Co-Optimization of Fuels & Engines

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

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Project ID: FT055

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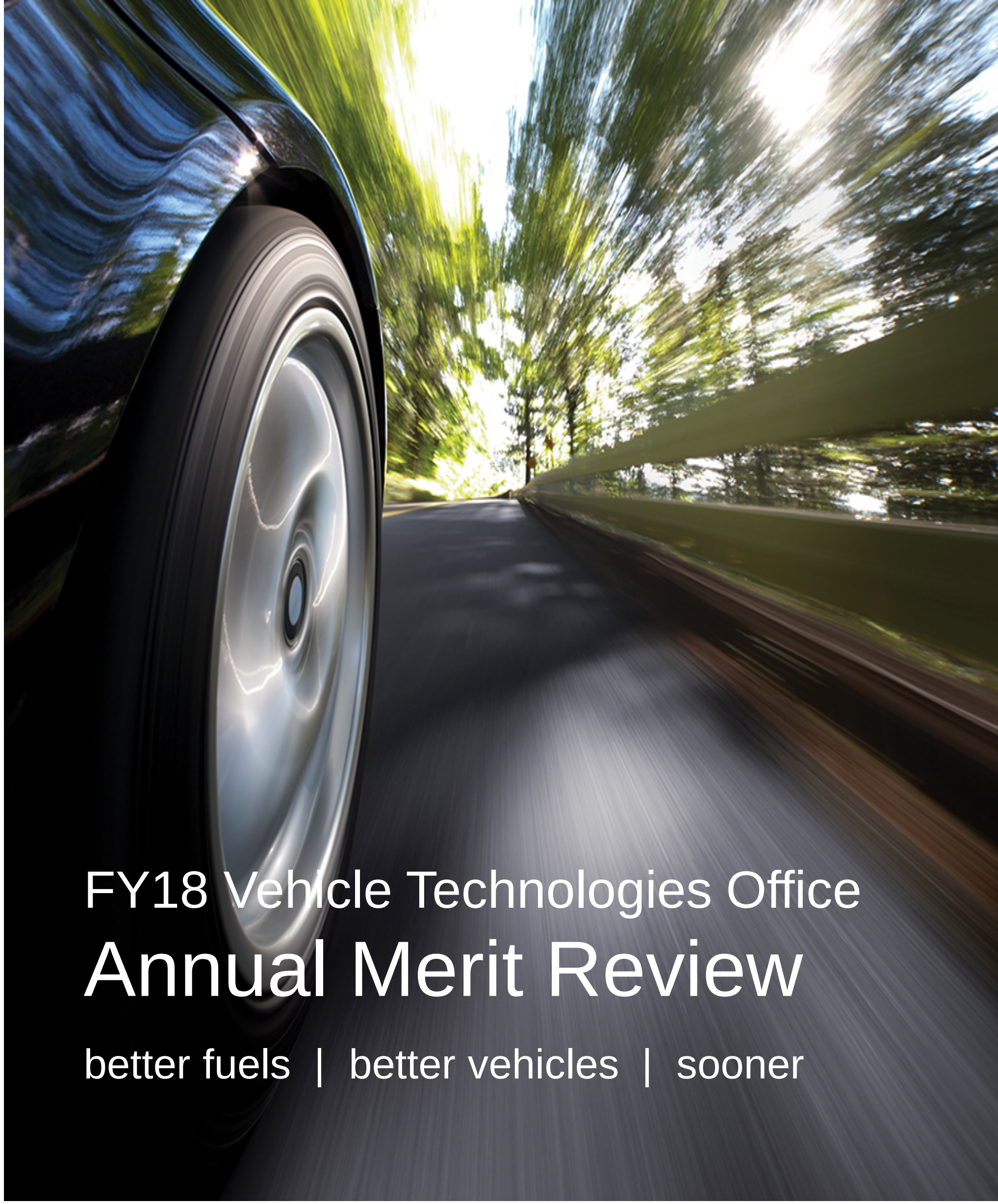


U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

VTO Program Managers: Gurpreet Singh, Kevin Stork, & Michael Weismiller

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			MM

* 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

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

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

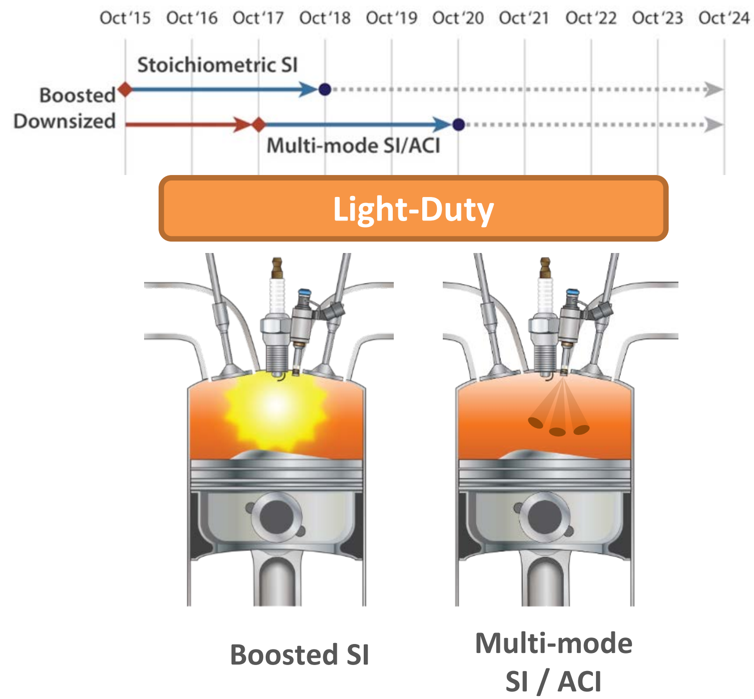
Partners

- 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*

**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

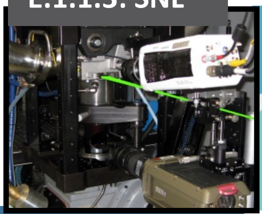
Milestones: Met or On Track

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

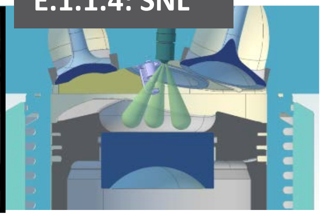
Overall Technical Approach: 5 tasks/ 3 labs + many collaborations

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

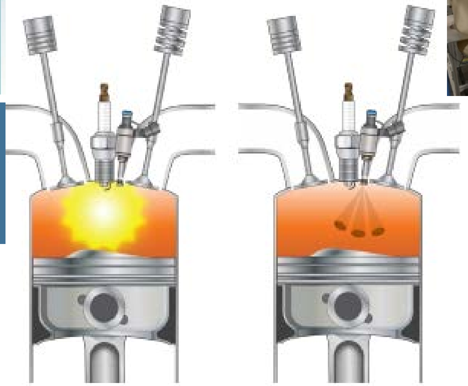
E.1.1.3: SNL



E.1.1.4: SNL



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



Boosted SI

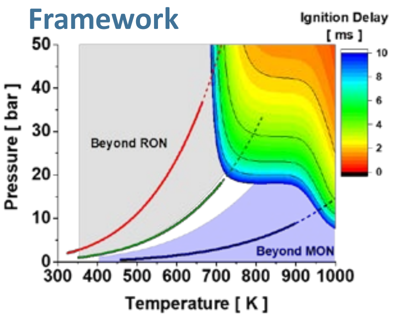
Multi-mode SI / ACI

E.1.2.6: ORNL

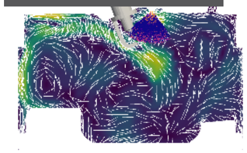
E.1.2.5: ANL

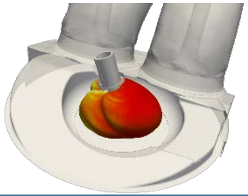
Multi-mode engine experiments to overcome technical barriers for achieving multi-mode goals

Temp-Press Trajectory Framework

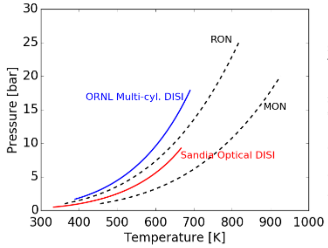


G.2.1: ANL

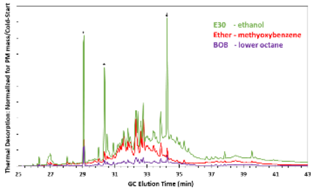




Collaborative Kinetics/ Toolkit tasks



Emissions Controls and Characterization Tasks



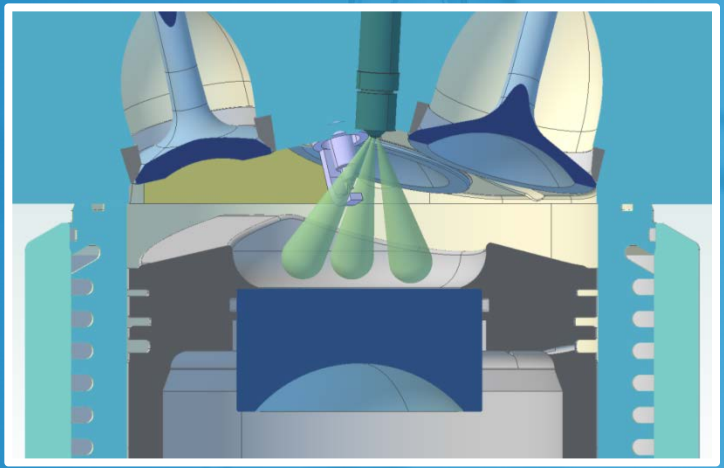
Enhance understanding and accelerate development through linked modeling efforts

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.

(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. 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.

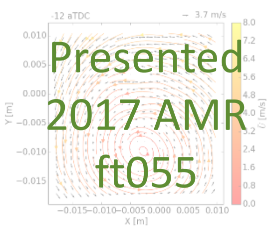
RIM = refractive index matching
PIV = particle image velocimetry
CR = compression ratio
IR = infrared

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



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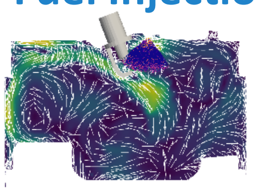
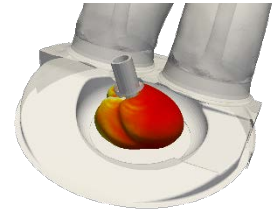
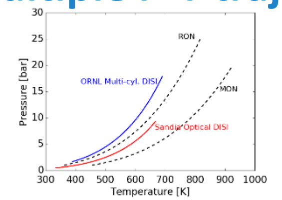
Motored with Fuel Injection



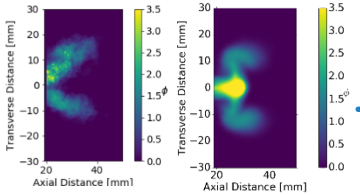
Combustion



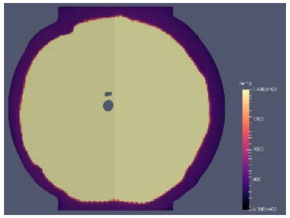
Multiple Conditions
Multiple P-T trajectories



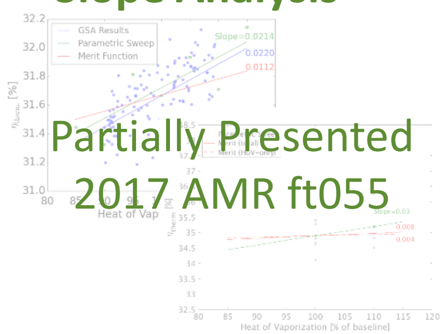
Spray Validation



Thermal Stratification



Merit Function Slope Analysis



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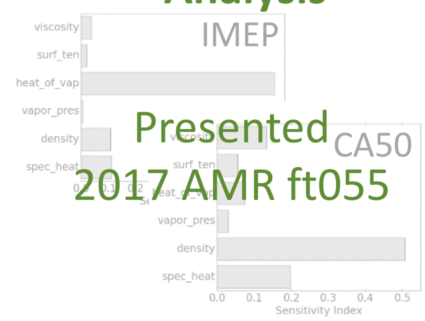
Global Sensitivity Analysis



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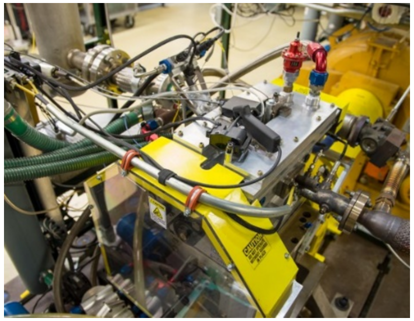
Approach – Multi-Mode Projects: 2 - Metal single-cyl. SI base engines (ANL/ORNL)

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

Utilize Co-Optima Core fuels and custom blends as needed

Technical Accomplishments Summary

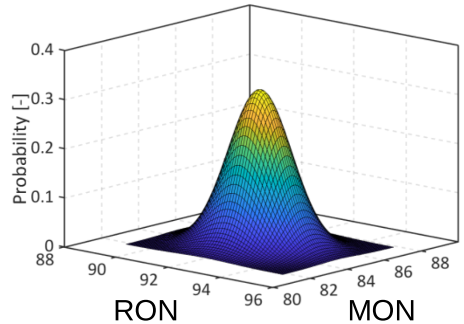
- **DISI @ SNL**
- Finished knock tests for a total of 9 fuels.
- Used uncertainty modeling to assess applicability of Octane-Index framework. Identified outliers like 2-butanol.
- Assessed relevance of PMI for 9 fuels across 3 well-mixed and 2 stratified operating strategies.
- Identified that alcohols 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

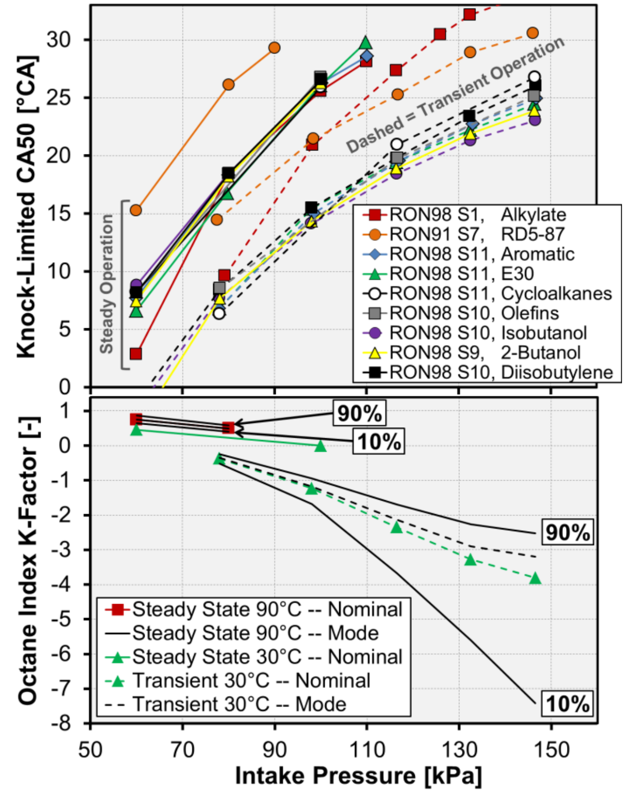
- **Multi-Mode @ ANL and ORNL**
- Minimum temperature allowing stable low load HCCI combustion (ANL)
- Maximum temperature still allowing knock-free high load SI combustion (ANL)
- ΔT metric for low load ACI and High load SI (ANL)
- Exploration of effect of multi-mode constraints and impact of range/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

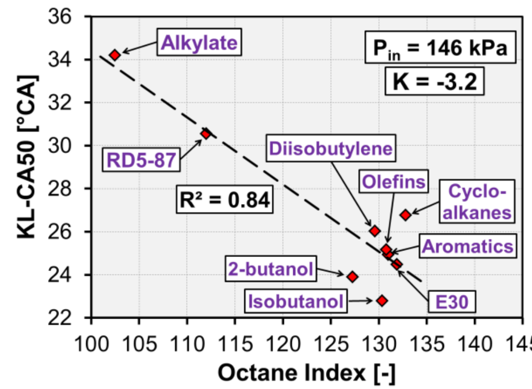
Stoichiometric Knock Limits for 9 Fuels

- 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.

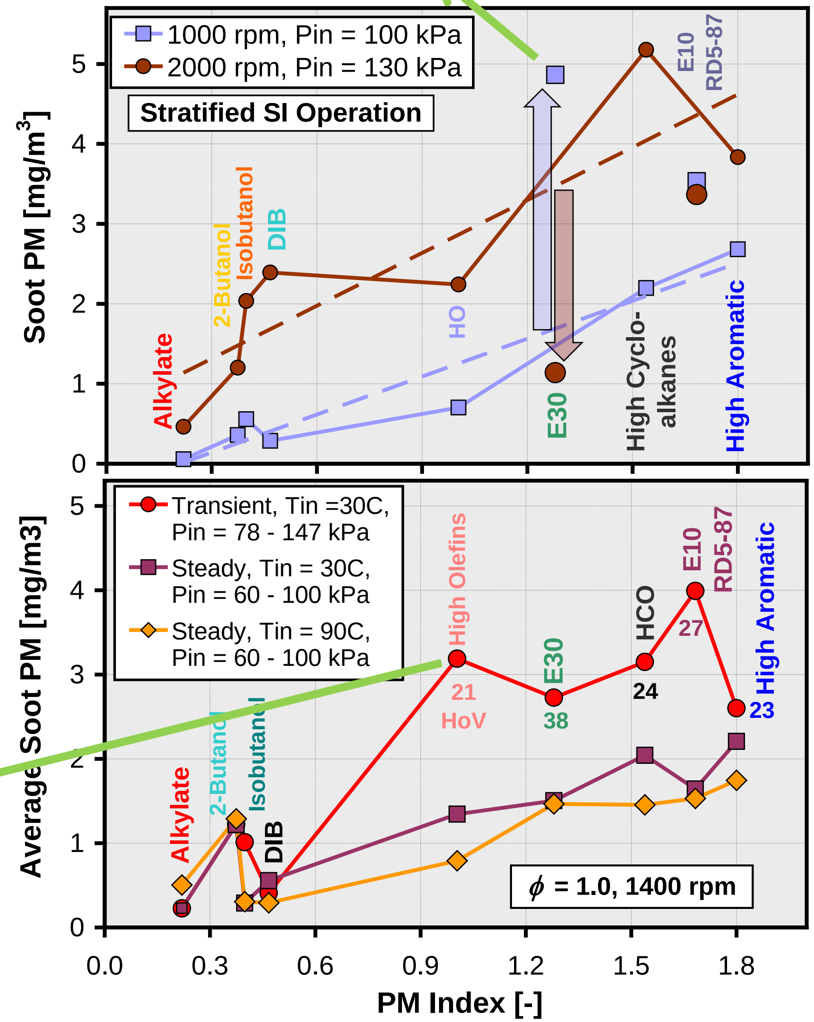




Assessment of PMI for Various Modes of Operation

- 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.

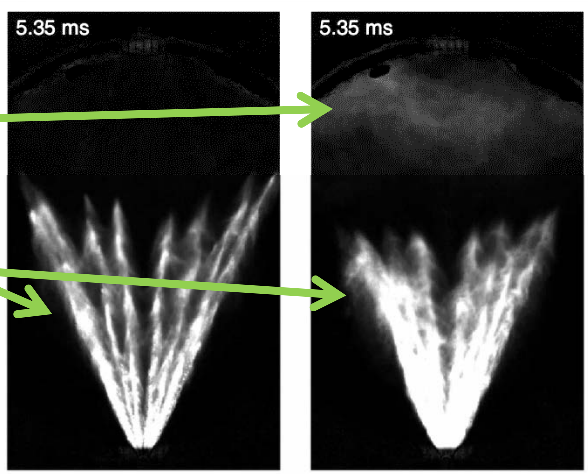
Pool fires for non-boosted operation.



DIB Blend **High-Olefin**

Lingering fuel from 2nd injection

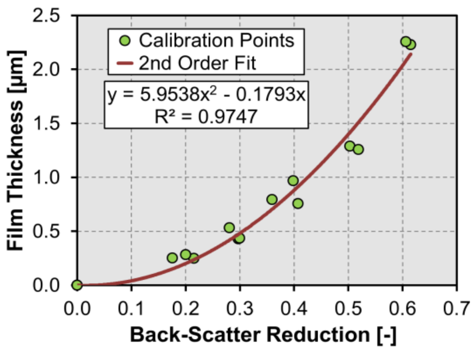
3rd injection



SNL Collaboration with Skeen *et al.*

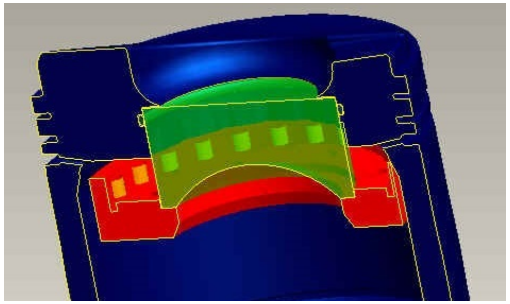
Development and Use of Wall-Wetting Diagnostics

- 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.

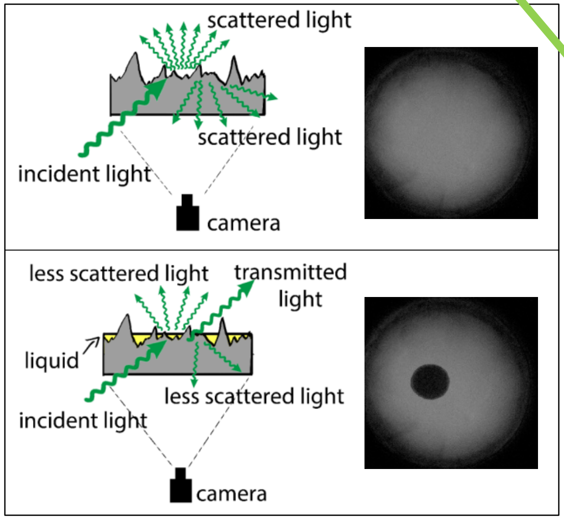


- Applied diagnostics to wide ranges of operating conditions, supporting interpretation of PMI efficacy and soot-production pathways.
  - Increased P_{in} strongly reduces wall wetting for E30.
  - Reduction of $T_{coolant}$ strongly increases **wall wetting** and **smoke** for E30.
- RIM will be applied for cold-start testing, as outlined by ACEC Tech Team.

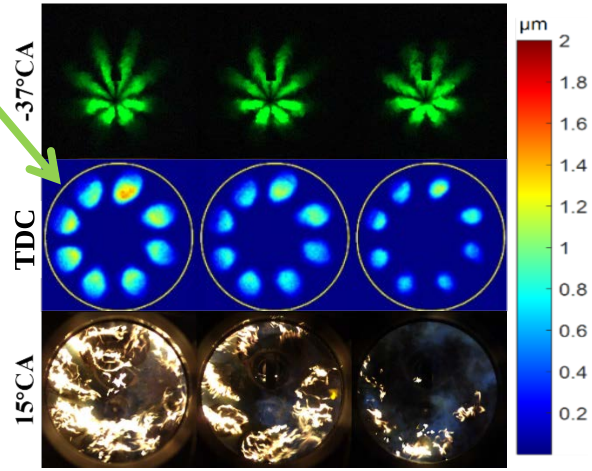
Side-based LED



Cross section of piston



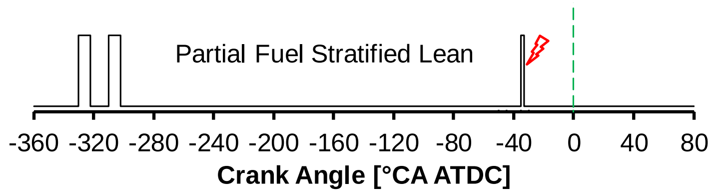
$T_{coolant}$ =	45	60	90	°C
Smoke =	1.14	0.69	0.068	FSN

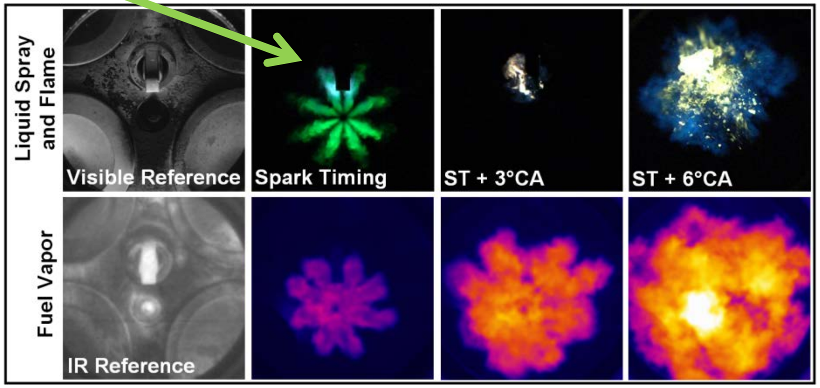


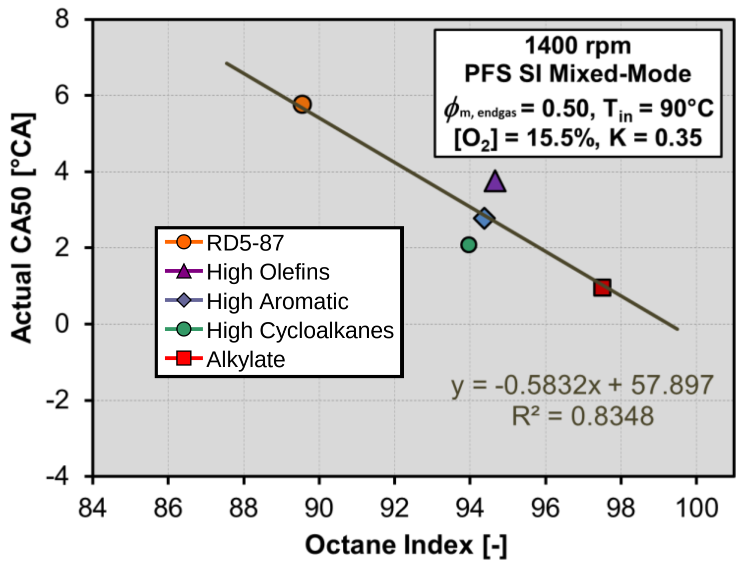
Illustrations by X. He, Beijing Institute of Technology.

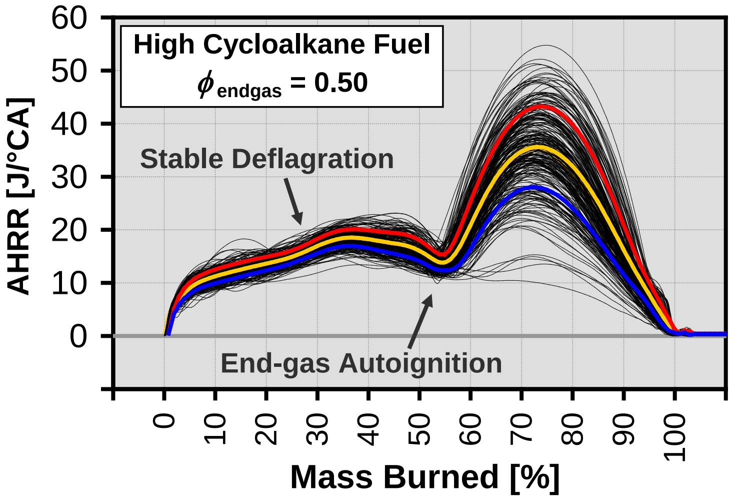
Mixed-mode Combustion for 5 Fuels

- 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 CA10-90 < 30°CA ⇒ 20% rel. eff. gain.
- Acquired data for ranges of ϕ, P_{in}, T_{in} and $[O_2]$.
- Octane-index ranking holds to first order.





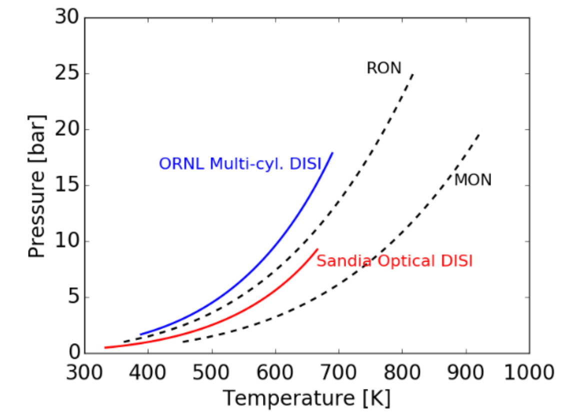


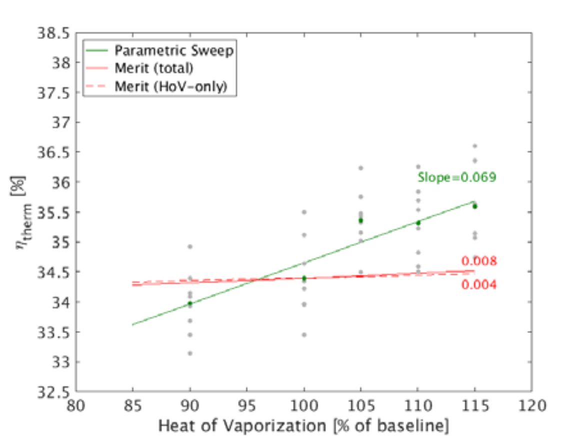


ANL: Advanced modeling efforts to enhance understanding and accelerate development

Expanding Merit Function analysis to new engines/operating points

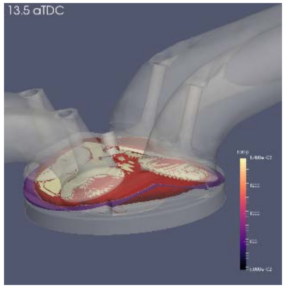
- ORNL multi-cylinder engine (see SI Combustion part I For more results)
- Knock-limited mid-load point

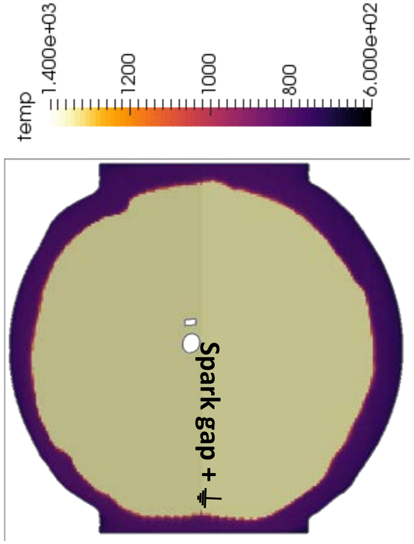


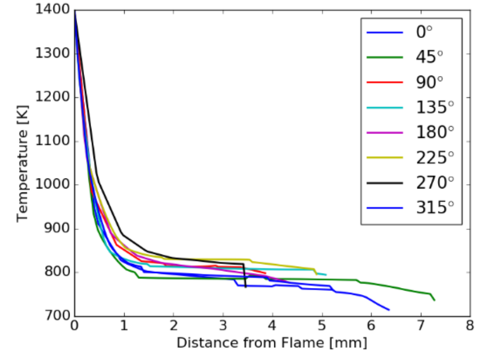


Thermal stratification can result in sequential auto-ignition

- Process relevant to both knock and SACI
- Providing information to more accurately model Sandia DISI engine with low-dimensional tools
  - o FT052: Fuel Kinetics & Simulation - for details





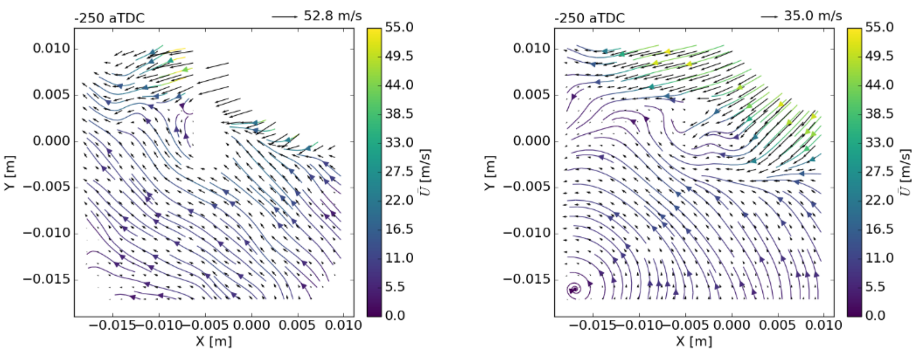


Temperature in the end-gas at CA50 - Sandia DISI engine Two planes approximately parallel to the pent-roof and through the center of the propagating flame.

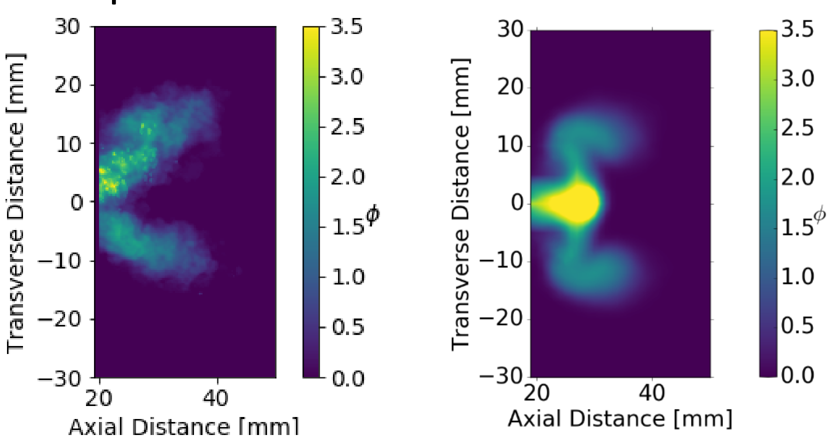
ANL DISI results: Furthering understanding of flow and mixing details

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**

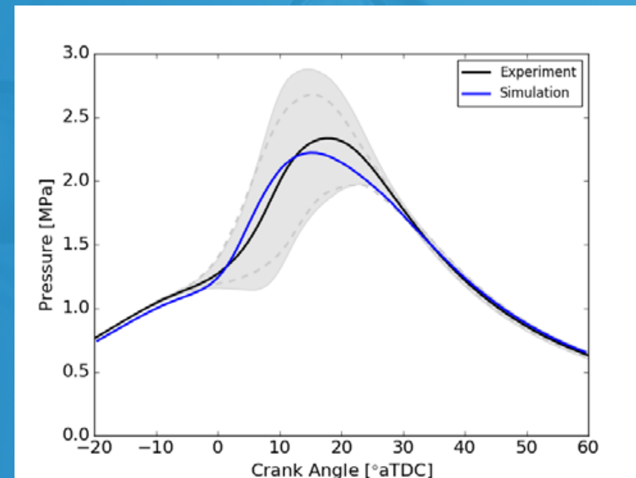


Experiment | Simulation



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**

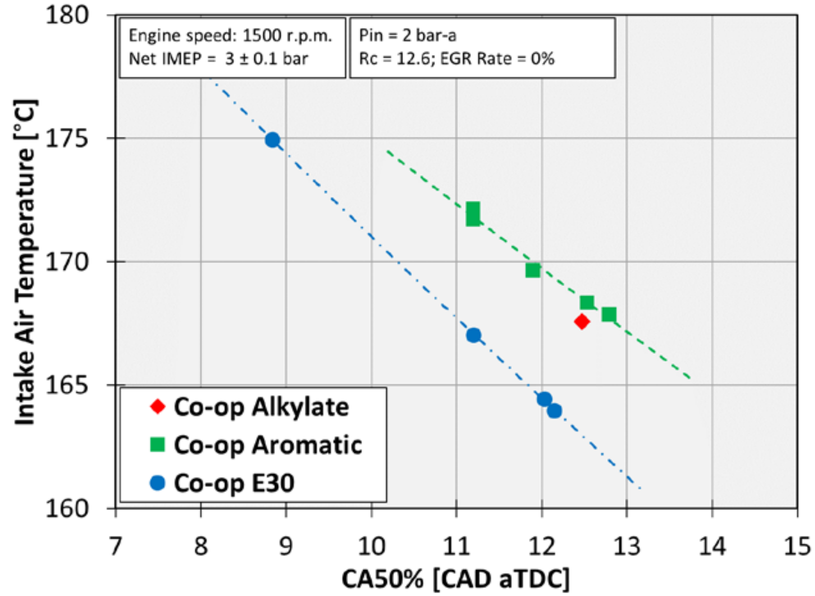


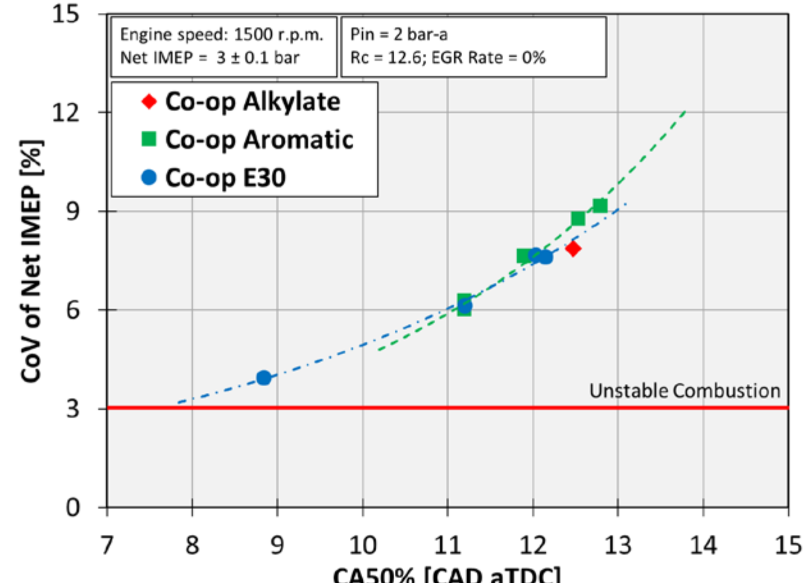
	Experiment	Simulation
CA10	3.4°	3.5°
CA50	11.9°	14.0°
CA90	23.7°	35.9°

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

Minimum temperature allowing stable low load HCCI combustion

- Preliminary results of testing with three co-optima core fuels show a weak corelation 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





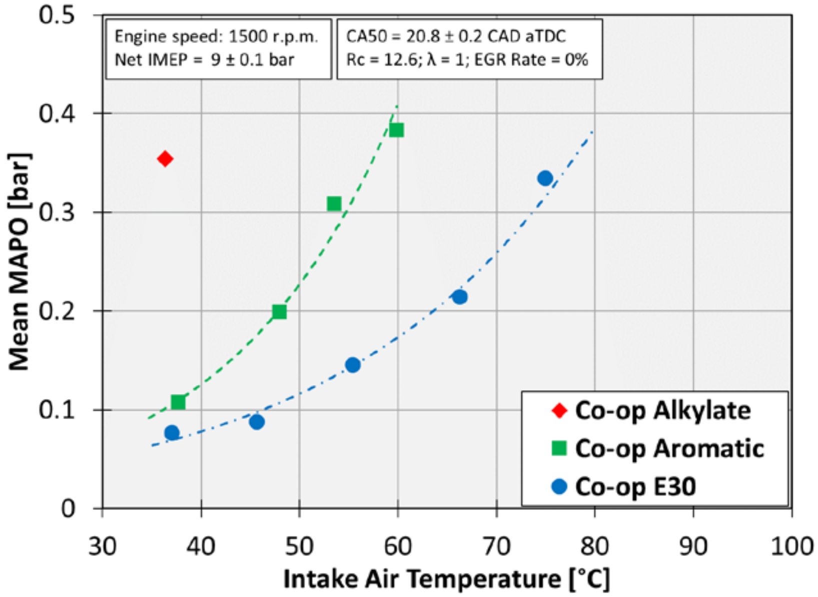
ANL: Fuel Properties which Enhance Mixed-Mode ACI/SI Engine Operation

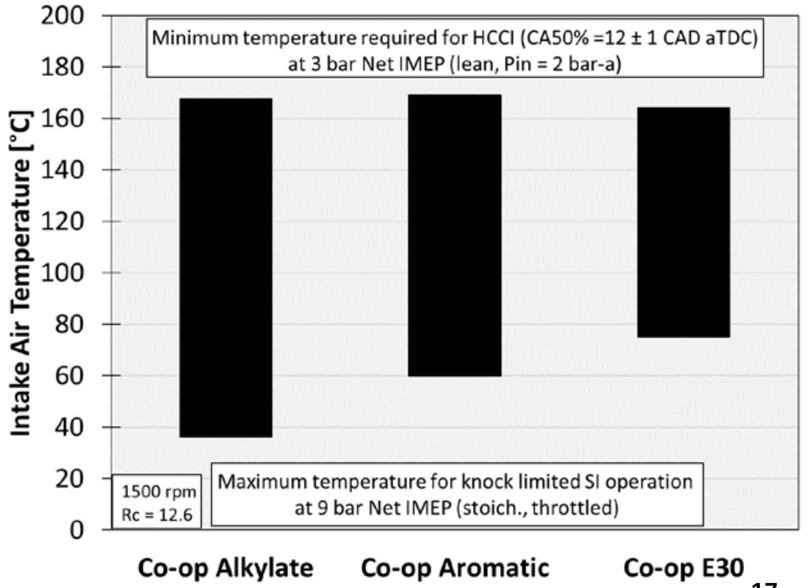
<u>Maximum temperature still allowing knock-free high load SI combustion</u>

- 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)

<u>ΔT metric for low load ACI and High load SI</u>

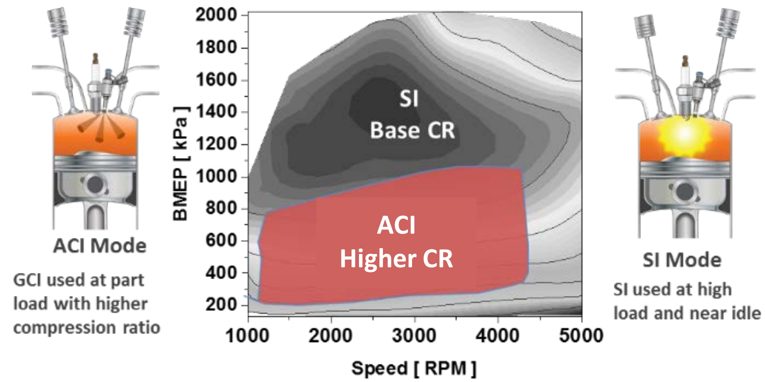
- Alkylate fuel showed maximum ΔT requirement of 130 °C
- Observed relationship between octane sensitivity and ΔT requirements suggests that in-cylinder P-T conditions are not high enough to capture fuel sensitivity effect at low load HCCI operation



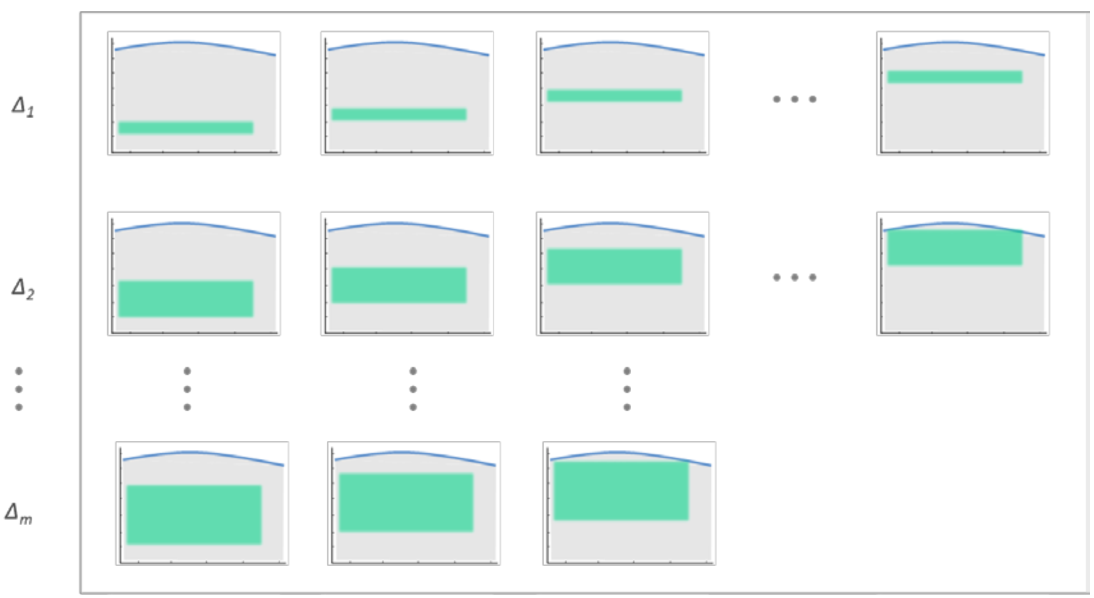


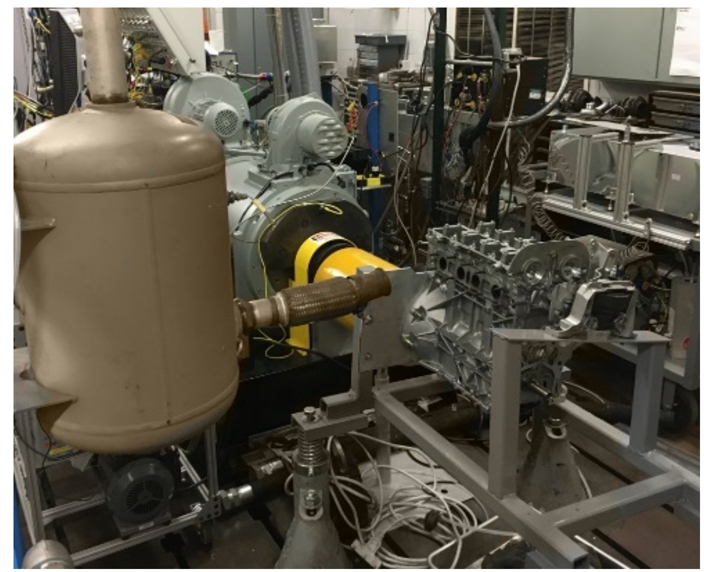
ORNL Multi-Mode SI-ACI

- 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



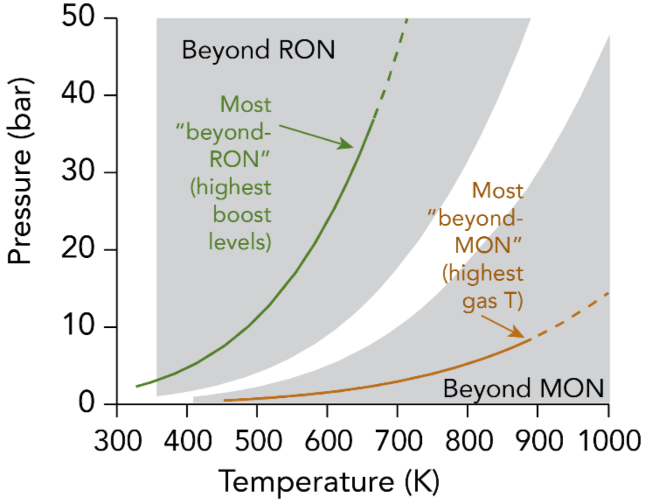


Links to boosted SI (Sluder) and previous multi-mode R&D provides insights into constraints needed for realistic results

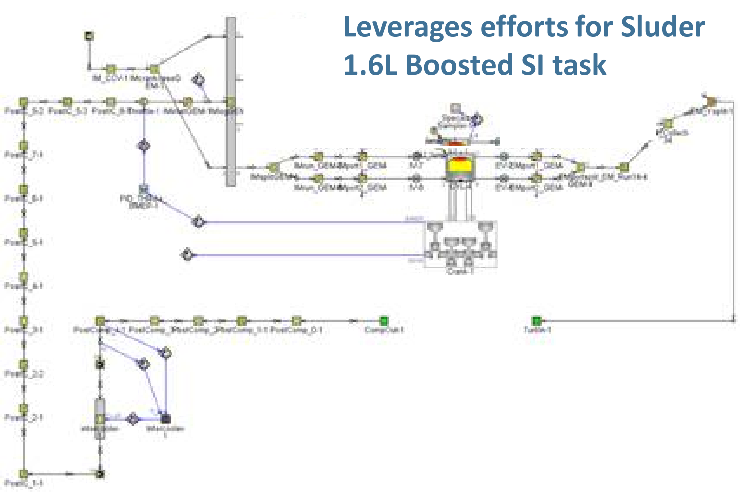
ORNL: Accelerating development with Tool-Kit and Fuel Properties team

- **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

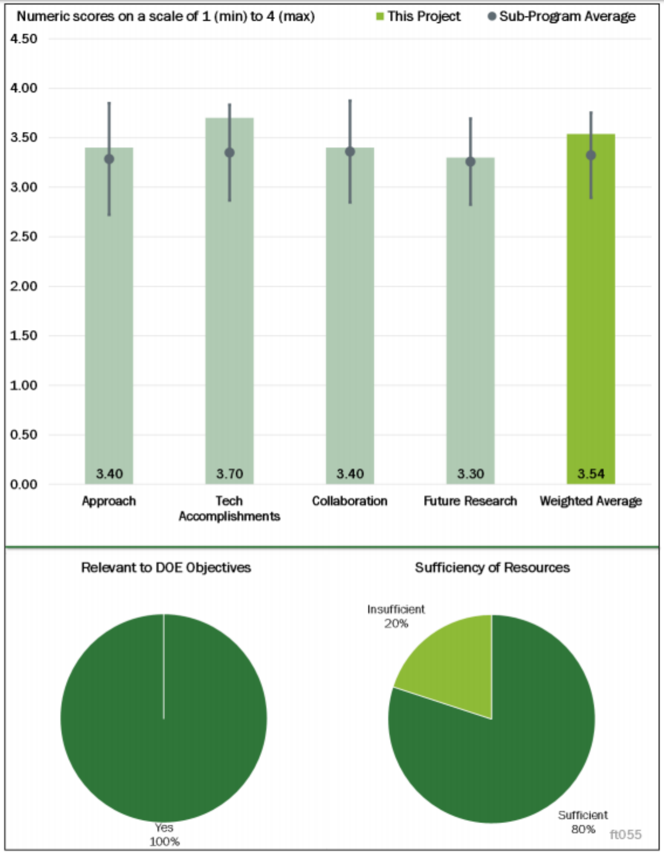


Figure 5-13 – Presentation Number: ft055 Presentation Title: Co-Optimization of Fuels and Engines (Co-Optima)—Multimode Lean Spark Ignition: Experiments and Simulation Principal Investigator: Magnus Sjoberg (Sandia National Laboratories)

Scores and comments from 2017 Annual Merit Review Report| https://www.energy.gov/sites/prod/files/2017/11/f39/05%20-%20Fuel%20and%20Lubricant%20Technologies.pdf

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
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 mechnisim
- 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

Remaining Challenges and Barriers

- 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

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

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

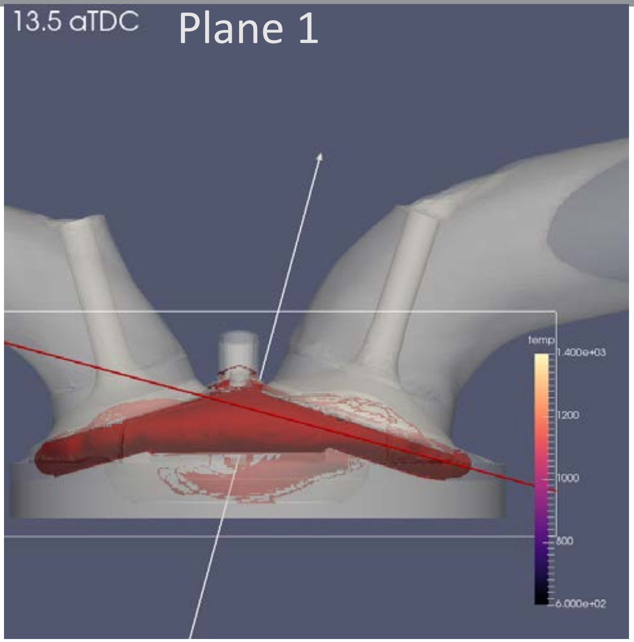
Fuel	Alkylate	E30	Aromatic
RON (-)	98.0	97.4	98.1
MON (-)	96.6	86.6	87.8
Sensitivity (-)	1.4	10.8	10.3
HoV (kJ/kg)	309	536	363
A/F_{st}	15.1:1	12.9:1	14.5:1
Paraffin (%vol)	3.0	12.9	8.2
I-Paraffin (%vol)	95.8	27.6	38
Aromatics (%vol)	0.7	13.8	39.8
Naphthenes (%vol)	0.02	7.0	8.0
Olefins (%vol)	0.08	5.6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

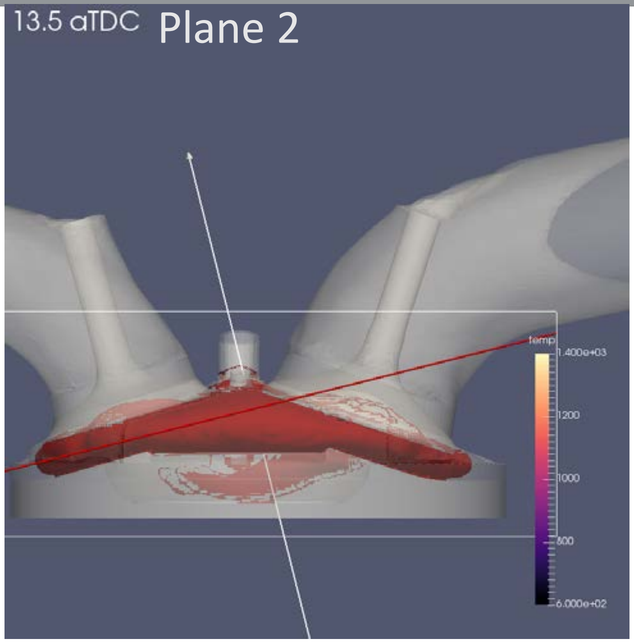
Test Conditions

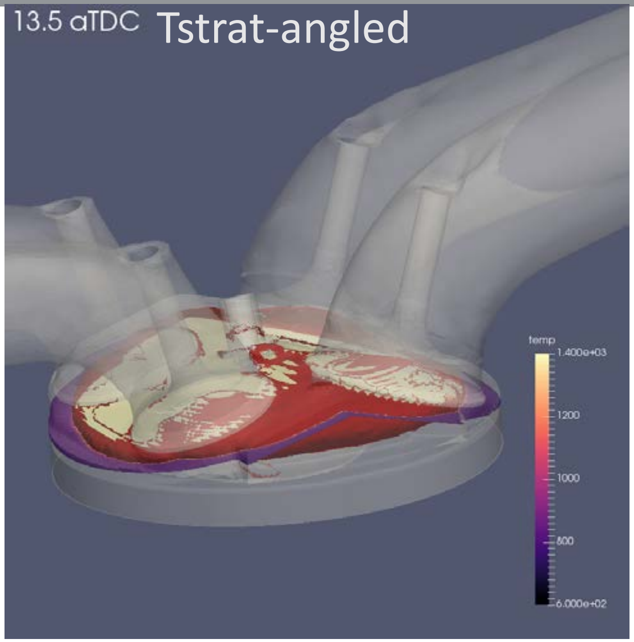
Condition	ACI	SI
NMEP (bar)	3	9
Speed (RPM)	1500	1500
EGR (%)	0	0
CA50 (°aTDC)	8	20.8
DI SOI (°bTDC)	300	
DI P_{inj} (bar)	150	
CoV of IMEP (%)	3	
MAPO* Limit (bar)	0.35	

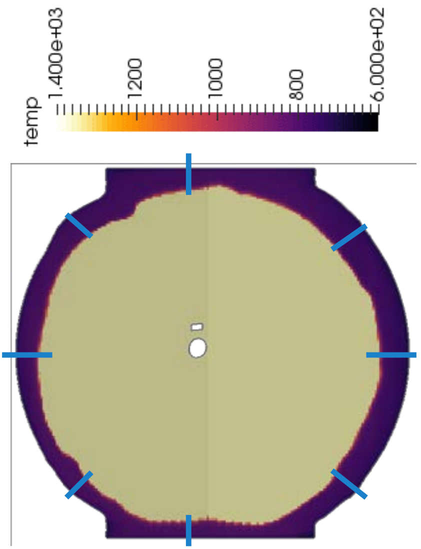
*Maximum Amplitude of Pressure Oscillations (MAPO)

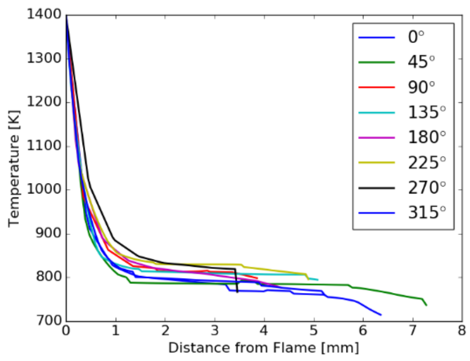
ANL CFD











- 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

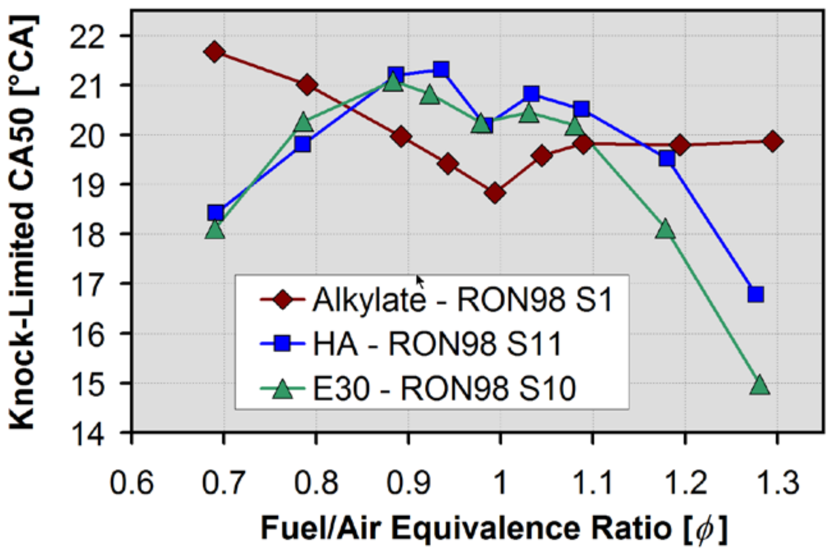
SNL - Fuel Properties Table

- 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.

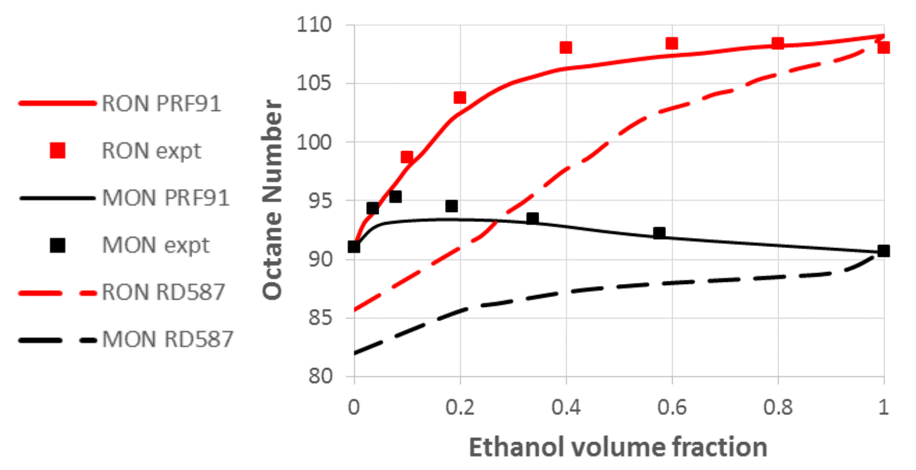
		Co-Optima Core Fuels							
	E10 RD5-87	Alkylate	E30	High Aromatic	High Olefin	High Cycloalkane	Isobutanol Blend	2-Butanol Blend	Diisobutyl-ene Blend
RON	90.6	98.0	97.9	98.1	98.3	97.8	98.1	98.2	98.3
MON	83.9	96.7	87.1	87.6	87.9	86.9	88.0	89.1	88.5
Octane Sensitivity	6.7	1.3	10.8	10.5	10.4	11.0	10.1	9.1	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

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 & Wagnon 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.

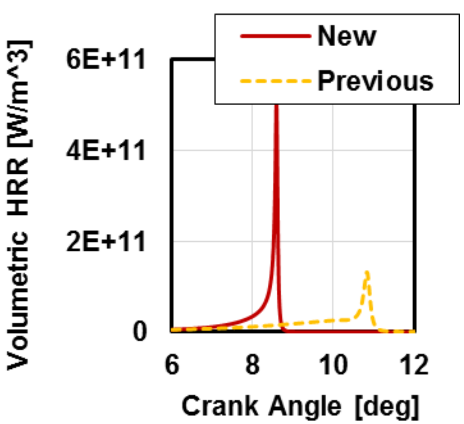


Fig 1. Comparison of predicted HRR of High Aromatic fuel under autoigniting condition

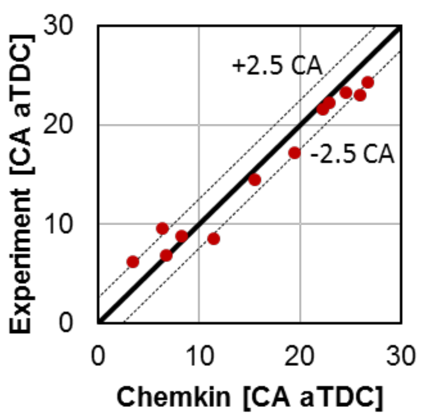


Fig 2. Comparison between measured and predicted autoignition timing

- 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, Wagnon 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)

Co-Optimization of Fuels & Engines