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Co-Optimization of
Fuels & Engines

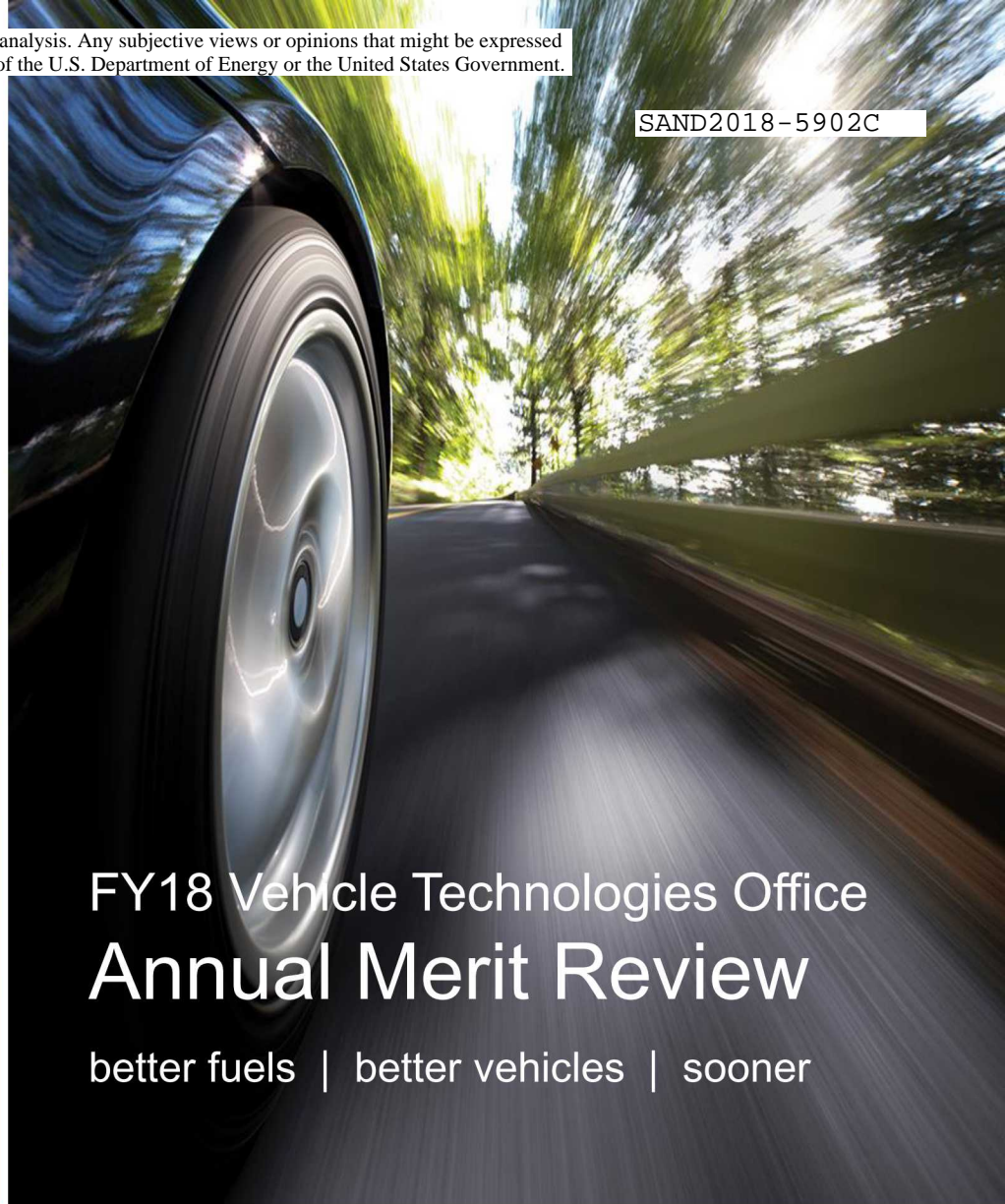
Co-Optima Boosted Spark-Ignition and Multi-Mode Combustion, Part 3

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SAND2018-5902C



FY18 Vehicle Technologies Office
Annual Merit Review

better fuels | better vehicles | sooner

U.S. DEPARTMENT OF
ENERGY

Energy Efficiency &

Sandia National Laboratories is a multission laboratory managed and operated by National Technology & 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.

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This presentation does not contain any proprietary, confidential, or otherwise restricted information.

Overview: Focus Light-Duty DISI → Multi-Mode



Advanced Engine Development: Transition from LD SI & ACI to ACI/SI Multi-Mode

Timeline*

| Task | FY16 | FY17 | FY 18 | FY19 | FY20 | |
|---------------|-------|------|-------|--------------|------|----|
| E.1.1.3: SNL | Start | → | End | New Proposal | | MM |
| E.1.1.4: SNL | Start | → | End | | | SI |
| G.2.1: ANL | Start | → | End | New Proposal | | SI |
| E.1.2.5: ANL | | | Start | | | MM |
| E.1.2.6: ORNL | | | Start | | | |

Barriers**

- 2020/2025 Stretch Efficiency Goals for downsize boosted engines
- 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

Budget

| Task | FY16 | FY17 | FY 18 |
|--|--------|--------|--------|
| E.1.1.3: Optical Diag.: Fuel Effects on Lean Homogen. and Stratified | \$652K | \$652K | \$475K |
| E.1.1.4: LD DISI relevance of RON & MON for lean/dilute + Knock | \$300K | \$300K | \$155K |
| G.2.1: DISI engine simulations | \$50K | \$255K | \$165K |
| E.1.2.5: Fuel properties enhance mixed-mode ACI/SI | NA | NA | \$315k |
| E.1.2.6: Multi-mode SI/ACI – stratification/fuel/dilute interact | NA | NA | \$325K |

Partners

- Co-optima partners include nine national labs, 13 universities, external advisory board, and stakeholders (77 organizations)
- 15 Industry partners in the AEC MOU
- Task specific partners
- General Motors - Hardware
- Toyota – Funds-in knock project
- Ford support for engine modifications
- LLNL (W. Pitz et al.) – Chemical kinetics
- G.2.5 Edwards - Toolkit
- + Many more – details in later slides

* Start and end dates refer to three-year life cycle of DOE lab-call projects. Co-Optima is expected to extend past the end of FY18

**https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf

Relevance



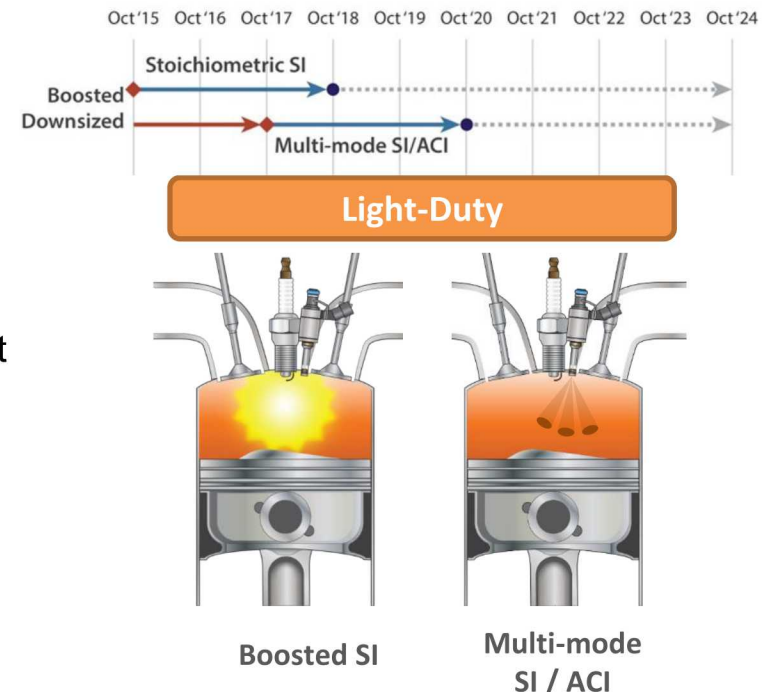
- Increased fuel economy requires engines with higher thermal efficiency, while complying with stringent exhaust requirements for clean air
 - **Mirrors the programmatic transition in Co-Optima from downsized boosted and light-duty ACI tasks to multi-mode SI-ACI R&D**
- These **light-duty engine development** and computational toolkit research tasks support:
 - **Near-term Co-Optima fuel-economy targets for conventional boosted SI**
 - **Longer-term development of fuels for advanced highly efficient SI combustion**

- **Boosted SI (DISI)**

- Continue to perform fuel studies to address barriers for achieving high thermal efficiency for boosted for **boosted stoichiometric SI operation**
- Emissions mitigation for more efficient **stratified-charge SI operation**
- Efficiency gains for **ultra-lean well-mixed SI operation** that utilizes mixed-mode combustion (with transition from deflagration to autoignition)

- **Multi-Mode (SI-ACI)**

- Address barriers to add to knowledge-base and modeling capabilities for **both SI and ACI modes**
- Inform industry of **fuel effects on multi-mode**
- **Link to emissions controls/ toolkit tasks** for accelerating development of multi-mode and addressing barriers



Overall Co-Optima Relevance
Farrell FT037

Milestones: Met or On Track



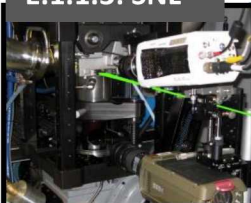
| Month/Year | Description of Milestone | Status |
|----------------------------|---|----------|
| March 2017, SNL E.1.1.4 | Provide fuel-efficiency and exhaust emissions data for SI operation for AKI87 and RON 98 to ASSERT team | Met |
| March 2017, ANL G.2.1 | Sensitivities to fuel properties at validation points for the SNL DISI engine | Met |
| June 2017, ANL G.2.1 | Dataset of simulations with virtual fuels to evaluate fuel property hypothesis | Met |
| Sept 2017, ANL G.2.1 | Sensitives to fuel properties at validation points for ACI engine | Met |
| 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 |
| Sept 2018, ANL E.1.2.5 | Evaluate relationship between fuel RON-MON sensitivity and temperature delta for ACI and SI | On Track |
| Sept 2018, ORNL E.1.2.6 | Make recommendation on viability of 2 step VCR as multi-mode enabler | On Track |

Overall Technical Approach: 5 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



E.1.2.6: ORNL

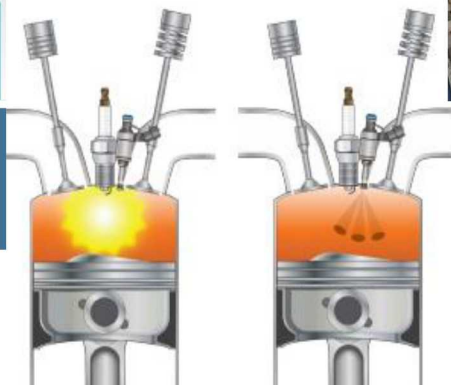


E.1.2.5: ANL



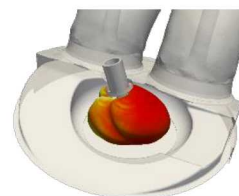
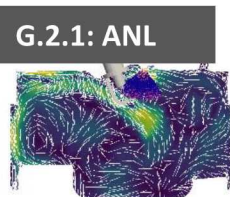
Combine metal- and optical-engine experiments and modeling: DISI combustion processes

Multi-mode engine experiments to overcome technical barriers for achieving multi-mode goals



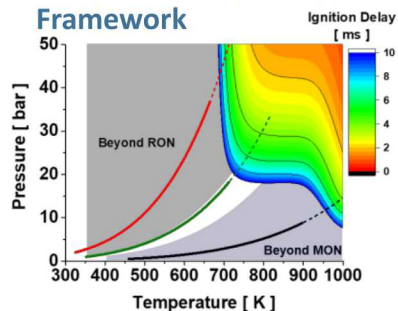
Boosted SI

Multi-mode SI / ACI

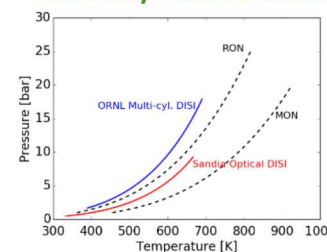


Enhance understanding and accelerate development through linked modeling efforts

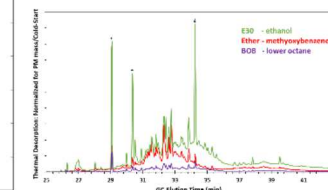
Temp-Press Trajectory Framework



Collaborative Kinetics/ Toolkit tasks



Emissions Controls and Characterization Tasks



Approach – SNL: Sjöberg



- 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 and promising blendstocks in mid-level RON98 surrogate blends.

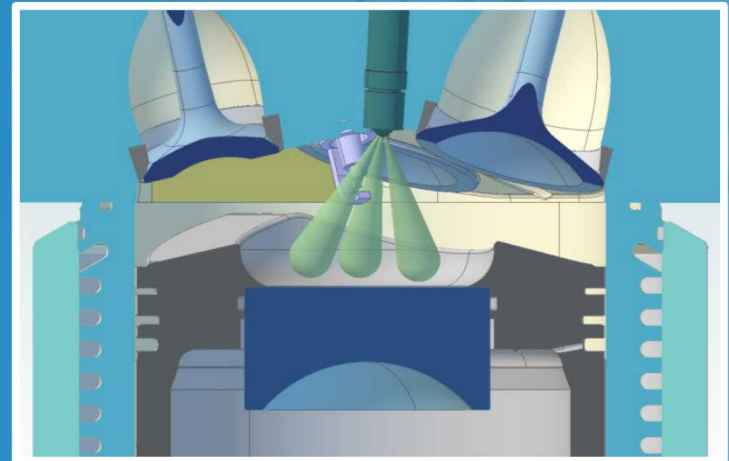
- First, conduct performance testing with all-metal engine over wide ranges of conditions.

- Assess relevance of Octane-Index framework for stoichiometric knock and 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.
- Provide conceptual understanding of advanced SI combustion modes.

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



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

ANL- CFD: Approach/Workflow



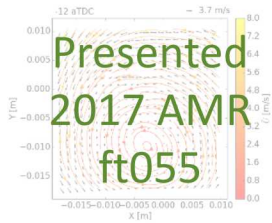
2 Turbulence models

- LES – more flow details
- RANS – higher throughput

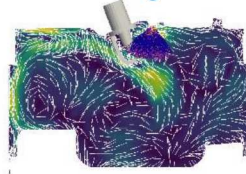
2 Turbulence-chemistry interaction models

- Well-stirred Reactor – easier implementation
- G-equation – improved flame description

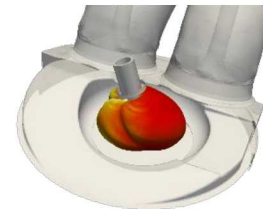
Motored Flow



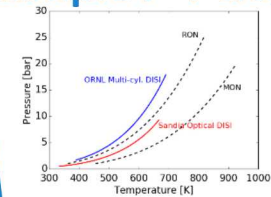
Motored with Fuel Injection



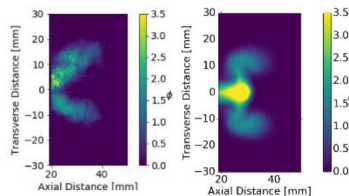
Combustion



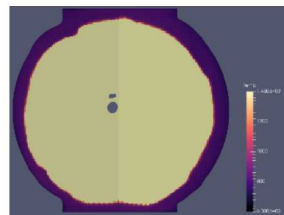
Multiple Conditions Multiple P-T trajectories



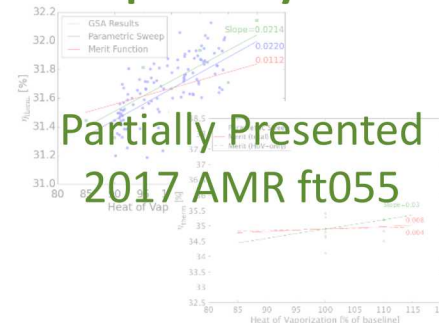
Spray Validation



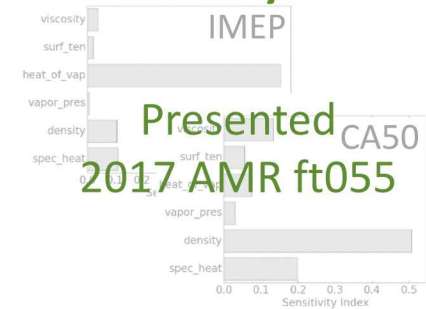
Thermal Stratification



Merit Function Slope Analysis



Global Sensitivity Analysis



Approach – Multi-Mode Projects:

2 - Metal single-cyl. SI base engines (ANL/ORNL)

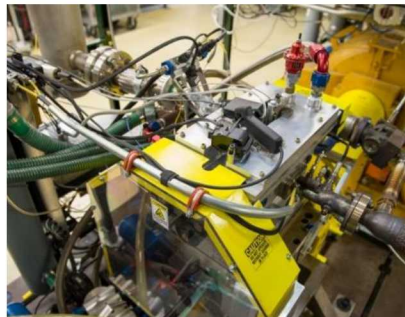


ANL – Kolodziej

- Fuel Properties which Enhance Mixed-Mode ACI/SI Engine Operation
 - Goal: Define a ΔT metric of low/high S fuels, using Co-Optima alkylate, E30, and aromatic gasolines
 - Question: “Does RON-MON sensitivity capture fuel auto-ignition and knock temperature dependencies?”
 - Engine parameter of interest: Temperature (modified by intake air heating)

ANL Single-Cylinder Engine Geometry:

| | |
|-------------------------|---------------------|
| CR (-) | 12.5:1* |
| Disp. (L) | 0.63 |
| Bore x Stroke (mm x mm) | 89.04 x 100.6 |
| Injection | PFI or DI (central) |



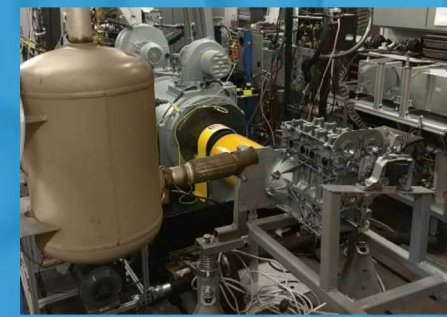
*Fixed compression ratio (CR)
Perform testing at 12.6:1 and 15:1 CR

ORNL - Curran

- Multi-mode SI/ACI: stratification/ fuel/ dilute interactions
 - Bridge foundational DOE CO-Optima research into fuel-property impacts on boosted SI efficiency and ACI efficiency and help understand fuel effects w/ tumble dominated combustion systems operating in both SI and ACI modes
 - Focus on quantifying the effects of octane number, S, and HOVat “SI” and “ACI” compression ratios @ multi-mode conditions.
 - Leverages boosted SI work by Sluder (same base engine)

ORNL Single-Cylinder Engine Geometry:

| | |
|-------------------------|------------------------|
| CR (-) - base | 10.1:1* |
| Disp. (L) | 0.40 |
| Bore x Stroke (mm x mm) | 79 x 81 |
| Injection | DI (central) Or PFI |



- *Assume a 2-step VCR mechanism
- Noted in 2018 ACEC Roadmap
 - Collaborate with toolkit team to accelerate

Technical Accomplishments Summary



ACCOMPLISHMENTS (0/11)

• DISI @ SNL

- Finished knock tests for a total of 9 fuels.
- Used uncertainty modeling to assess applicability of Octane-Index framework. Identified outliers like 2-butanol.

- Assessed relevance of PMI for 9 fuels across 3 well-mixed and 2 stratified operating strategies.

- Identified that alcohols and cooler engine conditions can induce shortcomings of PMI for soot predictions.

- Developed and used RIM diagnostics for fuel-film thickness measurements.

- Acquired mixed-mode combustion data for 5 fuels, spanning ϕ , P_{in} , T_{in} and $[O_2]$.

- Performed assessment of Octane-Index framework for ultra-lean conditions.

- Applied CHEMKIN to determine underlying autoignition sensitivities to intake $[O_2]$.

- Numerous technical publications.

• CFD @ ANL

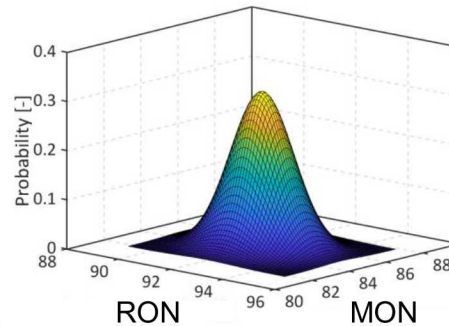
- Expansion of merit function analysis
- New understanding of thermal stratification on sequential autoignition
- Validated spray and detailed motored flow with fuel injection for SNL DISI
- G-equation combustion model used for lean-dilute combustion

• Multi-Mode @ ANL and ORNL

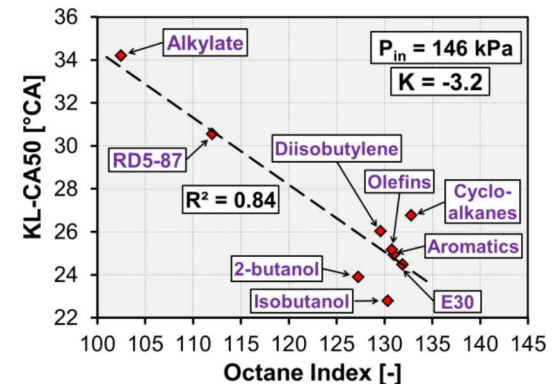
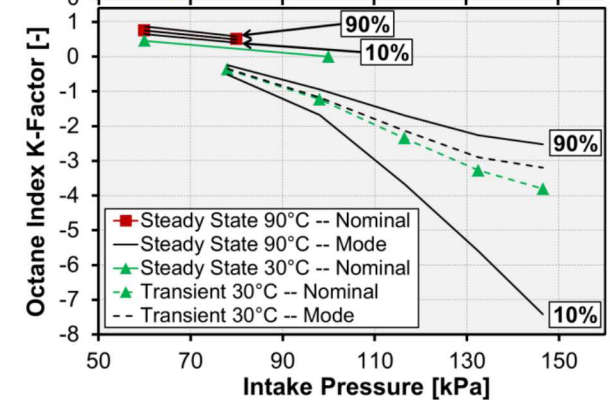
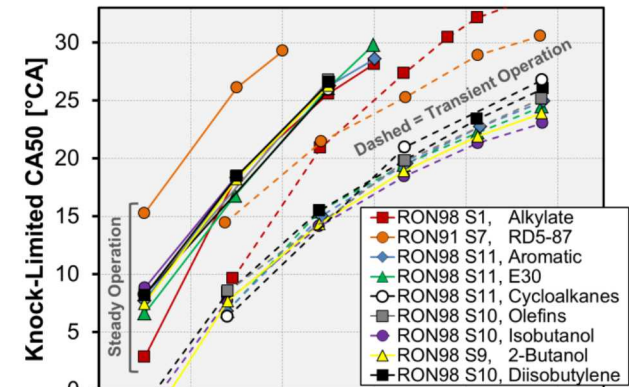
- Minimum temperature allowing stable low load HCCI combustion (ANL)
- Maximum temperature still allowing knock-free high load SI combustion (ANL)
- ΔT metric for low load ACI and High load SI (ANL)
- Exploration of effect of multi-mode constraints and impact of range/ location of ACI mode (ORNL)



- Intake-pressure sweeps reveal how fuels respond to load and engine conditions.
- Load-transient operation (dashed lines) allows more advanced CA50 due to cooler in-cylinder conditions.
- For boosted transient operation, K is highly negative. Here, fuels with high RON-MON sensitivity (S) show great benefits.



- RON, MON and knock limits all have quantifiable uncertainties.
- Performed Monto-Carlo simulations to assess robustness of Octane Index.
- Highly negative K becomes uncertain.
 - OI-based efficiency assessment remains useful.
- Iso-butanol and 2-butanol blends perform better than RON & S indicate; Cycloalkanes worse.
 - Uncertainly quantification suggests real fuel effects.

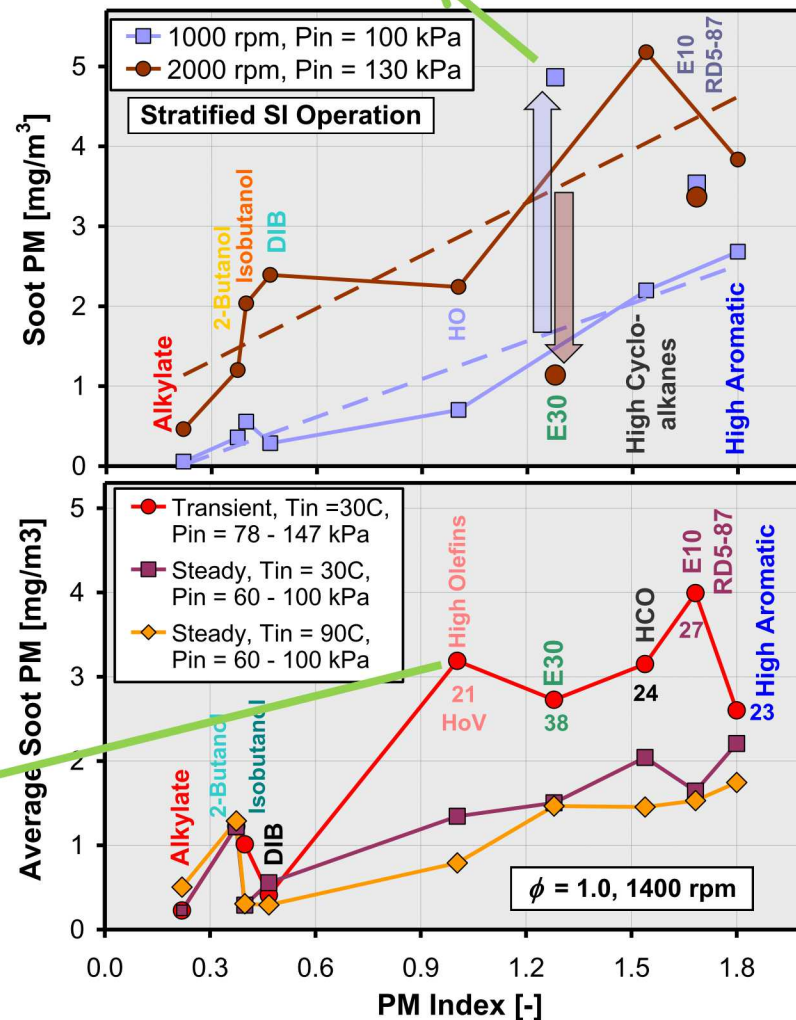
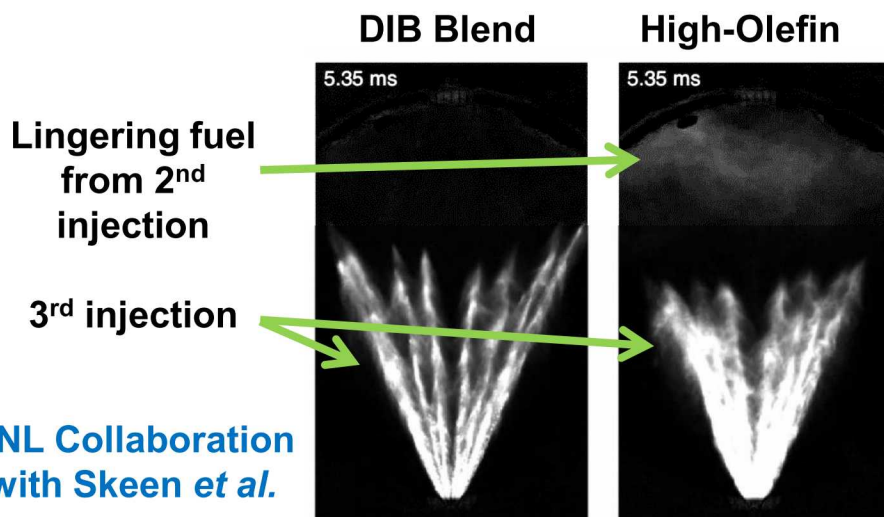




- How well engine-out soot scales with PMI was assessed for 9 fuels over 3 stoichiometric and 2 lean stratified-charge SI operating modes.
- Alcohol-containing fuels cause deviations.
 - E.g. E30 & E10 for stratified operation.
 - PMI does not account for oxygen content.
- High Olefin and Di-isobutylene blends show high variability between oper. conds.
- Spray-vessel experiments show strong fuel effects on spray and vaporization.
 - PMI does not account for spray variations.

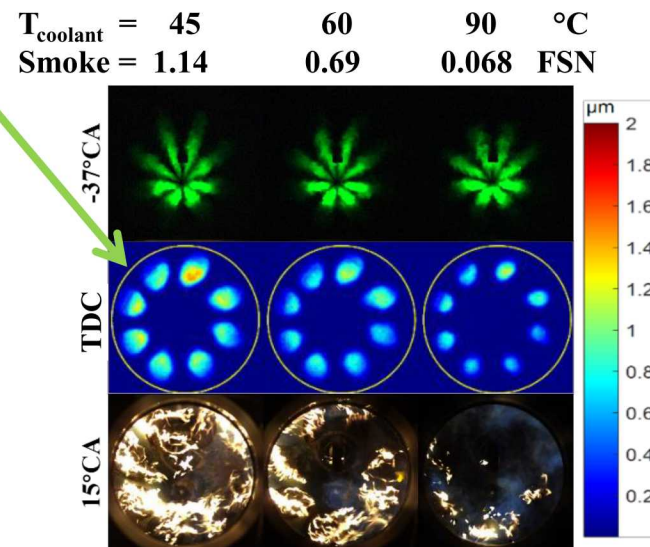
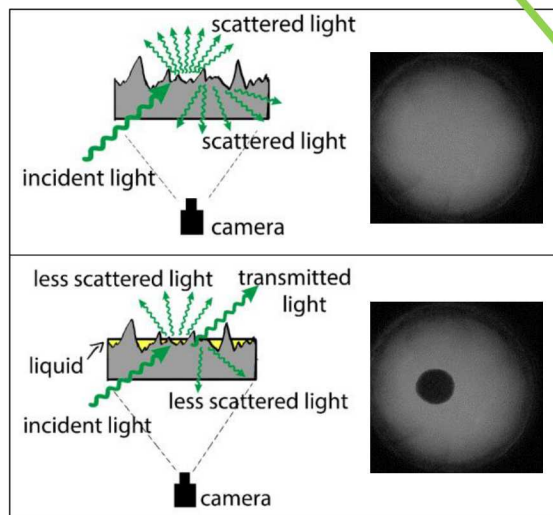
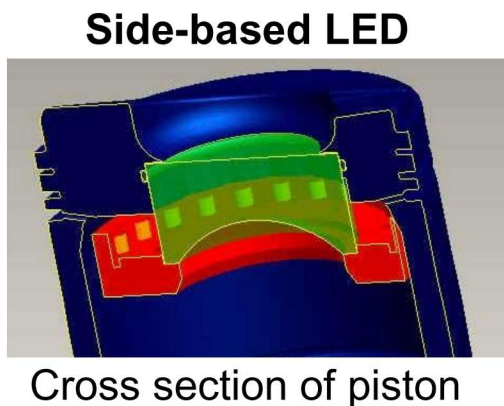
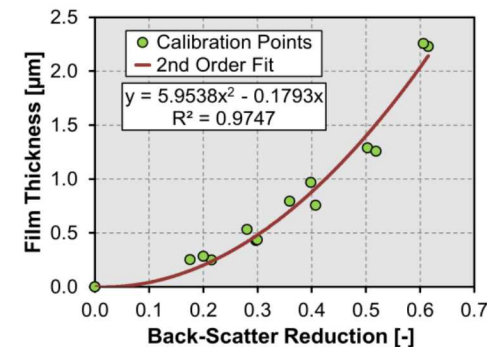


Pool fires for non-boosted operation.



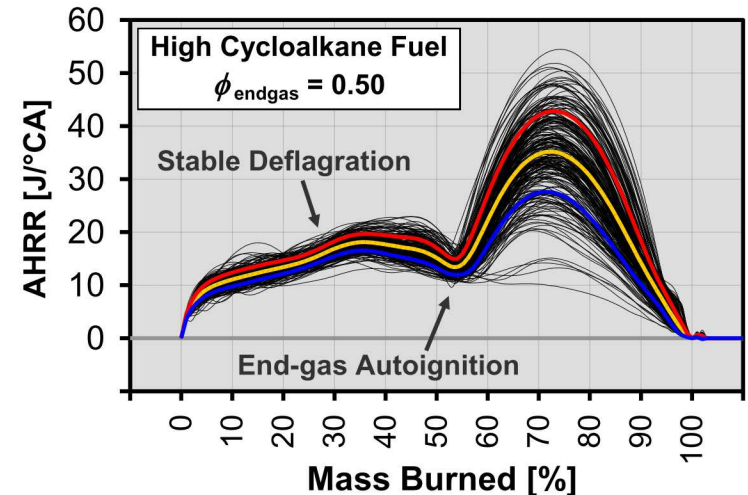
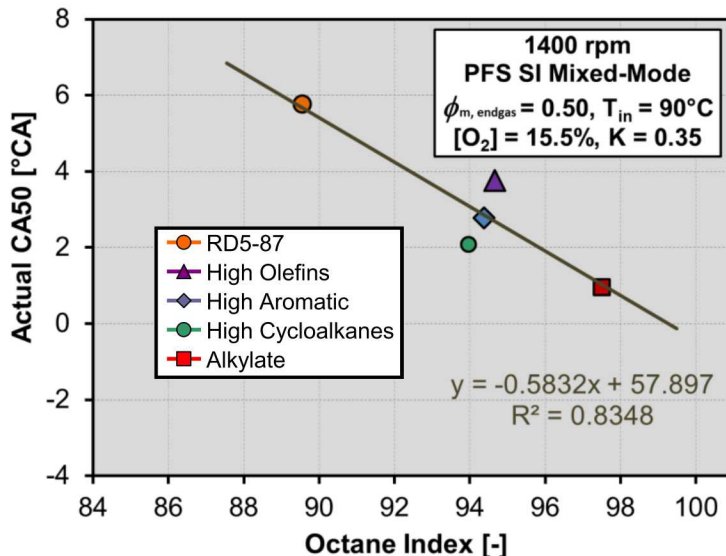
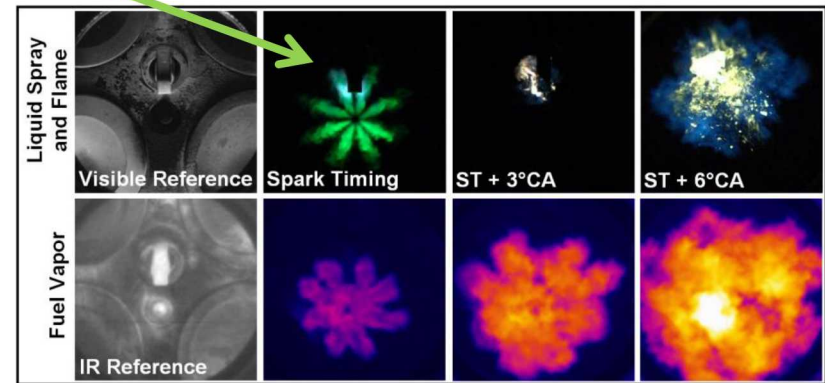
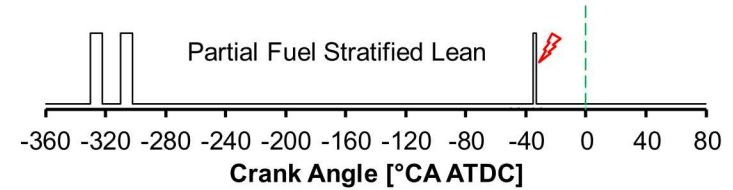


- Developed and used innovative LED-based side illumination for quantitative fuel-film thickness measurements.
- In-situ calibration yields relationship between relative reduction in back-scattered light and film thickness.
- Applied diagnostics to wide ranges of operating conditions, supporting interpretation of PMI efficacy and soot-production pathways.
 - Increased P_{in} strongly reduces wall wetting for E30.
 - Reduction of $T_{coolant}$ strongly increases **wall wetting** and **smoke** for E30.
- RIM will be applied for cold-start testing, as outlined by ACEC Tech Team.





- Established stratification approach to stabilize ultra-lean mixed-mode combustion.
 - Settled on 1.6 mg pilot. 3.6 mg in example.
- Use strong CA50 control authority to achieve stable end-gas autoignition for $CA_{10-90} < 30^\circ CA \Rightarrow 20\%$ rel. eff. gain.
- Acquired data for ranges of ϕ , P_{in} , T_{in} and $[O_2]$.
- Octane-index ranking holds to first order.



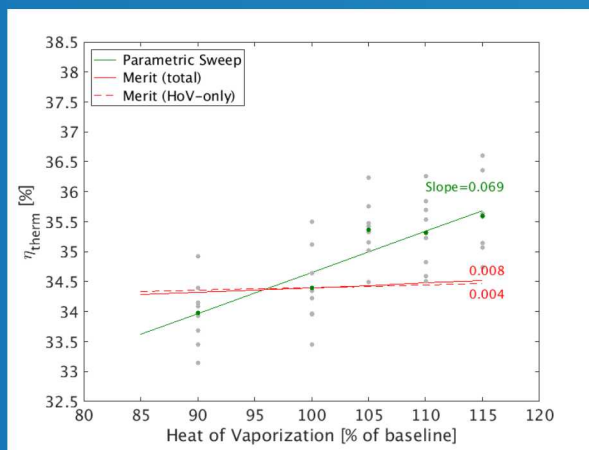
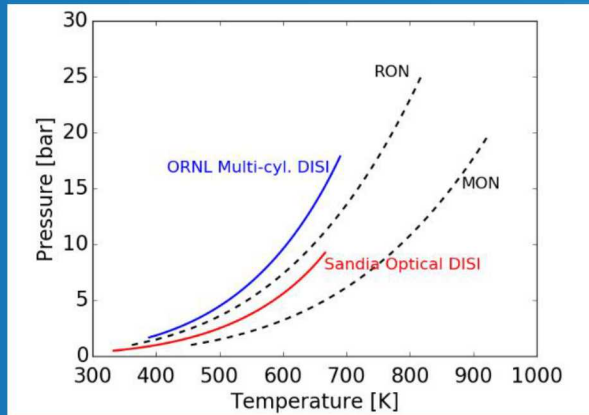
ANL: Advanced modeling efforts to enhance understanding and accelerate development



ACCOMPLISHMENTS (5/11)

Expanding Merit Function analysis to new engines/operating points

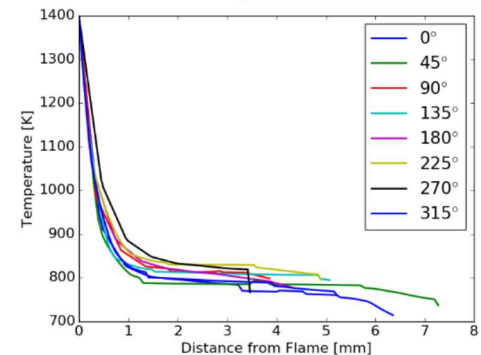
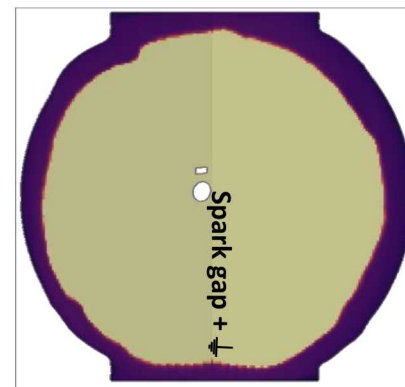
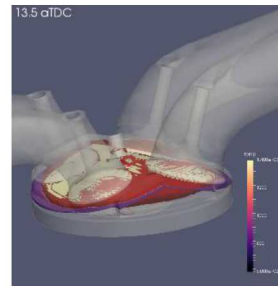
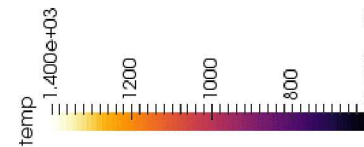
- ORNL multi-cylinder engine (see SI Combustion part I For more results)
- Knock-limited mid-load point



Thermal stratification can result in sequential auto-ignition

- Process relevant to both knock and SACI
- Providing information to more accurately model Sandia DISI engine with low-dimensional tools

○ FT052: Fuel Kinetics & Simulation - for details



Temperature in the end-gas at CA50 - Sandia DISI engine
Two planes approximately parallel to the pent-roof and through the center of the propagating flame.

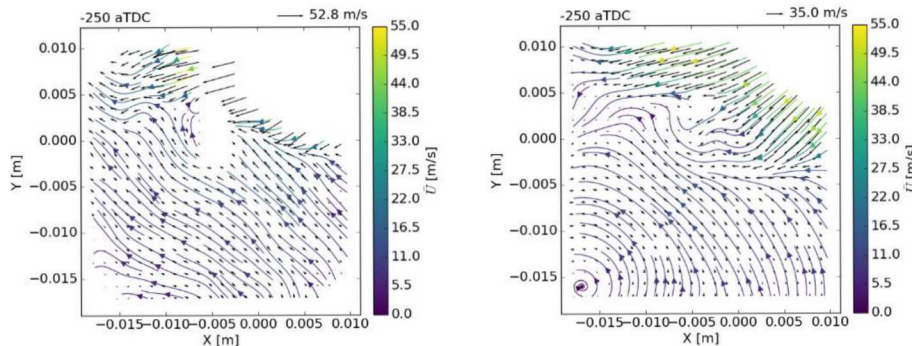
ANL DISI results: Furthering understanding of flow and mixing details



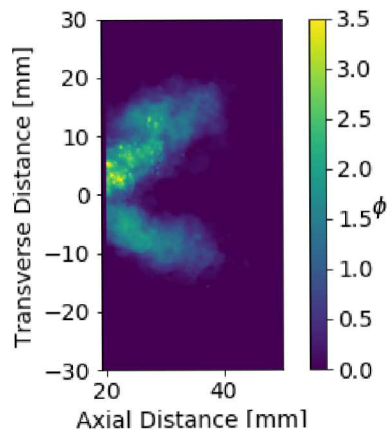
ACCOMPLISHMENTS (7/11)

Validated spray and detailed motored flow with fuel injection

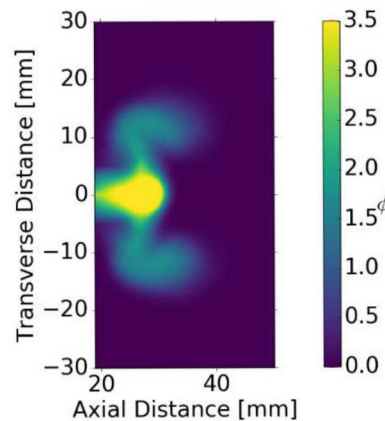
- Spray validated with data from Blessinger et al.
- 4.0% root mean square error in pressure
- **Results can be accelerated with confidence**



Experiment

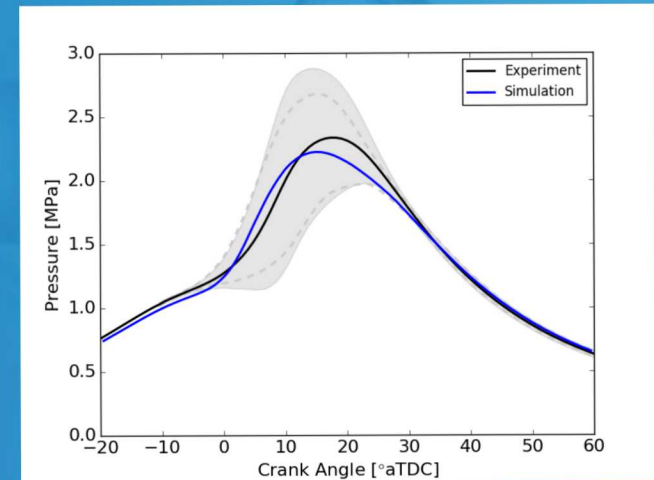


Simulation



G-equation combustion model able to match experimental pressures

- Uses a tabulated approach for robust flamespeeds at lean/dilute conditions
- **Important moving forward for MM**



| | Experiment | Simulation |
|-------------|------------|------------|
| CA10 | 3.4° | 3.5° |
| CA50 | 11.9° | 14.0° |
| CA90 | 23.7° | 35.9° |

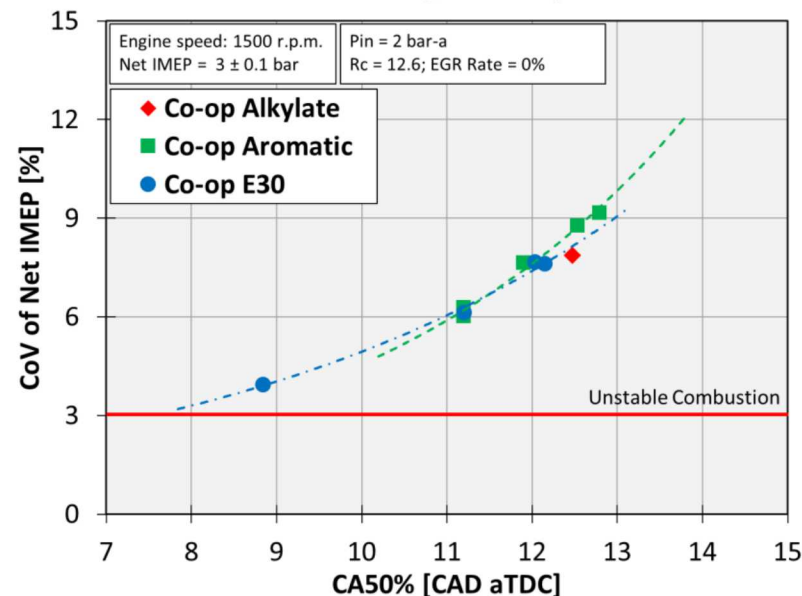
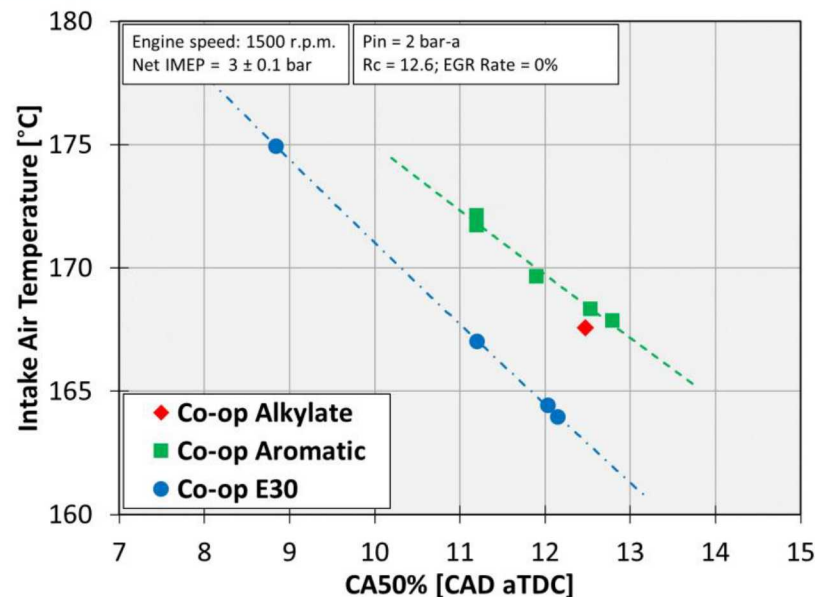
ANL: Fuel Properties which Enhance Mixed-Mode ACI/SI Engine Operation



ACCOMPLISHMENTS (8/11)

Minimum temperature allowing stable low load HCCI combustion

- Preliminary results of testing with three co-optima core fuels show a weak correlation between fuel's octane sensitivity and intake temperature requirements for low-load HCCI operation
- At 1500 rpm with 1 bar boost pressure, none of the tested fuels allowed stable (CoV < 3%) low-load HCCI operation with up to 175 °C intake temperature
 - Higher compression ratio and lower engine speed to be tested in the near future, both expected to lower intake temperature requirements for low-load ACI, but also lower high-load intake temperature tolerance



ANL: Fuel Properties which Enhance Mixed-Mode ACI/SI Engine Operation



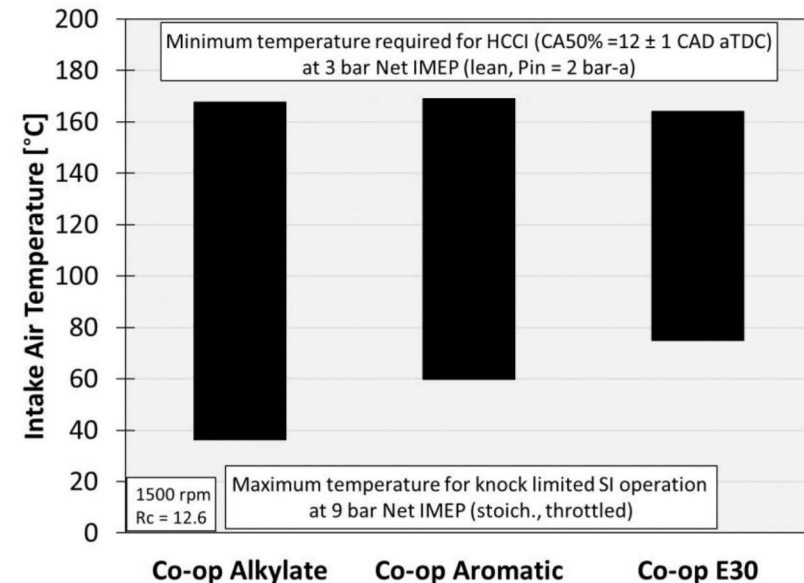
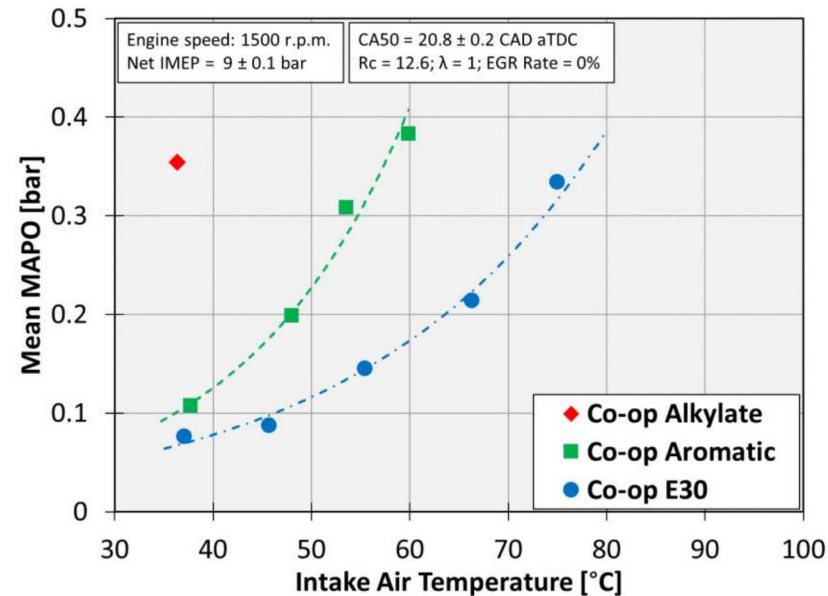
ACCOMPLISHMENTS (9/11)

Maximum temperature still allowing knock-free high load SI combustion

- The tested fuels show significantly different temperature tolerance at high load SI operation
- Observed differences seem to be also affected by fuel properties other than octane sensitivity (HoV effects)

ΔT metric for low load ACI and High load SI

- Alkylate fuel showed maximum ΔT requirement of 130 °C
- Observed relationship between octane sensitivity and ΔT requirements suggests that in-cylinder P-T conditions are not high enough to capture fuel sensitivity effect at low load HCCI operation



Co-op Alkylate

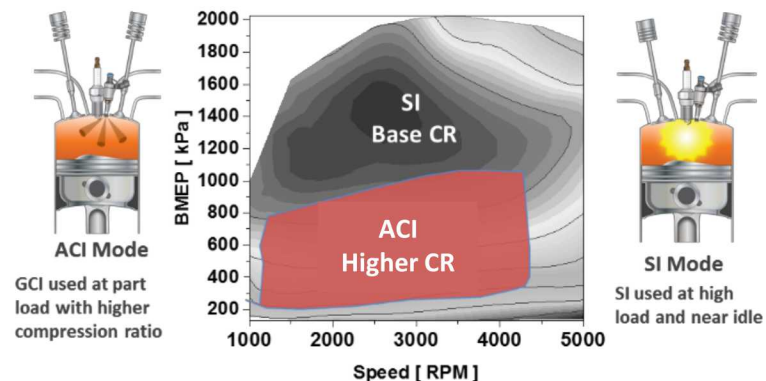
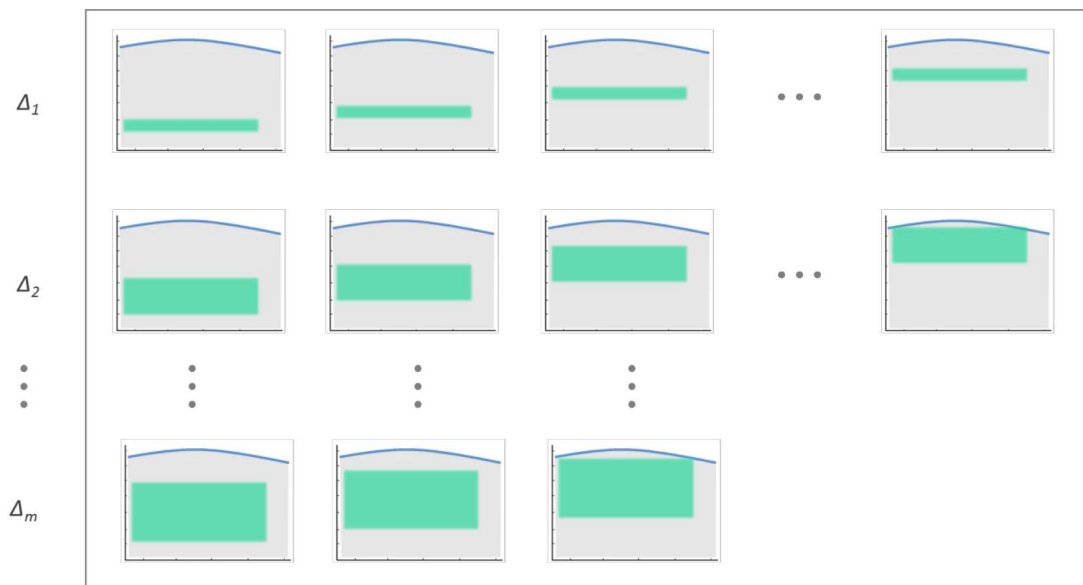
Co-op Aromatic

Co-op E30



- Understand fuel-property impacts on achieving stratified ACI with requirements of being able to run in SI mode part time
- Knowledge discovery and additional insights through modeling in collaboration with Co-Optima Toolkit development team project (Edwards ORNL)

Single-cylinder results inform what is possible for multi-mode ACI speed and load range and location as a function of fuel properties



Links to boosted SI (Sluder) and previous multi-mode R&D provides insights into constraints needed for realistic results

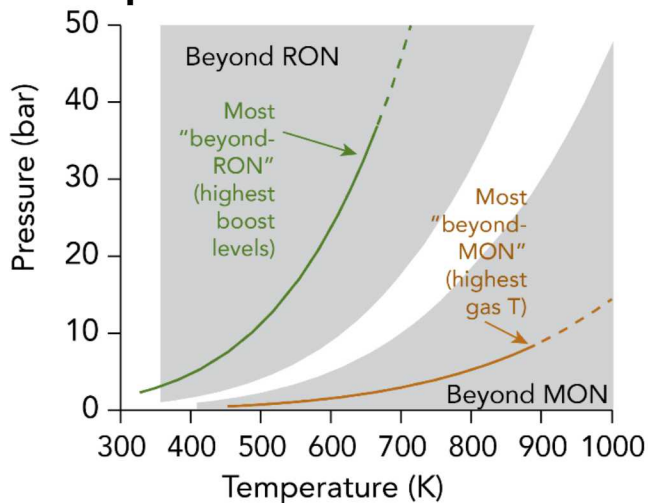
ORNL: Accelerating development with Tool-Kit and Fuel Properties team



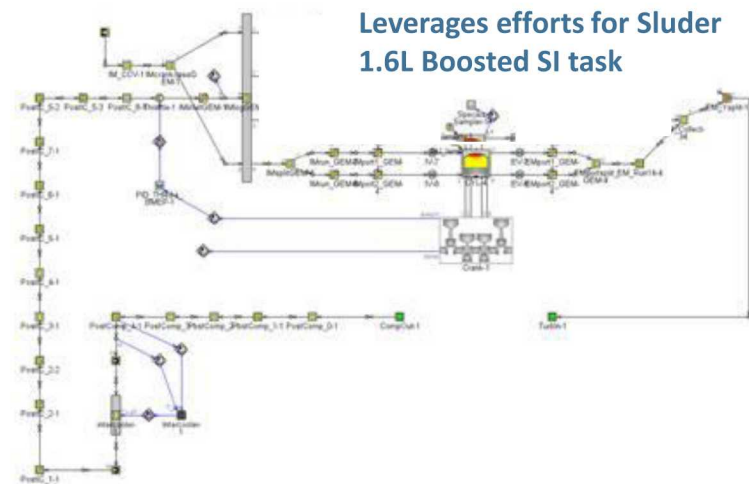
ACCOMPLISHMENTS (11/11)

- **Focus:** quantifying the effects of octane number, sensitivity, and heat of vaporization at “SI” and “ACI” compression ratios at prescribed experimental conditions relevant to multi-mode operation.
 - The ORNL multi-mode engine will **assume a two-step variable compression ratio mechanism** to enable mode transitions from SI to ACI which be completed using different custom piston configurations to enable different compression ratios.
 - To enable conditions for ACI modes, a custom intake manifold used to enable higher intake temperatures was used
- **Strong links to Co-Optima Tool-kit and Fuels Properties team**

Temperature - Pressure



Toolkit team



Responses to Previous Year Reviewers' Comments

Note: two new tasks not reviewed last year

Overall approach:

Reviewers noted “approach taken, of running both metal and optical engine experiments with CFD modeling, is very good (noted multiple times) “

Multi-mode comments:

–**Reviewer noted** approach adopted in this project not only supports refinement of the Merit Function for LD SI engines, but is also supporting development of diagnostic techniques that can help evaluate and troubleshoot engine operation for mixed-mode combustion regimes.

–**Reviewer commented** on the good progress made on Mixedmode combustion and transition.

Comments requiring addressing:

- **Reviewers noted** “...the scope of work is limited to low TRLs, practical considerations [aftertreatment requirements and transient controls] should be kept in mind ...”
 - Initial DISI work did look at in-cylinder and exhaust soot
 - Multi-mode project at ORNL will be engaged with emissions controls and characterization tasks
 - Engagement with industry on controls and transients – fundamental results informing the development
- **A reviewer noted** “...while the evaluation of particulate emissions is extremely valuable for current and near future production engines, it is not clear if the observed PM emissions were a consequence of the differences in the fuel properties or in the operating procedure.”
 - Good suggestion; fuel properties were isolated for five operating strategies, as shown in Accomplishments

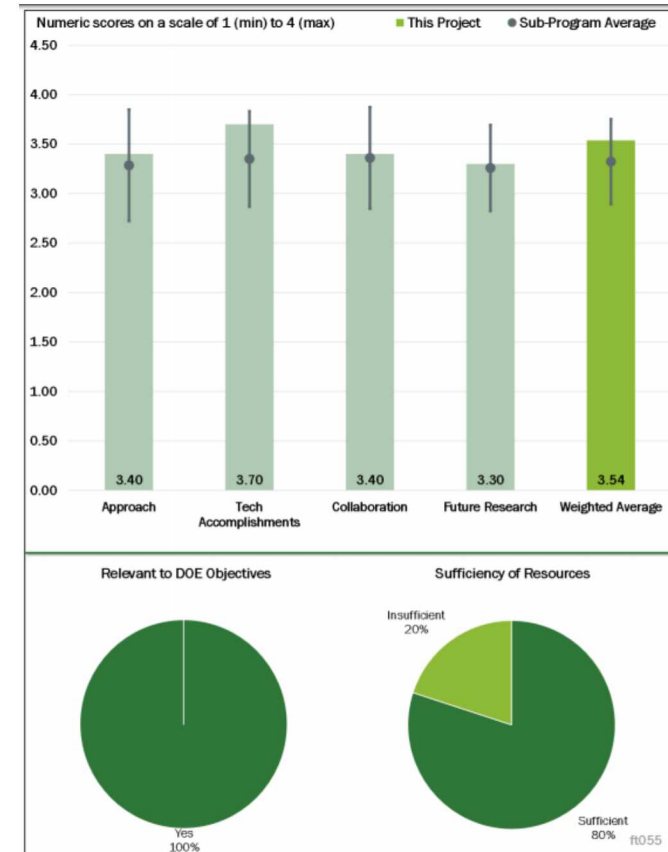


Figure 5-13 – Presentation Number: ft055 Presentation Title: Co-Optimization of Fuels and Engines (Co-Optima)—Multimode Lean Spark Ignition: Experiments and Simulation Principal Investigator: Magnus Sjoberg (Sandia National Laboratories)



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 E.1.1.3, E.1.1.4

- General Motors
- Funds-in knock project with Toyota.
 - Explores effect of deviations from non-dilute stoichiometric operation.
- Westbrook (LLNL) & Cernansky (Drexel)
 - Use of detailed chemical-kinetics to predict RON and MON of alternative fuel blends
- Pitz, Mehl & Wagnon at LLNL
 - Validate surrogate-gasoline mechanisms.
 - Identified areas that required corrections
- Direct with ANL on CFD
+ many more

ANL - CFD G.2.1

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

ANL – Multi-mode E.1.2.5

- Ford
- ORNL-multi-mode
- SNL DISI
- Merit-function development

ORNL – Multi-mode E.1.2.6

- Sluder boosted SI task
- Toolkit team – Edwards
- Kinetics team (Pitz, Wagnon et al.,)
- Fuel properties team (Szybist/ Splitter)
- Ford – support for engine modifications
- ANL multi-mode
- General Motors

Details in backup slides



- Developing combined experimental/ modeling approach to identifying fuel property/engine parameter impacts for wide array of ACI approaches suitable for multi-mode operation
- Identifying key fuel properties/engine parameters that provide efficiency, power density, and wide operability for kinetically controlled combustion
- Developing high-fidelity, computationally efficient kinetic and fluid dynamic models and high quality experimental data to validate
- Further work to address barriers in the 2018 ACEC roadmap around high efficiency SI-ACI multi-mode

Proposed Future Research*



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

SNL Mixed-mode combustion:

- Optically investigate fuel effects on flame structure in end-gas
- Use experiments and CHEMKIN to assess fuel effects on sensitivities to changes of ϕ , P_{in} , T_{in} and $[O_2]$.
- Add lower-RON fuels to test matrix, and determine effect on load coverage.
- Examine if there are specific chemical families that reduce applicability of octane-index framework.

SNL Stratified-charge SI operation:

- Determine fuel effects on load coverage.
- Focus on soot emissions and combustion stability for high-EGR, low- NO_x operation.
- Examine optically fuel/load combinations that have smoke or stability issues.
- Expand efforts on load transients, and start studies on cold-start effects.
 - Guidelines from ACEC Tech Team.
 - For both mixed-mode and stratified SI.

ANL CFD

- Develop and validate a CFD approach for lean SI combustion
- Parametric sweeps and/or GSA to identify influential fuel properties for multi-mode ACI operation using RANS-type turbulence modeling
- Sensitivities to fuel properties at validation points for multi-mode combustion and possibly update merit function [Q4 milestone]

Multi-mode

- Identify/define (new) fuel properties that impact engine performance under ACI operation
- Identify fuel property/engine parameters that:
- Improve ACI operability (simplify transient control/mode switching, expand speed/load range, improve cold start/low load performance)
- Reduce ACI combustion noise and engine-out emissions

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, metal-single engines, CFD

Technical Accomplishments

- Completed knock tests for 9 fuels - uncertainty modeling assess Octane-Index framework
- Assessed relevance of PMI for 9 fuels across 5 operating strategies
- Mixed-mode combustion data for 5 fuels, spanning ϕ , Pin, Tin and $[O_2]$.
- New understanding of thermal stratification on sequential autoignition
- ΔT metric for low load ACI and High load SI + data for both
- Exploration of effect of multi-mode constraints and impact of range/ location of ACI mode

Collaboration and Coordination

- 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

Proposed Future Research*

- Mixed-mode combustion + Stratified-charge SI operation
- CFD for accelerating development
- Multi-mode programmatic goals + Multi-mode + emission controls

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.
- ORNL multi-mode work was performed at the National Transportation Research Center (a U.S. Department of Energy User Facility), Oak Ridge National Laboratory, Knoxville TN. Oak Ridge National Laboratory is operated by UT-Battelle for the U.S. Department of Energy under contract DE-AC05-000R22725.

Technical Back-Up Slides



ANL: Initial Fuels and test conditions for multi-mode experiments



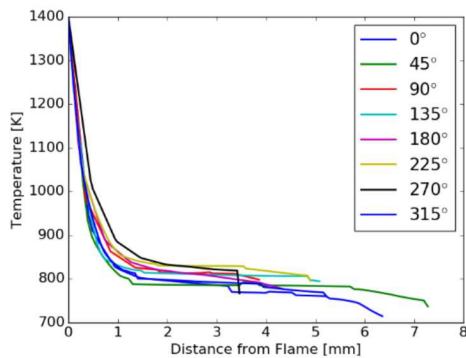
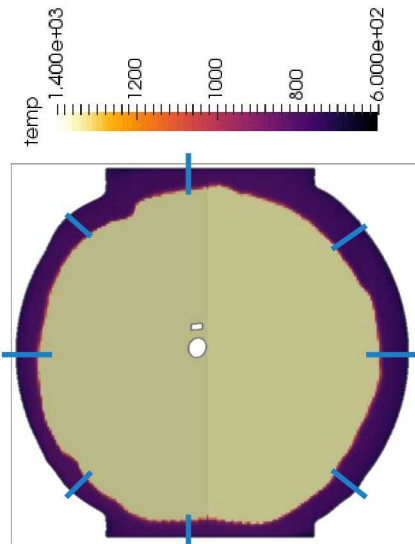
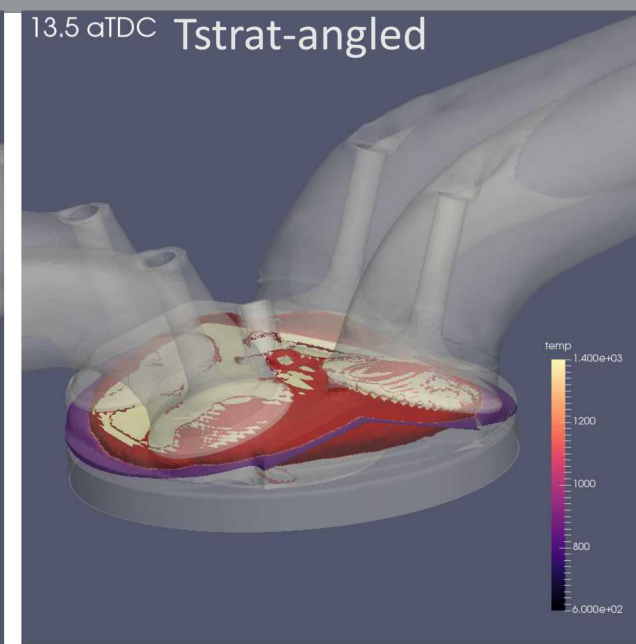
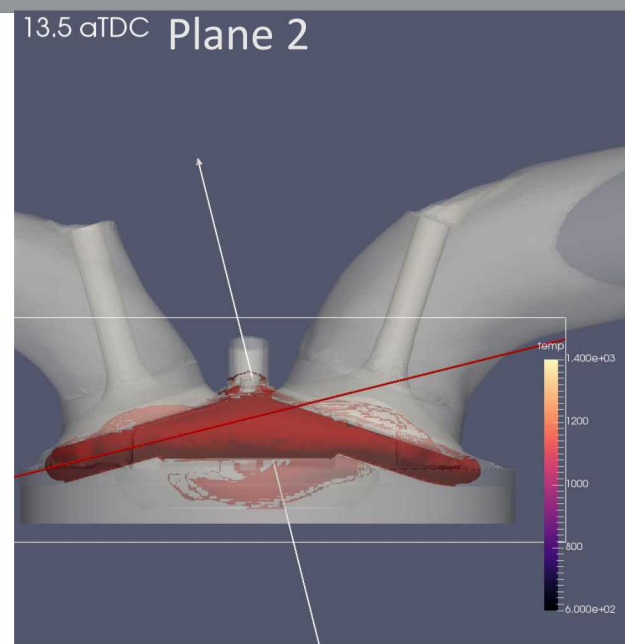
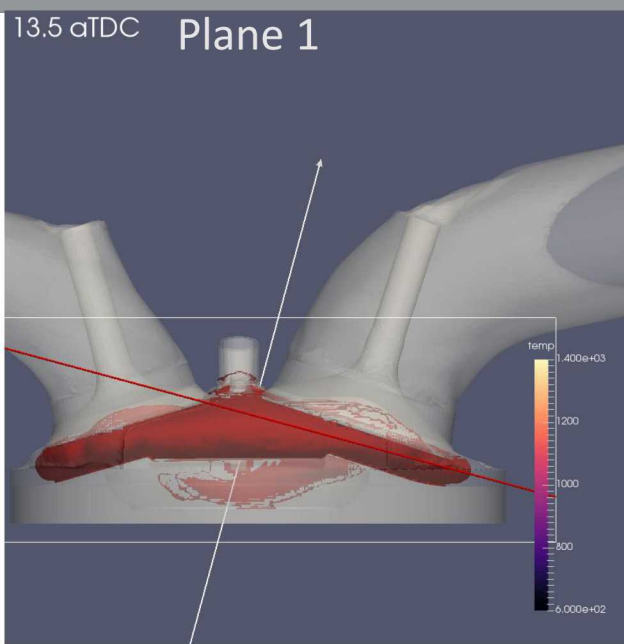
Fuels

| Fuel | Alkylate | E30 | Aromatic |
|-------------------|----------|--------|----------|
| RON (-) | 98.0 | 97.4 | 98.1 |
| MON (-) | 96.6 | 86.6 | 87.8 |
| Sensitivity (-) | 1.4 | 10.8 | 10.3 |
| HoV (kJ/kg) | 309 | 536 | 363 |
| A/F _{st} | 15.1:1 | 12.9:1 | 14.5:1 |
| Paraffin (%vol) | 3.0 | 12.9 | 8.2 |
| I-Paraffin (%vol) | 95.8 | 27.6 | 38 |
| Aromatics (%vol) | 0.7 | 13.8 | 39.8 |
| Naphthenes (%vol) | 0.02 | 7.0 | 8.0 |
| Olefins (%vol) | 0.08 | 5.6 | 4.5 |
| Oxygenates (%vol) | - | 30.4 | - |

Test Conditions

| Condition | ACI | SI |
|---------------------------|------|------|
| NMEP (bar) | 3 | 9 |
| Speed (RPM) | 1500 | 1500 |
| EGR (%) | 0 | 0 |
| CA50 (°aTDC) | 8 | 20.8 |
| DI SOI (°bTDC) | 300 | |
| DI P _{inj} (bar) | 150 | |
| CoV of IMEP (%) | 3 | |
| MAPO* Limit (bar) | 0.35 | |

*Maximum Amplitude of Pressure Oscillations (MAPO)



- Image presented - two planes that are angled ~ along the flame direction
- plane1 and plane2 show a side view with each plane; angled is at an angled view).
- Red iso-surface is the flame over semi-transparent surfaces of the domain

SNL - Fuel Properties Table



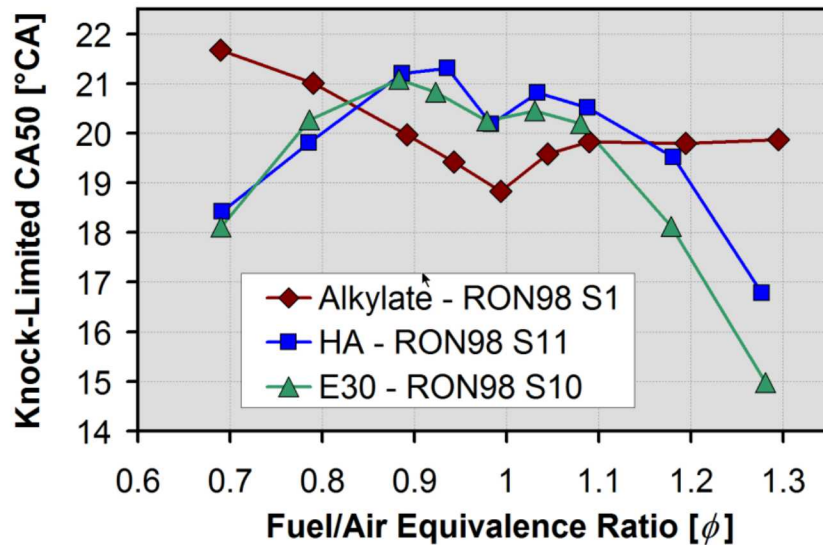
- One E10 regular gasoline, and eight RON = 98 fuels were studied in DISI engine at Sandia.
- Octane sensitivity, compositions, boiling points, heat of vaporization and PMI vary greatly.

| | Co-Optima Core Fuels | | | | | | | | |
|-----------------------------------|----------------------|----------|------|---------------|-------------|------------------|------------------|-----------------|---------------------|
| | E10 RD5-87 | Alkylate | E30 | High Aromatic | High Olefin | High Cycloalkane | Isobutanol Blend | 2-Butanol Blend | Diisobutylene 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 Stoichiometric | 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 |

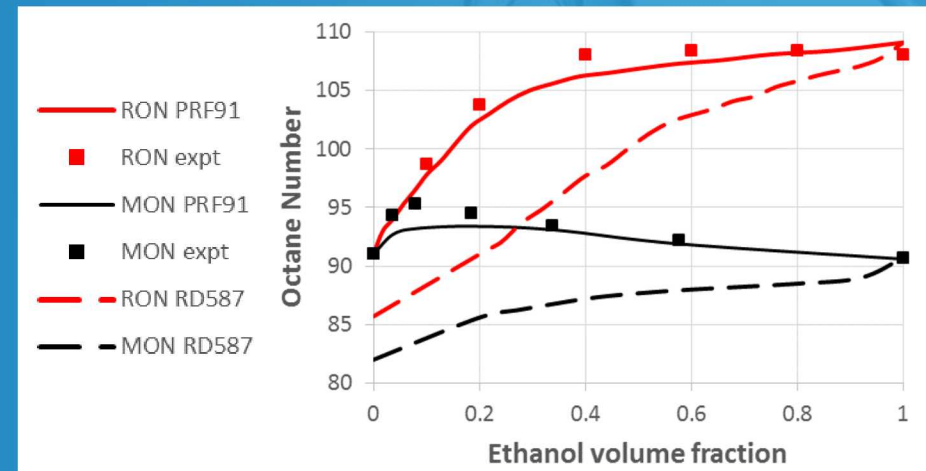
Collaborations (SNL)



- Funds-in knock project with Toyota.
- Explores effect of deviations from non-dilute stoichiometric operation.
- Knock limits change with ϕ .
 - Trends relate to RON-MON sensitivity.
- Insights complement Co-Optima studies of ultra-lean mixed-mode combustion.



- Collaborating with Westbrook (LLNL) & Cernansky (Drexel) on the use of detailed chemical-kinetics to predict RON and MON of alternative fuel blends.
 - Used RON- and MON-like DISI-engine data as input to CHEMKIN-PRO.



- Synergistic RON blending reproduced well.
- Non-monotonic MON trend for PRF91 fuel captured.
- Moving on to lean autoignition to support mixed-mode combustion.

Collaborations (SNL + ANL/ORNL)



SNL cont.

- Collaborating with Pitz, Mehl & Wagon at LLNL to validate surrogate-gasoline mechanisms.
- Identified various areas that required corrections, e.g.:
 - NO_x influence on autoignition.
 - Burn rate of trimethylbenzene.
- Corrected mechanism captures well DISI engine autoignition timings for both stoichiometric and lean conditions for Co-Optima Core fuels.



- CFD
 - Direct SNL on DISI activities
 - UConn (Prof. Lu) for chemical mechanism
 - Fuel properties for E30 SNL
 - ORNL engine (Sluder, Yue)
- ANL Multi-Mode
 - Ford
 - ORNL-multi-mode, SNL DISI
- ORNL Multi-Mode
 - ANL multi-mode
 - Sluder boosted SI task
 - Toolkit team – Edwards
 - Kinetics team (Pitz, Wagon et al.,)
 - Fuel properties team (Szybist/ Splitter)
 - Ford – support for engine modifications

AEC MOU & ACEC Interactions with industry for project updates and feedback (multiple times per year)
Co-Optima

- Collaboration across 9 NLS 2 DOE offices
- Eight universities
- Stakeholders (129 individuals from 77 organizations)

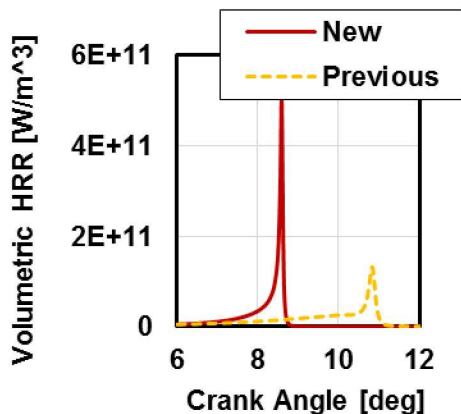


Fig 1. Comparison of predicted HRR of High Aromatic fuel under autoigniting condition

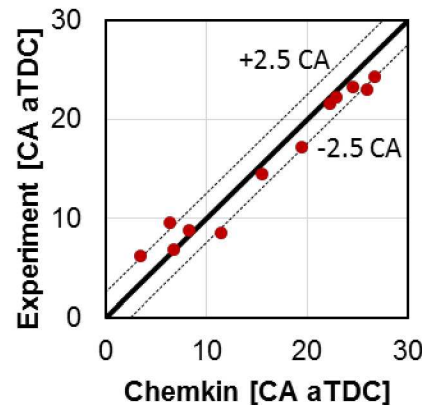


Fig 2. Comparison between measured and predicted autoignition timing



Reviewer Only Slides





SNL

- D. Vuilleumier and M. Sjöberg, “The Use of Transient Operation to Evaluate Fuel Effects on Knock Limits Well Beyond RON Conditions in Spark-Ignition Engines”, SAE paper 2017-01-2234, presented at SAE International Powertrains, Fuels and Lubricant meeting.
- M. Sjöberg and X. He, “Combined effects of intake flow and spark-plug location on flame development, combustion stability and end-gas autoignition for lean spark-ignition engine operation using E30 fuel”, IJER, Vol 19, Issue 1, pp. 86 – 95, January 2018.
- C.P. Ding, M. Sjöberg, D. Vuilleumier, D.L. Reuss, X. He, and B. Böhm, “Fuel-film thickness measurements using refractive index matching in a stratified-charge SI engine operated on E30 and alkylate fuels”, Exp Fluids (2018) 59: 59.
- 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", in press for Combustion and Flame.
- 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", accepted for presentation at Symposium on Combustion.
- 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”, submitted to SAE International Journal of Fuels and Lubricants.

ANL/SNL

- N. Van Dam, M. Sjöberg, and S. Som, “Large-eddy Simulations of Spray Variability Effects on Flow Variability in a Direct-injection Spark-ignition Engine Under Non-combusting Operating Conditions”, SAE Technical Paper 2018-01-0196, presented at SAE International World Congress Experience, April 2018.
- N. Van Dam, S. Som, W. Zeng and M. Sjöberg, “Parallel Multi-cycle Large-eddy Simulations of an Optical Pent-roof DISI Engine”, presented at ASME 2017 Internal Combustion Fall Technical Conference ICEF2017, Oct 2017, Paper # ICEF2017-3603.

ANL/SNL

- J. Drallmeier, S. Curran, M. Wissink, and R. Wagner, “Ignition Delay in Low Temperature Combustion”, SAE Technical Paper, SAE 2018-01-1125, 2018

Presentations



SNL:

- M. Sjöberg, "An Introduction to DOE's Co-Optima Initiative", International Wkshp on Fuel & Engine Interactions, China, Aug 2017.
- D. Vuilleumier and M. Sjöberg, "Assessment of Octane-Index Framework for Stoichiometric Knock Limits of Tier III Fuel Blends", AEC Program Review Meeting at USCAR, Aug 2017.
- M. Sjöberg and D. Vuilleumier, "The Use of Transient Operation to Evaluate Fuel Effects on Knock Limits Well Beyond RON Conditions in Spark-Ignition Engines", Co-Optima Stakeholders meeting, Oct 2017.
- M. Sjöberg, "Mitigation of Cycle-to-Cycle Combustion Variability to Enable Highly Efficient DISI Engines", 2017 VERIFI meeting.
- M. Sjöberg, D. Vuilleumier, N. Kim, D.L. Reuss, X. He and C. Ding, "Ability of PMI to Predict Soot Emissions from Lean Stratified-Charge and Well-Mixed Stoichiometric SI Operation using Alternative Fuels", AEC Program Review Meeting at ANL, Jan 2018.
- D. Vuilleumier, M. Sjöberg and N. Kim, "Applicability of the Octane-Index Framework for Stoichiometric and Lean End-gas Autoignition in a DISI Engine", AEC Program Review Meeting at ANL, Jan 2018.
- M. Sjöberg, D. Vuilleumier, D.L. Reuss, X. He, and C. Ding, "Combined Effects of Gasoline Composition and Operating Strategies on Soot-Production Pathways for Stratified-Charge SI Operation", presented at SAE World Congress Experience, April 2018.
- 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", presented at SAE International World Congress Experience, April 2018.

ANL

- N. Van Dam, P. Pal, Z. Yue and S. Som, "Overview of Co-Optima Engine CFD Simulations," Co-Optima Stakeholder Teleconference, July 2017.
- N. Van Dam, Zeng, W., M. Sjöberg, and S. Som, "Fuel Property GSA and Investigating Merit Function Terms with CFD", AEC Program Review Meeting at USCAR, Aug 2017.
- N. Van Dam, Z. Yue, P. Pal, and S. Som, "Simulations Enabling Co-Optimization of Engines and Fuels," CONVERGE User Conference North America, Dearborn, MI, Sep 2017.
- N. Van Dam, W. Zeng, M. Sjöberg, R. Scarcelli, S. Som, "Simulations of Flow, Spark and Combustion Variability in an Optically Accessible DISI Engine," VERIFI 3.0 Meeting at ANL, Nov 2017.
- N. Van Dam, M. Sjöberg, E. Boink, Z. Yue, S. Som, "Fuel Property Sensitivity Analysis for Input to the Merit Function," Co-Optima All-hands Lightning Round Presentation at ANL, Mar 2017.

ORNL

- S. Curran, "Addressing Barriers to LTC from an International Perspective" 38th Task Leaders Meeting in Baiona, Spain, 2017

Critical Assumptions and Issues



- **Multi-Mode – ORNL**

- Multi-mode strategy requires two step variable compression ratio mechanism. The limits of the compression ratios will be matched to what has been demonstrated by Nissan/ Infinity
- For more details - Kiga, S., et al., “The world’s first Production Variable Compression Ratio engine -The new Nissan VC-T (Variable Compression-Turbo) engine” Vienna Motor Symposium, 2017

- **Emissions compliance**

- Research in this presentation focused 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
- Co-optima collaborations across tasks are working to provide fundamental knowledge for this area

- **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.).