and Stratified	$475k	$320k
E.1.1.4: SNL, Metal DISI Engine: Fuel Effects on Lean Mixed-Mode Combustion	$155k	$320k
G.2.1: ANL, Sandia DISI Engine Simulations (Sensitivity Analysis)	$165k	$175k
G.5.7: LLNL, Multi-mode co-optimization via data consolidation and analysis	NA	$164k

* Start and end dates refer to three-year life cycle of DOE lab-call projects, corresponding to Phase 1 and Phase 2 of Co-Optima.

Barriers**

- Lack of robust lean-burn and EGR-diluted combustion technology and controls.
- Determine the factors limiting range of LTC /develop methods for extending the 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

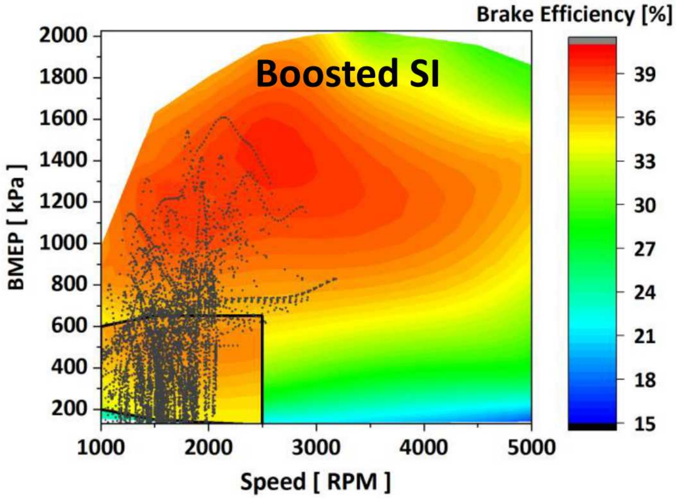
- General Motors – Hardware.
- Toyota – Funds-in knock project.
- LLNL (Pitz & McNenly) – Kinetics and solvers.
- Convergent Science Inc. – Software.
- *+ Many more – details in later slides*

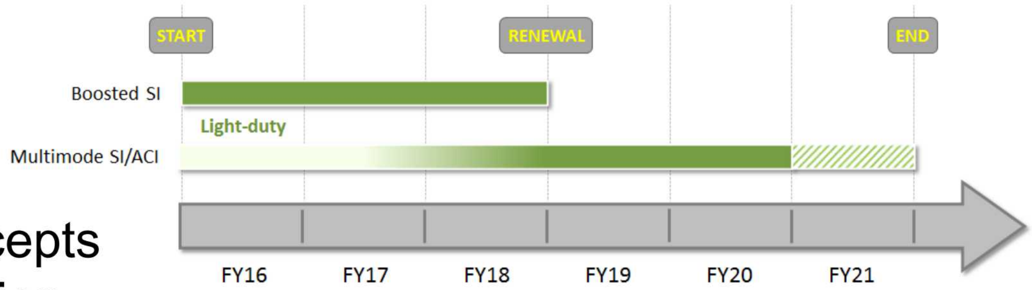
**2018 U.S. DRIVE ACEC Tech Team Roadmap

Relevance

- Broader Co-Optima effort; pre-competitive, early-stage research aims to develop better understanding how fuel properties affect 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 stratified-charge SI operation**
    Deflagration-based combustion.
    Focus on emissions mitigation.
  - **Lean mixed-mode combustion**
    Deflagration and autoignition.
    Octane-appetite assessment.
- Other advanced combustion concepts are integrated via data consolidation and analysis.

Figure Source | J. Szybist, ORNL





Resources

Task	FY18 Budget	FY19 Budget	PI, NL Researchers	Facilities	Equipment / Tools
E.1.1.3: SNL, Optical Diagnostics: Fuel Effects on Lean Well-mixed and Stratified	$475k	$320k	M. Sjöberg, D. Vuilleumier, N. Kim D. Reuss	Alternative Fuels DISI Engine Lab in Combustion Research Facility	Optical single-cylinder lean-burn spray-guided stratified-charge DISI engine. Exhaust emissions analyzers. Multiple optical diagnostics.
E.1.1.4: SNL, Metal DISI Engine: Fuel Effects on Lean Mixed-Mode Combustion	$155k	$320k	M. Sjöberg, D. Vuilleumier, N. Kim D. Reuss	Alternative Fuels DISI Engine Lab in Combustion Research Facility	Metal single-cylinder lean-burn spray-guided stratified-charge DISI engine. Exhaust emissions analyzers. GT-Power and CHEMKIN models.
G.2.1: ANL, Sandia DISI Engine Simulations (Sensitivity Analysis)	$165k	$175k	S. Som, C. Xu	Computational Multi-physics Section	Laboratory computing resource center for HPC. CONVERGE CFD tools. In-house codes.
G.5.7: LLNL, Multi-mode co-optimization via data consolidation and analysis	NA	$164k	D. Flowers	NA	In-house codes, gaussian process model tools, GT-power, zero-RK

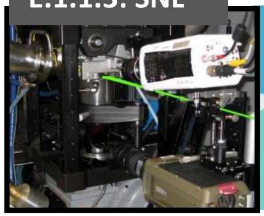
Milestones: Met or On Track

Month/Year	Description of Milestone	Status
March 2018, SNL E.1.1.3	Fuel sooting behavior- Compare sooting tendencies of three Tier 3 fuel blends for stratified-charge SI operation.	Met
Dec 2018, LLNL G.5.7	Define framework requirements & MVP for year 1 - stat model inputs, existing engine and simulation data, data exchange process, and downselect from provisional set of figures of merits.	Met
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.	Local SA performed, Global SA in progress
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.	Met

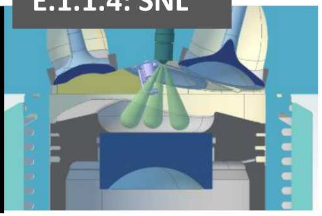
Overall Technical Approach:
4 tasks / 3 labs + many collaborations

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

E.1.1.3: SNL

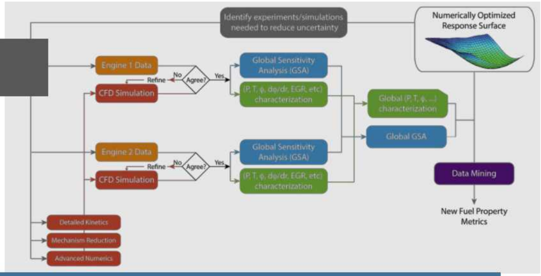


E.1.1.4: SNL



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

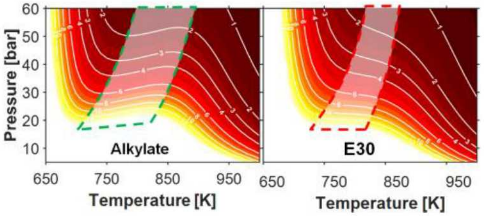
G.5.7: LLNL



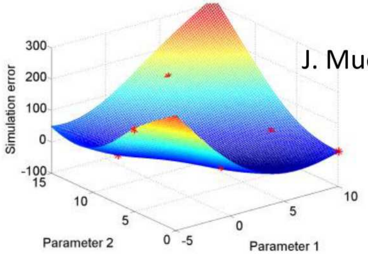
Consolidate and analyze data to identify multi-mode approaches with high co-optimization potential.

Multi-mode SI / ACI

Use Fundamental Knowledge Base

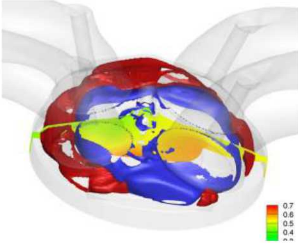


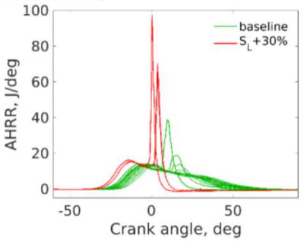
Collaborative Kinetics/ Toolkit tasks



J. Mueller, LBL

G.2.1: ANL





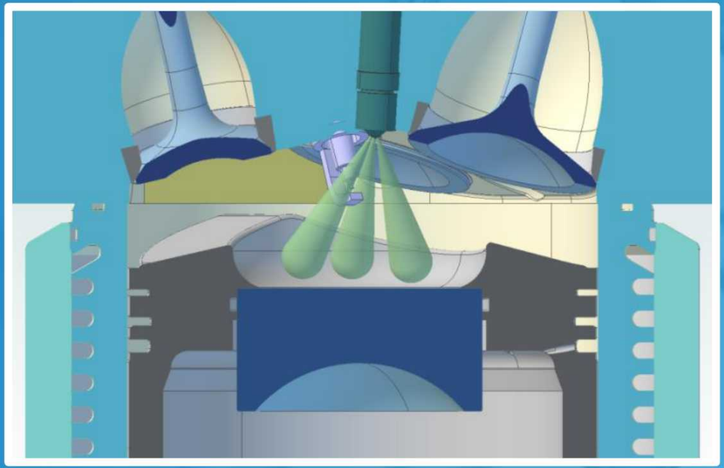
Enhance understanding and accelerate development through linked modeling efforts.

Approach – SNL DISI

- Combine metal- and optical-engine experiments and modeling 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).
- Second, apply optical diagnostics to:
  - Clarify shortcomings of PMI.
  - Probe spray development.
- Third, extend scope of fuel studies through the use of validated GT-Power and CHEMKIN models.

(SACI) = spark-assisted compression ignition

- 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 injection for well-mixed oper.



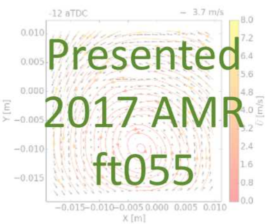
- Identical geometry for all-metal testing and optical diagnostics.
  - PIV - Flows, Mie or DBI - Liquid Spray, RIM - Wall Wetting, IR - Fuel Vapor, Plasma & flame imaging, DBI - soot mass.

RIM = refractive index matching
PIV = particle image velocimetry
IR = infrared
DBI = diffused back illumination

Approach / Workflow: ANL - CFD

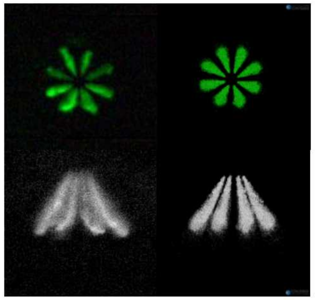
Turbulence model: RANS – higher throughput enabling sensitivity analysis
Spray: State-of-art Lagrangian models allowing for fuel-stratification studies
Turbulence-chemistry interaction: Hybrid model (G-equation + Well-stirred Reactor) – improving mixed-mode prediction

Motored Flow



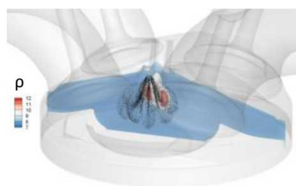
Presented 2017 AMR ft055

Spray Validation

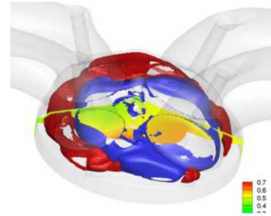


EXP CFD

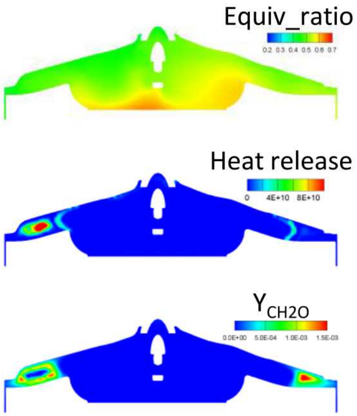
Motored with Fuel Injection



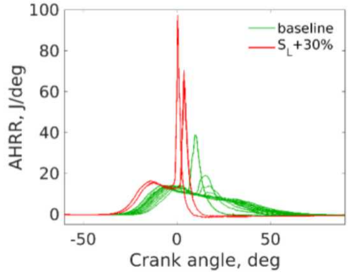
Combustion



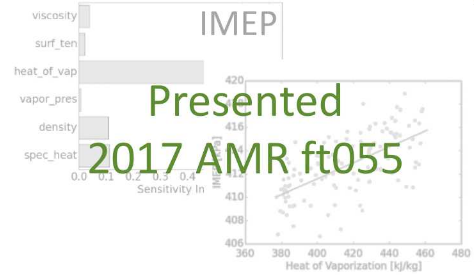
Probing underlying physics



Local sensitivity Analysis



Global Sensitivity Analysis



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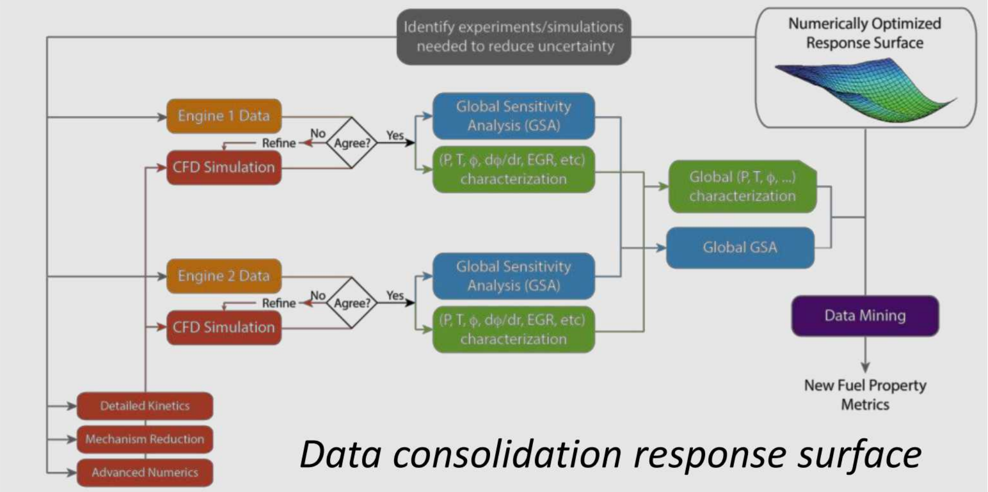
Approach: LLNL

Multi-mode co-optimization via data consolidation and analysis

- Simulation and experiments conducted at partner labs are investigating different ACI strategies for multi-mode engines.
- This task focuses on developing an analytical framework for comparing data across different experimental and simulation efforts.
  - Identifying existing data sets.
  - Evaluating options for collecting and consolidating data from different sources into a common framework.
  - Developing analytical methods for data evaluation.
  - Identifying modes with high co-optimization potential.



Data consolidation response surface

This task seeks to provide a rigorous comparative basis for selection of multi-mode fuel and engine characteristics that can provide most potential for fuel economy improvement.

Technical Accomplishments Summary

- **DISI @ SNL**
- Continued assessment of relevance of PMI for 9 fuels across 3 well-mixed and 2 stratified operating strategies.
- Identified that both ethanol and a diisobutylene blend can induce shortcomings of PMI for soot predictions.
- Developed and used DBI for in-cylinder soot diagnostics of select fuels.
- Used RIM and spray imaging to assess spray dynamics responsible for piston-top fuel-film formation, including cold-start conditions with E30.

- Developed and used an experimentally based methodology to determine the octane appetite of mixed-mode combustion using GT-Power and CHEMKIN.

- Led team efforts within Co-Optima and IEA's Low-Temperature Combustion task.

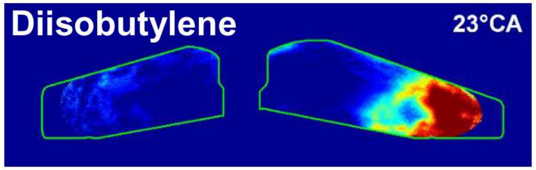
- Numerous technical publications.

- **CFD @ ANL**
- Validated CFD models for lean, mixed-mode engine operation with E30.
- Leveraged a hybrid combustion modeling approach to accurately predict both flame propagation and end-gas autoignition.
- Investigated sensitivities of mixed mode engine performance to laminar flame speed and HoV.
- Validated spray and vapor penetration for operation with partial fuel stratification.

- **Data Consolidation @ LLNL**
- Completed multi-mode data survey across Co-Optima tasks.
- Identified initial data-set for multi-mode statistical analysis.
- Completed initial analysis using statistical surrogate modeling approach.
- Multi-mode fuel and operating point search for 3, 4, 6, 8 & 9 comp. surrogates.

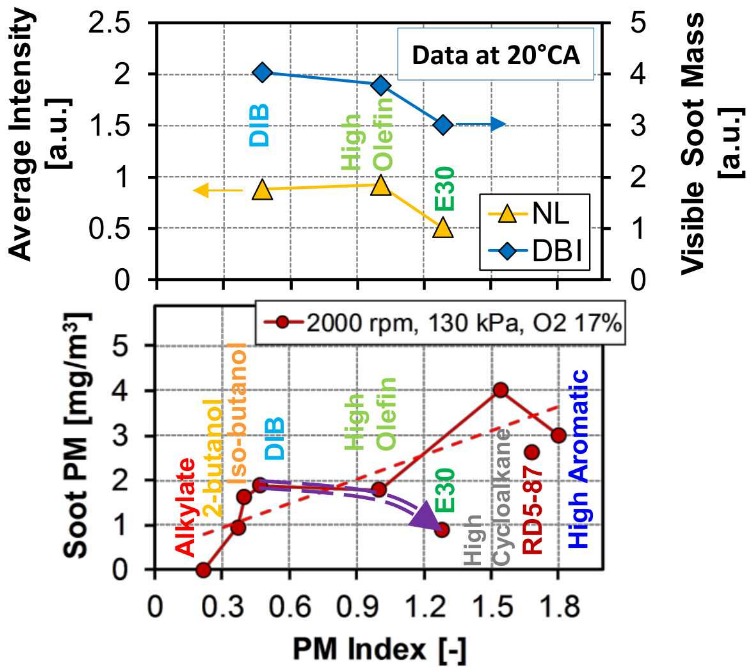
DBI-based In-Cylinder Diagnostics of Bulk-gas Soot

- For moderately boosted lean stratified-charge operation, E30 produces less, diisobutylene (DIB) blend more smoke than PMI predicts.
- Diffused back illumination (DBI) light extinction was developed and used to determine reasons for PMI discrepancies.

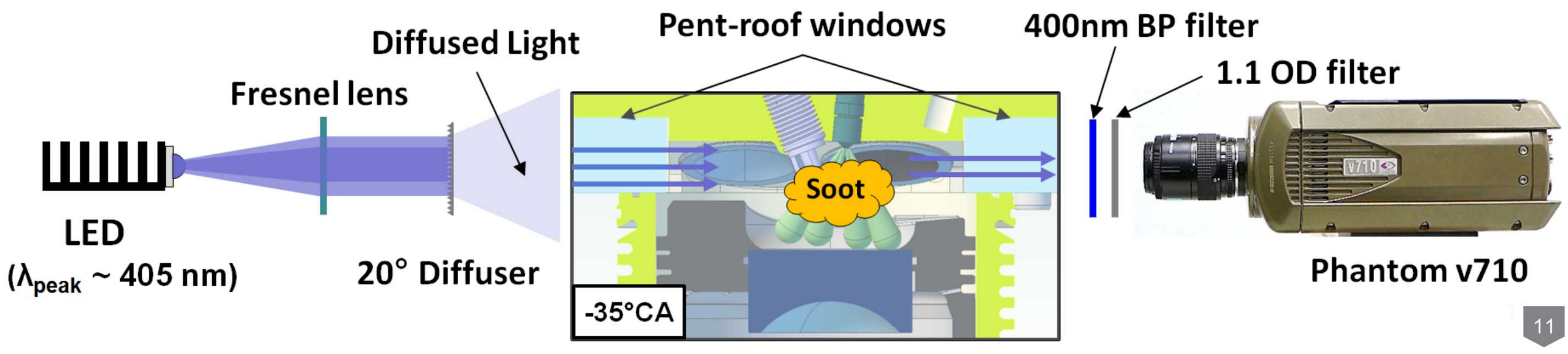


- Consistent with smoke levels, both in-cylinder flame luminosity and soot mass are lower for E30 and higher for DIB blend.

- Suggests that soot-formation differences are responsible for PMI discrepancies, not soot-oxidation differences.



DBI development guidance by S. Skeen.



Accomplishments (SNL)
Reasons for Shortcomings of PMI

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

DBE_i : *double bond equivalent*
$VP\ (443K)_i$: *Vapor pressure at 443K*
Wt_i : *Mass fraction*

Effect of Stoich. A/F Ratio on Local ϕ

- For lean stratified operation, air-fuel mixing is concurrent with combustion.
- Stoichiometric A/F ratio of E30 is relatively low. ($AFR_{stoich,\ Diisobutylene}$ = 14.7 vs. $AFR_{stoich,\ E30}$ = 12.8)
- Difference in AFR_{stoich} can influence local ϕ.
  - For example, assume that the same degree of mixing of air and fuel is achieved in a region.

m_{air} = 1 [mg], m_{fuel} = 0.15 [mg] → AFR_{local} = 6.7

$\phi_{local,\ HO,\ diisobutylene}$ = 2.21 vs. $\phi_{local,\ E30}$ = 1.92

Effect of Oxygen Content on Local ϕ_Ω

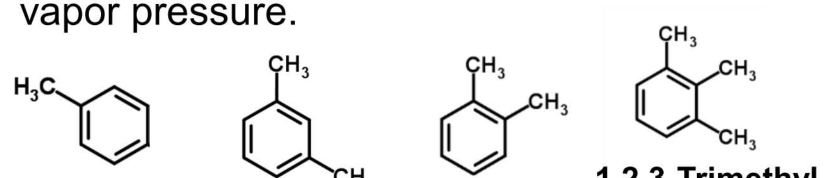
- Even for equal ϕ, the oxygen equivalence ratio (ϕ_Ω) indicates an effectively leaner E30 mixture*.

$\phi_{\Omega,\ local,\ HO,\ diisobutylene}$ = 2.21 vs. $\phi_{\Omega,\ local,\ E30}$ = 1.86

- Neither **lower AFR_{stoich}** of E30, nor **oxygen** in ethanol, is accounted for in PMI, and both can contribute to reduced soot formation.

Effect of Vapor Pressure on PMI

- For boosted stratified operation, wall wetting becomes insignificant.
- PMI of toluene is much smaller than other similar aromatic species due to its higher vapor pressure.



Toluene | **m-Xylene** | **o-Xylene** | **1,2,3-Trimethyl-benzene**

	C	H	DBE	VP [kPa]	PMI_m
Toluene	7	8	4	424.5	1.18
m-Xylene	8	10	4	217.3	2.30
o-Xylene	8	10	4	189.4	2.64
1,2,3-Trimethyl-benzene	9	12	4	85.5	5.85

- PMI may underestimate bulk-gas sooting propensity of toluene in diisobutylene blend for boosted stratified operation.

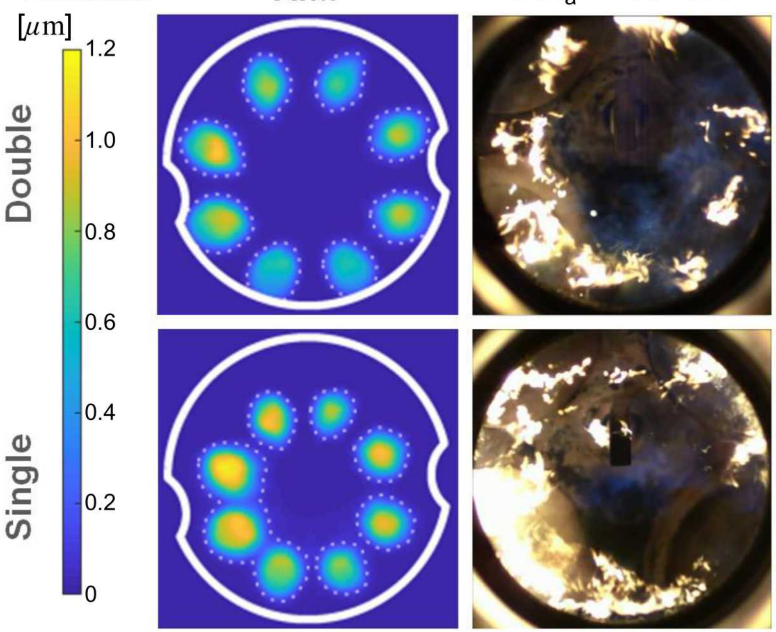
*see SAE 2005-01-3705.

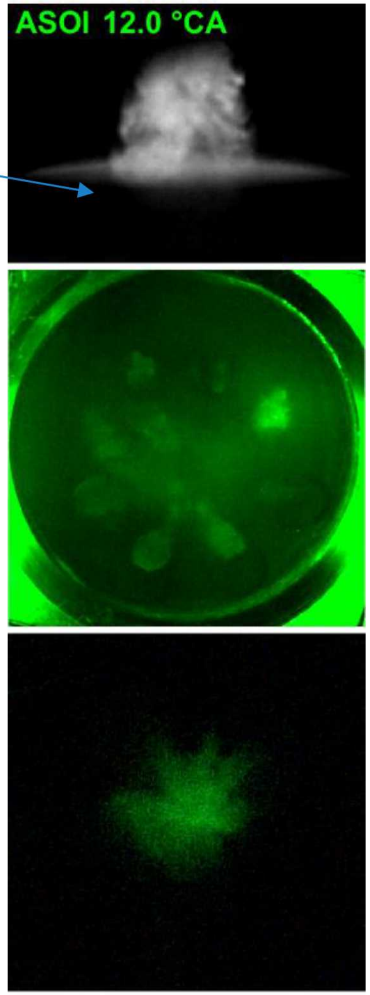
Accomplishments (SNL)

Use of Wall-Wetting and Spray Diagnostics

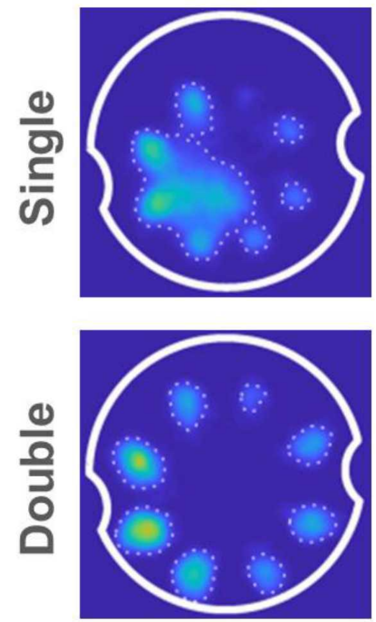
- Applied previously developed RIM diagnostics to wide ranges of operating conditions.
  - Focused on E30 fuel, which is particularly challenging due to elevated vaporization cooling.
- Including cold-start testing, as outlined by ACEC Tech Team (see back-up).
- Add spray, flame and soot-deposit imaging for holistic assessment.
  - Contrast single- and double-injection strategies.
  - Fuel effects.

P_{in} = 100 kPa
Inj. Dur = 1600 μs
SOI_a = -31 °CA





[SOI] = Early

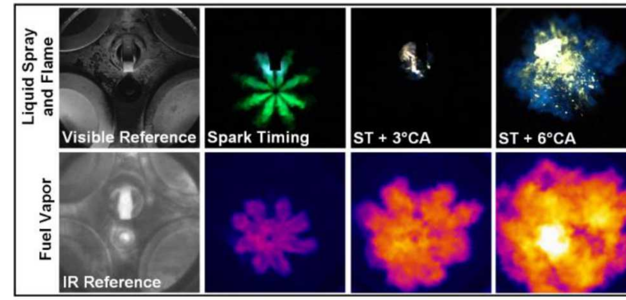


- Builds solid knowledge base for spray-wall interactions.

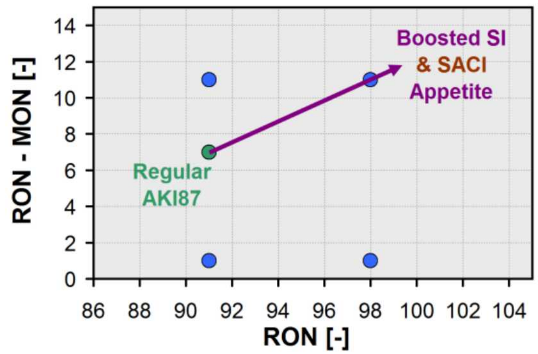
- Contrast conditions with and w/o spray collapse.
- Pickett *et al.* connection.

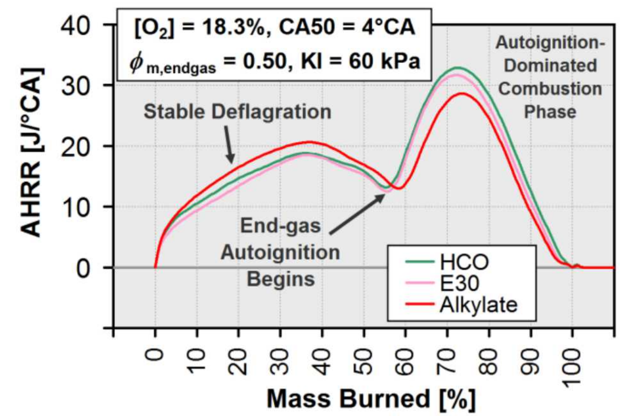
Accomplishments (SNL): Developed Methodology for Determining Octane Appetite of Mixed-mode Combustion

- Small pilot injection (PFS) used to stabilize ultra-lean mixed-mode combustion (SACI).



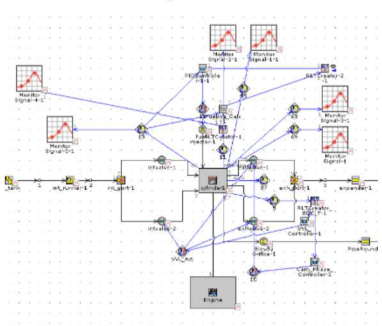
- What is the fuels appetite of SACI?
  - Fuel properties that support high efficiency, large load range, and robust implementation.
  - Compatible with RON & S appetite of boosted SI?



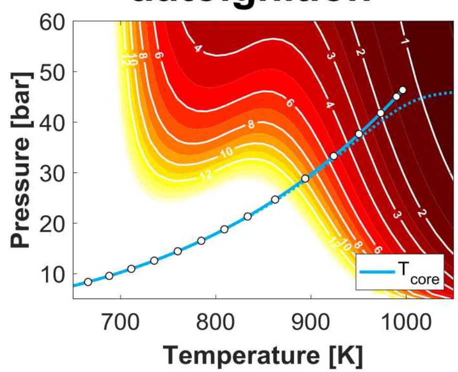


- Need lower-order modeling for first-order assessment:

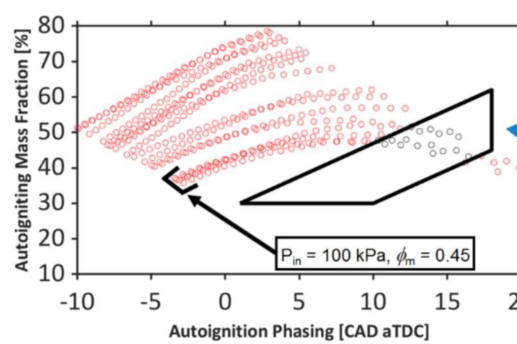
1. GT-Power for T-P trajectories.

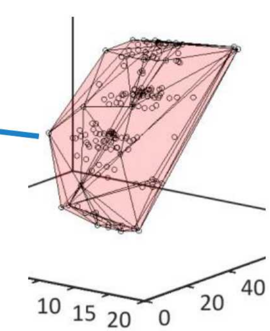


2. CHEMKIN for autoignition



3. Screen for feasibility

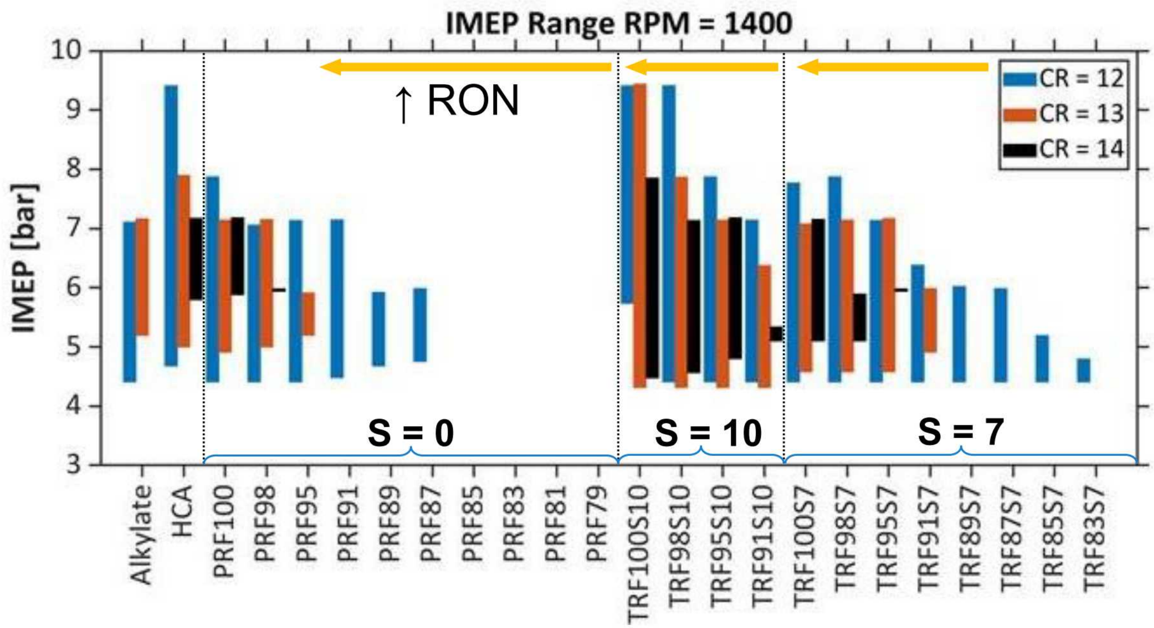




Accomplishments (SNL): Fuels Appetite of Mixed-Mode Combustion Found to Be Compatible with Boosted SI

- Span relevant ranges for ACI implementation in a mixed-mode SI engine.
  - Engine speed; 1000, 1400, 2000 rpm.
  - CR; 12, 13, 14
  - P_{in}; 100, 130 kPa.
  - IVC T; 85 – 130 °C, via trapped residuals.
  - ϕ_m; 0.45, 0.55

$$\phi_m \equiv \frac{\left(F/C\right)_{Actual}}{\left(F/A\right)_{Stoichiometric}}$$

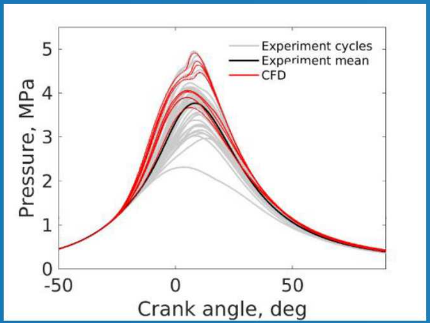


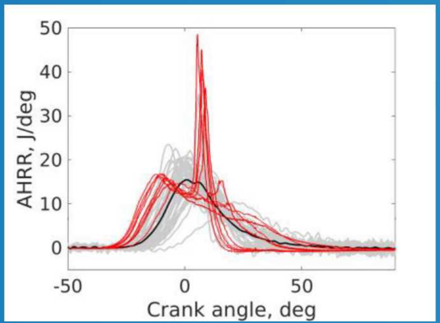
- A certain autoignition resistance is required to achieve reasonable load.
- For a given RON, higher-S fuels are more tolerable to high-CR implementation.
- Based on this first-order modeling, the octane appetite of mixed-mode combustion is strikingly similar to that of stoichiometric boosted SI.
- Additional experimental validation underway for select fuel combinations.
- Optimal fuel search being performed in collaboration with LLNL.

ANL Accomplishments: Predicting and Probing Mixed-Mode Combustion

CFD simulations are able to match experimental measurements

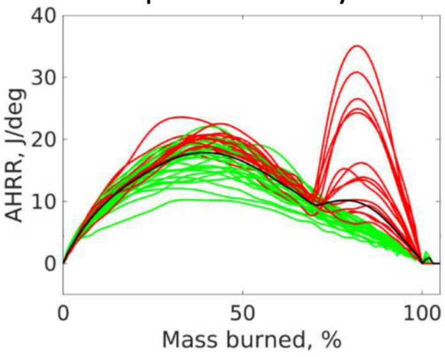
- The previous CFD model was validated only for stoichiometric engine operations.
- Significant improvements were made to accommodate the lean, mixed-mode operating condition featuring large cycle-to-cycle variability (CCV).
- A hybrid combustion model was leveraged to predict both flame propagation and end-gas auto-ignition.
    - Tabulated flame speed for flame tracking.
    - Online chemistry for auto-ignition.
- **This demonstrated the fidelity and capabilities of CFD tools.**



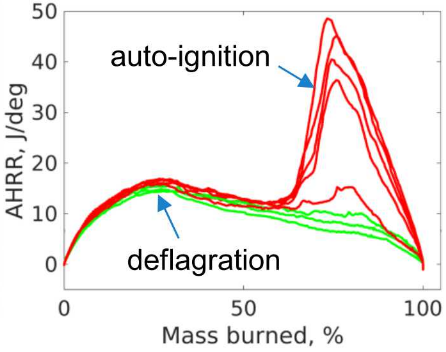


Distinctive features between purely deflagrative and mixed-mode cycles are captured and visualized.

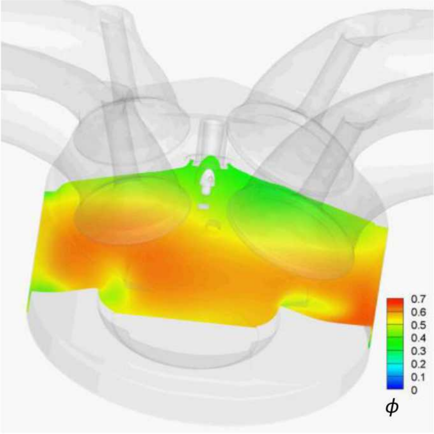
Experimental cycles



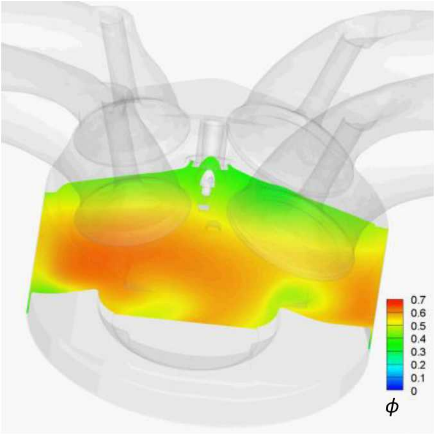
Simulation cycles



Deflagration cycle



Mixed-mode cycle

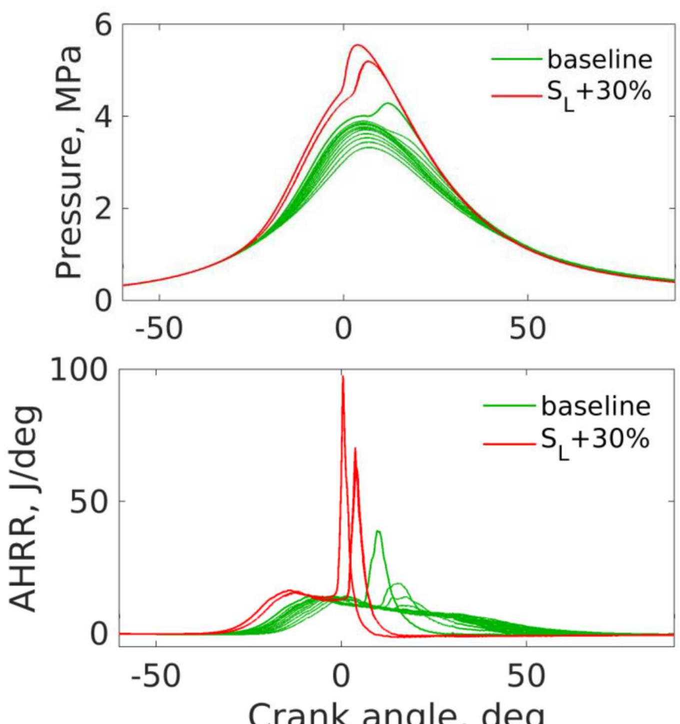


Blue: deflagrative fronts Red: auto-ignition fronts

ANL Accomplishments:
Enabling Sensitivity Analysis of Fuel Properties

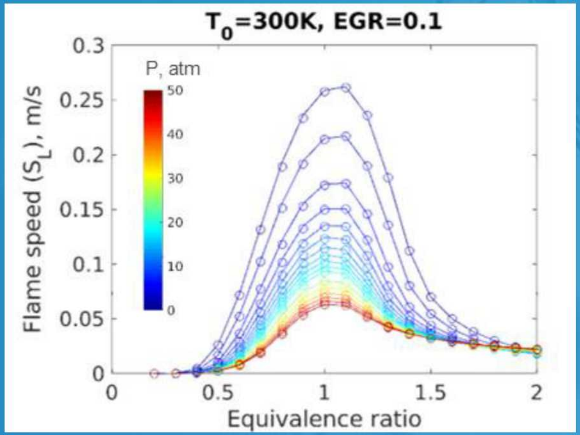
Advanced modeling enables sensitivity analysis for searching optimal fuels

- Local sensitivity to laminar flame speed was explored using the validated CFD model.
- Increasing S_L was found to enhance both deflagrative flame propagation and end-gas autoignition.
- **This approach can be readily extended to global sensitivity analysis and other fuel properties.**



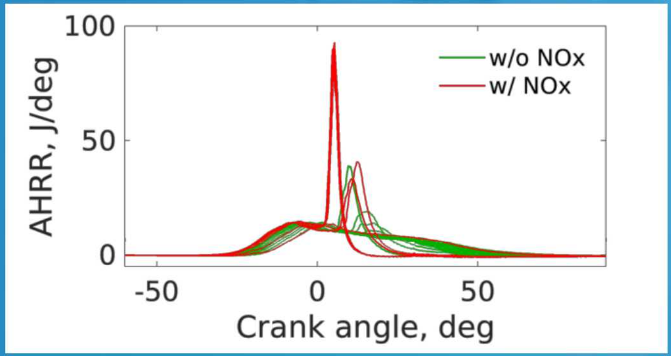
Investigated effects of NO_x chemistry on mixed-mode combustion simulations

- NO_x chemistry has negligible effect on the laminar flame speed calculations, while significantly enhances end-gas auto-ignition prediction.
- **NO_x chemistry is demonstrated to be an essential element for MM simulations.**



1D laminar flame speed calculations

Lines: w/o NOx
Symbols: w/ NOx



3D mixed-mode calculations

Validations of Spray and Vapor Penetrations

<u>Performed detailed validation of spray and vapor penetration for engine operation with partial fuel stratification (PFS)</u>

- Spray models validated against high-speed liquid spray and infrared fuel-vapor imaging by Sjöberg *et al.*
- Spray settings for previous experience with GDI simulations is employed and it matches experimental data well; in particular, non-axisymmetric features are captured (see from bottom view)
- **Results provide confidence for planned studies of PFS-assisted mixed-mode comb.**

Liquid penetration

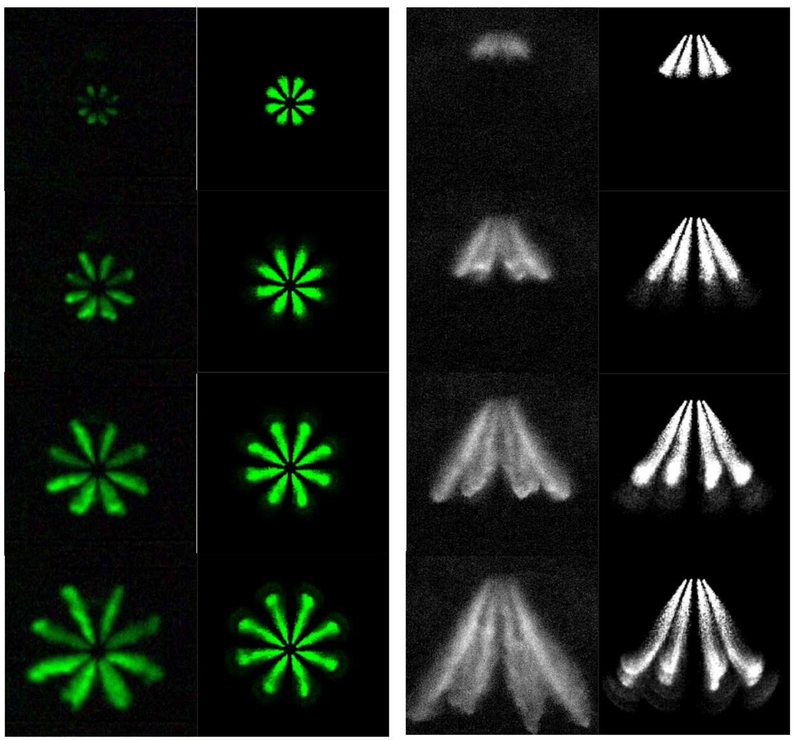
EXP CFD EXP CFD

SOI+ 0.2 CAD

0.4 CAD

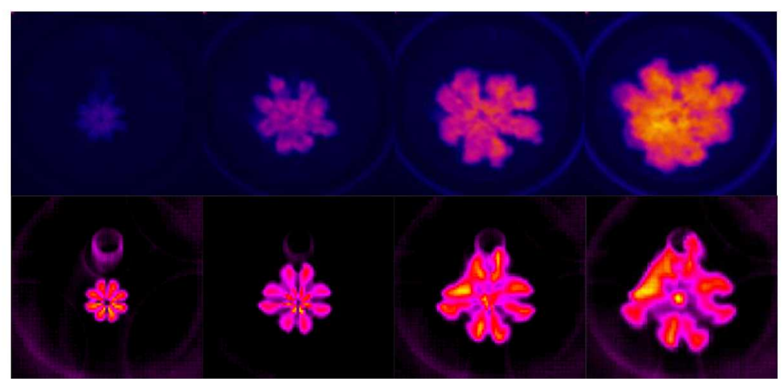
0.6 CAD

0.8 CAD



bottom view side view

Vapor penetration



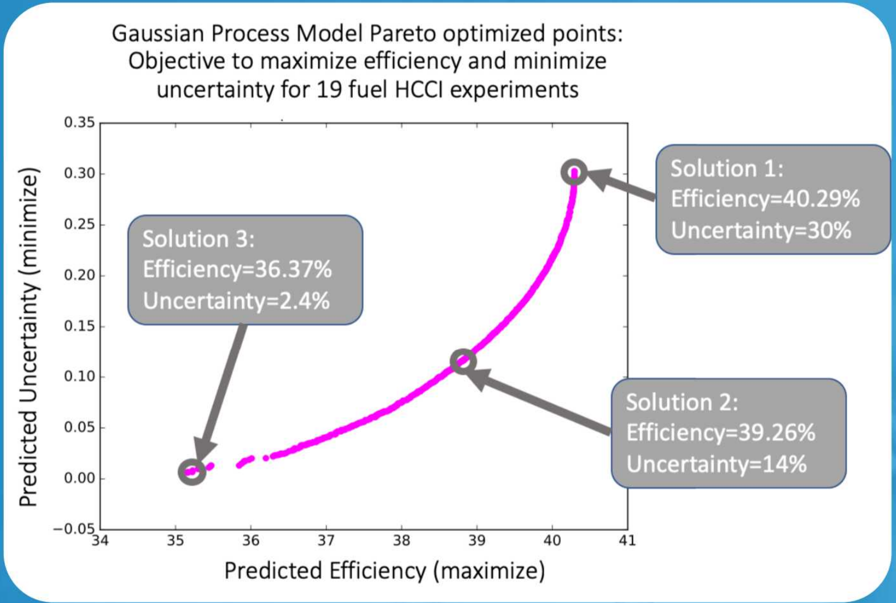
EXP

CFD

SOI+0.5 CAD SOI+1.5 CAD SOI+2.5 CAD SOI+3.5 CAD

LLNL Accomplishments: ACI fuel parameter selection with Gaussian Process Model

- Developed response surface approach using ACI data.
- 19 fuels evaluated for single HCCI condition (2000 RPM, 2 bar BMEP) and boosted SI condition.
- Up to 19 fuel/engine analysis parameters considered (RON, S, Aromatics, Saturates, Olefins, Oxygenates, T90, LHV, …)
- Gaussian process model developed to predict efficiency based on fuel characteristics.
- Bi-objective optimization for maximizing efficiency, minimizing uncertainty.
- Collaboration with J. Mueller (LBNL) and J. Szybist (ORNL).



Tradeoff between uncertainty and efficiency for optimized points.

Framework can identify general data needs (*e.g.* number and types of inputs, number of unique operating points) to find maximum efficiency with acceptable uncertainty.

LLNL Accomplishments:
Fuel Search for Mixed-mode Combustion

- Wide range of engine parameters:
  - Spark timing, engine speed, intake pressure, compression ratio, BDC temperature, equivalence ratio.
  - 864 combinations for a single fuel, cannot be explored through experiments or CFD alone.

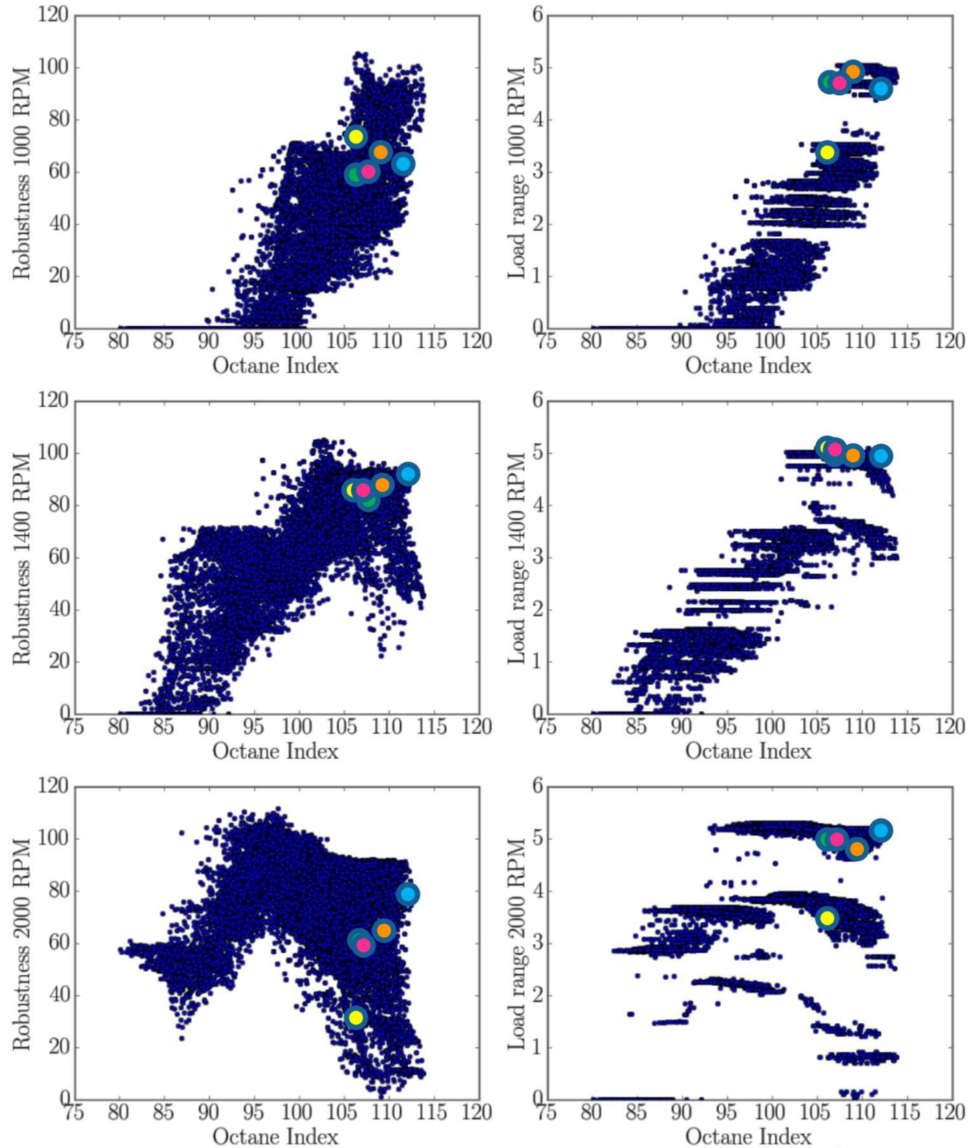
- Modeling approach from Vuilleumier and Sjöberg [AEC, Jan 2019]:
  - GT-power engine model calculates the pressure time history for each engine condition.
  - Pressure history serves as input to 0D variable pressure reactor.
  - 0D model computes the autoignition phasing.
  - Screen feasible conditions using experimentally-informed operating ranges (avoid knock, slow burn, etc.) and compute load range (max IMEP-min IMEP).

- LLNL Fuel search:
  - Find fuels which maximize the number of operating points (robustness) and the load range.
  - Parallel Zero-RK reactor model allows to test tens of thousands of fuels/day using detailed Co-Optima gasoline surrogate mechanism.
  - Employ different optimization strategies: gradient-based methods, genetic algorithms, etc.

Fuel Search for Mixed-mode Combustion

- **Preliminary fuel search results:**
- Simulated 50,000 fuels from three-component TRF to nine-component surrogates.
- High RON and high sensitivity fuels tend to perform well, but there is large scatter at fixed RON/MON.
- Plots show robustness and load range at different RPMs vs. octane index (OI = RON - K•S, with K = -1).
- Found high load range fuels for the different fuel compositions:

# components	Highest load range
3	12.18
4	14.61
6	14.65
8	14.86
9	14.88



Responses to Previous Year Reviewers' Comments
Note: one new task not reviewed last year

Overall approach:

A reviewer noted "The reviewer indicated that the team is performing well in this project with a healthy blend of experimental work and numerical computations. This is a well-designed project." **Another reviewer echoed this sentiment:** "The reviewer stated that employing measurements in metal and optical engines and using CFD modeling are good approaches to enhancing synergistic work performance and effectively addressing the technical barriers of the research scope."

Accomplishments:

A reviewer noted "The reviewer praised this project as having made good progress over the past year and summarized some of the notable accomplishments of the project, including engine-out soot measurements as a function of particulate matter index (PMI) for nine different fuels. The work that is focused on variations in spray characteristics that influence particulate emissions but are not accounted for by PMI is valuable and should be pursued further." Also "The reviewer thought that the quantitative wall-wetting diagnostic technique is a powerful tool for studying soot production." Response: Encouraged by this, the suite of optical diagnostics has been expanded to include diffused-back illumination (DBI) light extinction for in-cylinder soot quantification. We have also utilized the RIM techniques further to understand the effects of fuels, injection strategies, and spray dynamics / collapse on wall wetting and the associated PM challenges.

Collaboration and Coordination:

A reviewer noted "The reviewer found excellent collaboration among participating national laboratories as well as industry partners. The reviewer said that it is worth noting that coordinating the activities across multiple teams/researchers requires a lot organization and the effort is worth applauding."

Proposed Future Research:

A reviewer noted "The project has made good progress thus far and the reviewer encouraged continuation of several of the ongoing efforts. For the Sandia National Laboratories (SNL) mixed-mode/SI work, the reviewer said that, in addition to lower RON fuels, the impact of low MON should also be investigated to determine the effect on load range." Response: We have added new fuel blends to the test matrix for mixed-mode combustion (SACI), including low-RON fuels with varying octane sensitivity.

A reviewer noted "While the scope of work is limited to low technology readiness levels (TRLs), the reviewer asserted that the project should keep practical considerations such as aftertreatment requirements and transient controls in mind while analyzing results and assessing the feasibility of the combustion concepts being proposed." Response: Cold-start conditions have been incorporated into the experimental matrix, and future work will include transient PM/PN measurements.

Collaborations

Leveraging Co-Optima Collaborations:

- **Strong industry engagement including industry-led external advisory board, monthly stakeholder phone calls, and annual stakeholder meeting.**
- **Collaboration across nine national laboratories, two DOE offices, and thirteen universities.**

15 Industry partners in the AEC MOU

- **Meet two times a year to share information with industry partners.**
- **Other national labs and University partners as well.**

Task Specific Collaborations [Strong links between task PIs]

SNL - DISI
E.1.1.3, E.1.1.4

- General Motors.
  - Hardware support.
- Direct with ANL on CFD.
- Funds-in knock project with Toyota.
  - Explores combined effects of EGR, fuel type and CR on knock.
- Pitz & Wagnon at LLNL
  - Surrogate-gasoline mechanisms.
- McNenly & Lapointe at LLNL
  - Optimal fuel search for SACI.
- 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.* for spray insights.
- Skeen *et al.* for DBI setup.

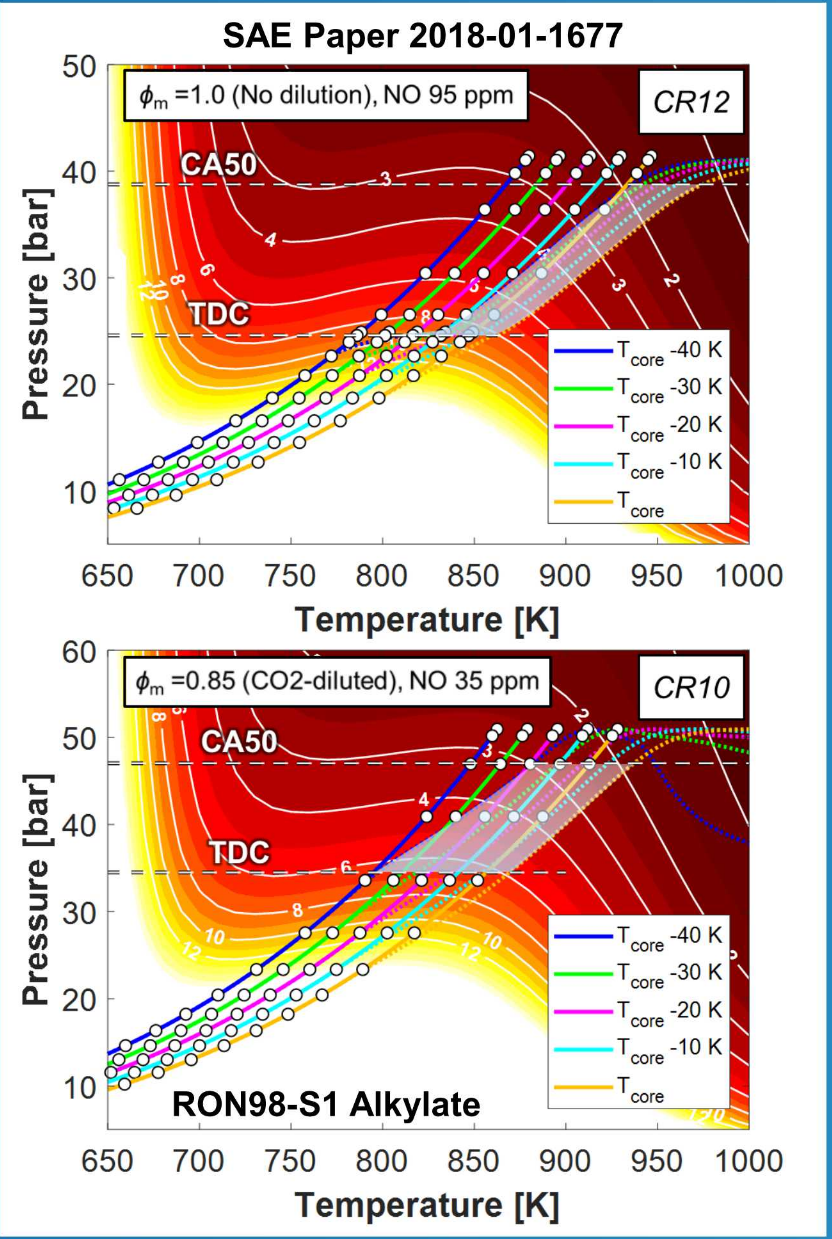
ANL - CFD
G.2.1

- Direct collaborations with SNL on DISI activities.
- Convergent Science Inc. for software.
- UConn (Prof. Tianfeng Lu) for chemical mechanism.
- Fuel properties for E30 SNL.
- Surrogate model for E30 (McNenly LLNL, Pal ANL).
- ORNL engine (Sluder, Yue).

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.

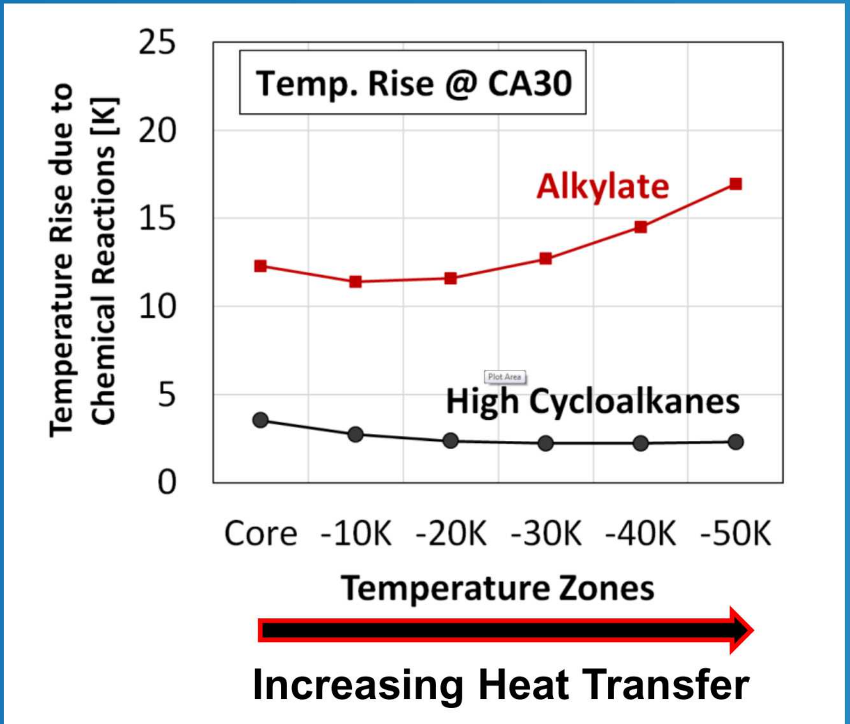
Collaborations (SNL)



- Funds-in knock project with Toyota.
  - Open literature dissemination.
- Explores effect of deviations from non-dilute stoichiometric operation.
- Knock limit and knock intensity are not solely explained by autoignition timing of core zone.
- Low- and intermediate-temperature heat release interacts with thermal stratification.
  - Influences rate of sequential autoignition and acoustic-knock generation.
- Effect is dependent on fuel type, dilution type, and CR.
- Insights complement Co-Optima studies of ultra-lean mixed-mode combustion.
  - Guide the implementation of multi-zone CHEMKIN models for optimal fuel search.

Remaining Challenges and Barriers

- **DISI @ SNL**
- Single-zone CHEMKIN model does not account for fuels' differing ability to utilize thermal stratification to smooth HRR for mixed-mode combustion.
- ⇒ *Use systematic assessment of knock generation across load and speed map + CFD modeling insights to generate a higher-order multizone model.*



- **CFD @ ANL**
- Mixed-mode CFD simulations are sensitive to boundary conditions, *e.g.*, cylinder wall temperature, for which detailed measurement from experiments are not available yet. ⇒ *Use conjugated heat transfer to alleviate the model dependence on the wall temperature.*
- High quality experimental data are needed to perform comprehensive model validation. ⇒ *Direct collaboration with SNL.*

- **Data Consolidation @ LLNL**
- No agreed upon set of conditions for comparison of multi-mode simulation and experimental efforts ⇒ *Getting input from multi-mode stakeholders.*
- Data population is limited for some strategies, due to throughput limitations for experiments and CFD simulations ⇒ *Light-weight 0D/1D modeling approach can augment experiments and CFD.*

Proposed Future Research*

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

SNL Mixed-mode combustion:

- Validate modeling results for key fuels.
- Assess fuel effects on drive-cycle fuel economy.
- Test optimized fuel from LLNL fuel search.
- Refine CHEMKIN modeling strategy to account for thermal- and fuel-stratification.
  - Based on knock assessment, CFD guidance, and optical diagnostics of end-gas conditions.

SNL Stratified-charge SI operation:

- Focus on soot emissions and combustion stability for high-EGR, low-NO_x operation.
- Examine optically fuel/load combinations that have PM or stability issues.
- Expand efforts on load transients, and pursue studies on cold-start effects.
  - Guidelines from ACEC Tech Team.
  - Monitor exhaust enthalpy and thermally affected PM / PN transients.
- Identify fuel properties that support robust implementation and clean exhaust.

ANL CFD

- Develop and validate a CFD approach for lean mixed-mode combustion with partial fuel stratification, by exploring both RANS and LES-type approaches.
- Investigate roles of both thermal- and mixture-stratification on mixed-mode performance, and provide physical insights for reduced-order modeling.
- Parametric sweeps and/or GSA to identify influential fuel properties for multi-mode ACI operation using RANS-type turbulence modeling. Identify beneficial fuel properties based on insights from GSA.

LLNL Data Consolidation

- Establish and use common comparative conditions for multi-mode operation across Co-Optima efforts.
- Build framework to allow for high confidence estimation of multi-mode improvement to fuel economy on drive-cycle and real-world basis.
- Develop low-dimension engine model (*e.g.* GT-power) that can be used to trial statistical analysis and response surface approaches.

Summary

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

- Developed and used DBI for in-cylinder soot diagnostics of select fuels. Identified that both ethanol and an diisobutylene blend with toluene and can induce shortcomings of PMI.
- Used RIM and spray imaging to assess spray dynamics responsible for piston-top fuel-film formation, including cold-start conditions with E30.
- Developed an experimentally based methodology to determine the octane appetite of mixed-mode combustion (SACI) using first-order modeling with GT-Power and CHEMKIN.
- Used Zero-RK reactor model to perform an initial search over 50,000 fuels.
- Validated the CFD model for mixed-mode engine operation.
- Demonstrated the capability of performing sensitivity analysis using CFD.
- Validated spray models allowing for simulations of partial fuel stratification.

Collaboration and Coordination

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

Proposed Future Research*

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

- Expand test matrix to include fuel effects on PM/PN dynamics of cold starting and load transients. Test new "optimal" fuels and assess FE benefits over drive cycles.
- CFD for accelerating development.
- Establish and use common comparative conditions for multi-mode operation across Co-Optima efforts.

Acknowledgements

- The experimental work supporting tasks E.1.1.3, E.1.1.4 and G.2.1 was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
- The CFD + ANL multi-mode work was done by UChicago Argonne, LLC, Operator of Argonne National Laboratory (Argonne). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DEAC02-06CH11357.
- The data consolidation work in task G.5.7 was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Technical Back-Up Slides

(Include this “divider” slide if you are including back-up technical slides **[maximum of five]**. These back-up technical slides will be available for your presentation and will be included in the USB drive and Web PDF files released to the public.)

SNL - Fuel Properties Tables

- 24 different fuels were simulated in CHEMKIN for assessing the octane appetite of mixed-mode combustion.

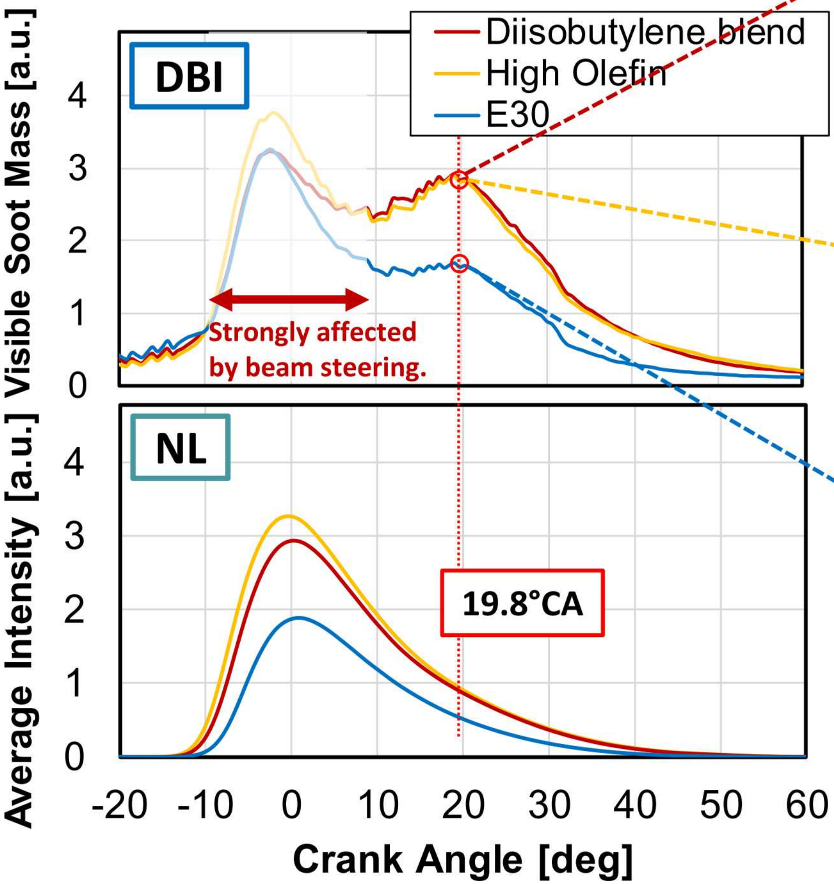
#	Name	RON	S
1	Alkylate	98	1
2	HCA	98	10
3	PRF100	100	0
4	PRF98	98	0
5	PRF95	95	0
6	PRF91	91	0
7	PRF89	89	0
8	PRF87	87	0
9	PRF85	85	0
10	PRF83	83	0
11	PRF81	81	0
12	PRF79	79	0
13	TRF100S10	100	10
14	TRF98S10	98	10
15	TRF95S10	95	10
16	TRF91S10	91	10
17	TRF100S7	100	7
18	TRF98S7	98	7
19	TRF95S7	95	7
20	TRF91S7	91	7
21	TRF89S7	89	7
22	TRF87S7	87	7
23	TRF85S7	85	7
24	TRF83S7	83	7

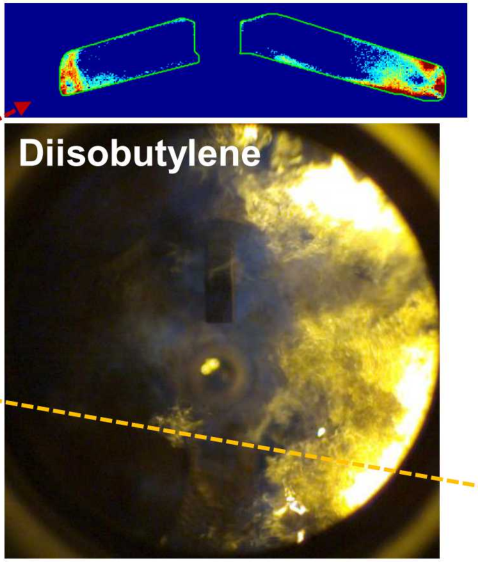
- One E10 regular gasoline, and eight RON98 fuels were used in stratified-charge studies in DISI engine at Sandia.

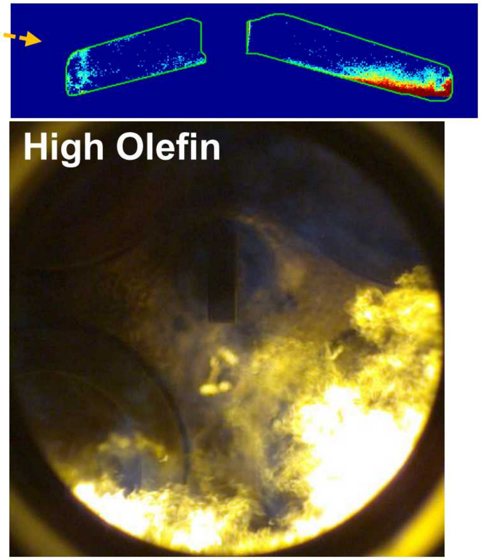
		Co-Optima Core Fuels							
	E10 RD5-87	**Alkylate**	**E30**	**High Aromatic**	**High Olefin**	**High Cycloalkane**	**Isobutanol Blend**	**2-Butanol Blend**	**Diisobutyl-ene Blend**
RON	90.6	98.0	97.9	98.1	98.3	97.8	98.1	98.2	98.3
MON	83.9	96.7	87.1	87.6	87.9	86.9	88.0	89.1	88.5
Octane Sensitivity	6.7	1.3	10.8	10.5	10.4	11.0	10.1	9.1	9.8
Oxygenates [vol.%]	10.6	0.0	30.6	0.0	0.0	0.0	24.1	28.4	0.0
Aromatics [vol.%]	22.8	0.7	13.8	39.8	13.4	33.2	19.0	17.9	20.1
Alkanes [vol.%]	48.7	98.1	40.5	46.2	56.4	40.6	53.1	50.1	56.3
Cycloalkanes [vol.%]	12.1	0.0	7.0	8.0	2.9	24.2	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
T10 [°C]	57	93	61	59	77	56	63	63	63
T50 [°C]	98	100	74	108	104	87	-	-	-
T90 [°C]	156	106	155	158	136	143	111	111	111
Net Heat of Combustion [MJ/kg]	41.9	44.5	38.2	43.0	44.1	43.2	40.6	40.1	43.2
Heat of Vaporization [kJ/kg]	412	308	532	361	333	373	412	415	337
AFR Stochiometric	14.1	15.1	12.9	14.5	14.8	14.5	13.8	13.6	14.7
HoV [kJ/kg stoichiometric charge]	27.3	19.1	38.4	23.3	21.1	24.0	27.9	28.5	21.5
Particulate Matter Index	1.68	0.22	1.28	1.80	1.00	1.54	0.40	0.37	0.47

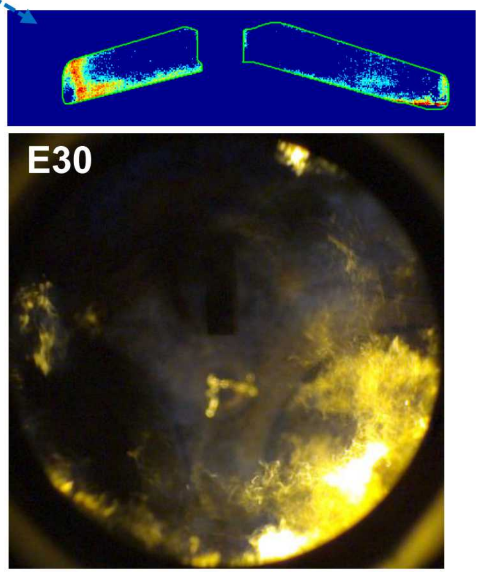
DBI-based In-Cylinder Diagnostics of Bulk-gas Soot

Still images from representative cycle







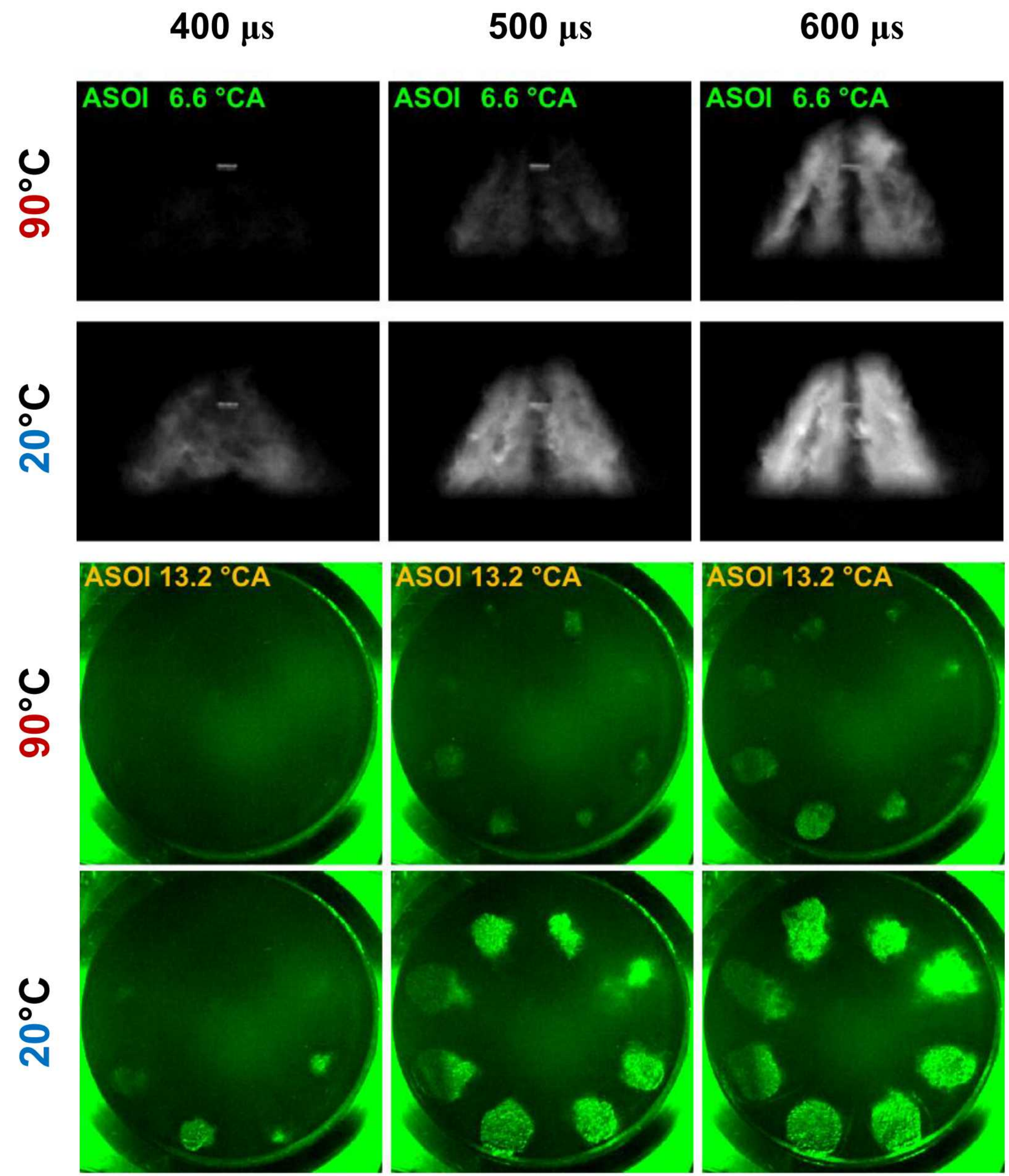


Accomplishments (SNL): Effect of Coolant Temperature on Wall Wetting

P_{in} ≈ 100 kPa, SOIa ≈ -41°CA

- When $T_{coolant}$ is reduced from 90 to 20°C:
  - Ligaments from spray persist longer.
  - Fuel-film area increases dramatically.
- Here, temperature of fuel varies with $T_{coolant}$ (just like in a real engine).
- To maintain similar intake pressure, flow rate was adjusted for each $T_{coolant}$.
  - 4.60 g/s (90 °C) vs. 5.05 g/s (20 °C)

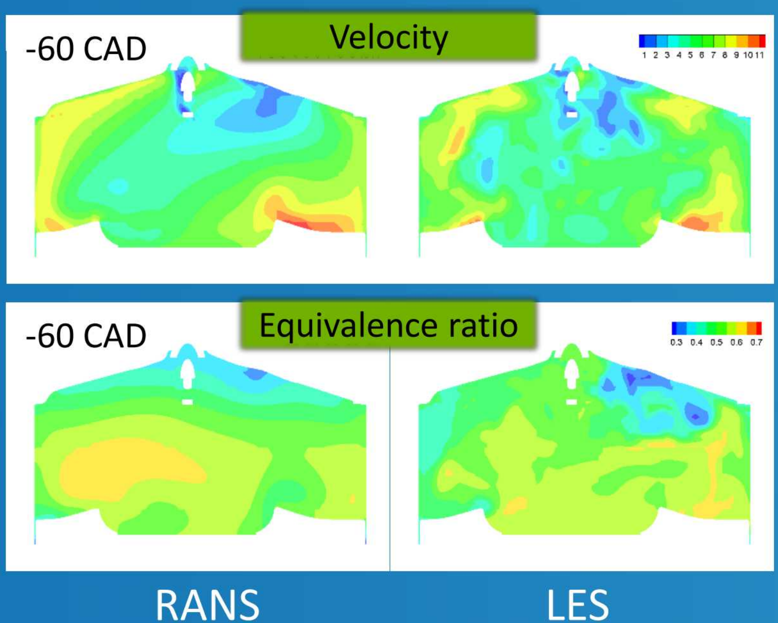
- Injection strategy has to be tailored to the thermal state of the engine.

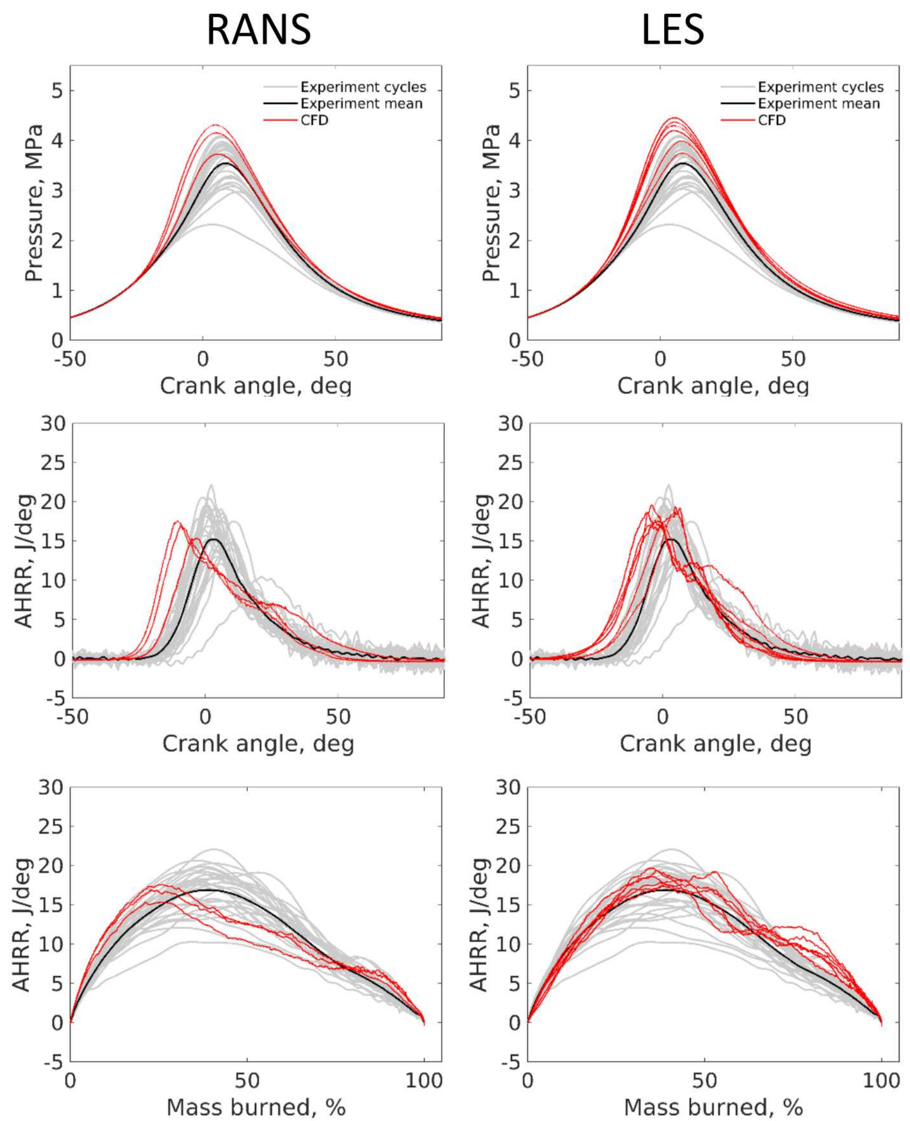


Leveraging High-Fidelity Large Eddy Simulations

<u>High-fidelity large eddy simulations (LES) are performed to improve model prediction and to gain in-depth understanding of physics</u>

- LES resolves finer flow structure and mixture distribution
- LES is able to capture the flame propagation better than RANS at the expense of more computational resources
- **This provides additional insights to the effects of mixture stratification on combustion processes**





Reviewer-Only Slides

(Include this "divider" slide between those to be presented and the "Reviewer-Only" slides. These slides will be removed from the presentation file and the USB drive and Web PDF files.)

Publications

SNL:

- C. K. Westbrook, M. Sjöberg, and N.P. Cernansky, "A New Chemical Kinetic Method of Determining RON and MON Values for Single Component and Multicomponent Mixtures of Engine Fuels", Combustion and Flame, Vol. 195, pp. 50-62 (2018), doi: 10.1016/j.combustflame.2018.03.038
- X. He, Y. Li, M. Sjöberg, D. Vuilleumier, C.P. Ding, F. Liu and X. Li, "Impact of coolant temperature on piston wall-wetting and smoke generation in a stratified-charge DISI engine operated on E30 fuel", Proceedings of the Combustion Institute 37(4): 4955-4963, 2019, doi: 10.1016/j.proci.2018.07.073
- D. Vuilleumier, X. Huan, T. Casey and M. Sjöberg, "Uncertainty Assessment of Octane Index Framework for Stoichiometric Knock Limits of Co-Optima Gasoline Fuel Blends", SAE International Journal of Fuels and Lubricants 11(3):247–269, 2018, doi: 10.4271/04-11-03-0014.
- C.-P. Ding, D. Vuilleumier, N. Kim., D.L. Reuss, M. Sjöberg, and B. Böhm, "Effect of Engine Conditions and Injection Timing on Piston-Top Fuel Films for Stratified DISI Operation using E30", accepted for IJER special issue on Spray-Wall Interactions.
- 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", submitted to IJER.

ANL:

- C. Xu, S. Som, N. Van Dam, and M. Sjöberg, "Numerical investigation of mixed-mode combustion in a direct-injection spark-ignition engine", abstract submitted to ASME ICEF 2019, manuscript in preparation

LLNL:

- None (new task FY19).

Presentations

SNL:

- D. Vuilleumier, X. Huan, T. Casey, and M. Sjöberg, "Uncertainty Assessment of Octane Index Framework for Stoichiometric Knock Limits of Co-Optima Gasoline Fuel Blends", Co-Optima Stakeholders meeting, May 2018.
- M. Sjöberg, "Light-duty Multimode Engine Operation", IEA Combustion TCP Task Leaders Meeting, Fréjus, France, June 2018.
- X. He, Y. Li, M. Sjöberg, D. Vuilleumier, C.P. Ding, F. Liu, and X. Li, "Impact of coolant temperature on piston wall-wetting and smoke generation in a stratified-charge DISI engine operated on E30 fuel", presented at the 37th International Symposium on Combustion, Dublin, Ireland, Aug. 2018.
- D. Vuilleumier, "Advanced Gasoline Combustion: Mixing and Autoignition", presented at Beijing Institute of Technology, Aug. 2018.
- D. Vuilleumier, N. Kim, and M. Sjöberg, "Lean End-Gas Autoignition: Motivations and Results", AEC Program Review Meeting at USCAR, Aug 2018.
- N. Kim, D. Vuilleumier, E. Cenker, S. Skeen, and M. Sjöberg, "The Use of In-cylinder Soot Diagnostics to Understand Shortcomings of PMI for Stratified-Charge SI Combustion", AEC Program Review Meeting at USCAR, Aug 2018.
- M. Sjöberg, D. Vuilleumier, N. Kim, D. Reuss, X. He, and C.-P. Ding, "Effect of Fuel Type and Operating Conditions on Piston-Top Fuel Films in a DISI Engine", presented to Coordinating Research Council, Nov 2018.
- D. Vuilleumier, N. Kim and M. Sjöberg, "Fuel Effects on Mixed-Mode Combustion in a DISI Engine", AEC Program Review Meeting at ORNL, Jan 2019.
- N. Kim, D. Vuilleumier, D. Reuss, M. Sjöberg, X. He, and C.-P. Ding, "Influence of Injection Strategies and Spray Dynamics on Wall Films and Soot Formation for Lean Stratified SI Engine Operation using E30", AEC Program Review Meeting at ORNL, Jan 2019.

ANL:

- Z. Yue, C. Xu, P. Pal, J. Kim, R. Scarcelli, and S. Som, "Update on CFD Simulations of mixed-mode and multi-mode combustion for Co-Optima", AEC Program Review Meeting at ORNL, Jan 2019.

LLNL:

- None (new task FY19)

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 particularly challenging for lean operation since lean-NOx 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 overarching 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.
  - Overarching 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.*).