Co-Optimization of
Fuels & Engines

MM/ACI Combustion Part II (FT071)

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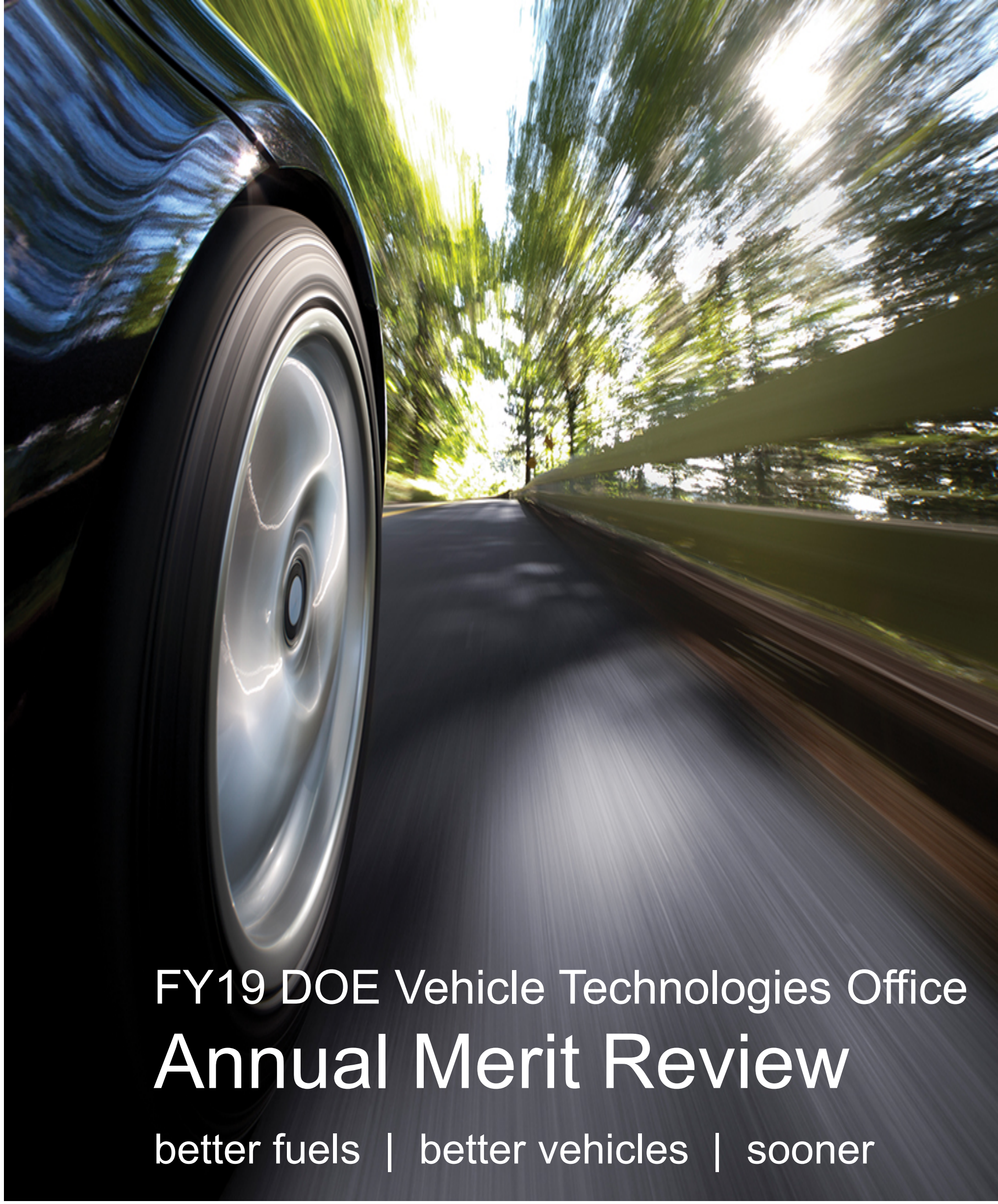
Project # FT071

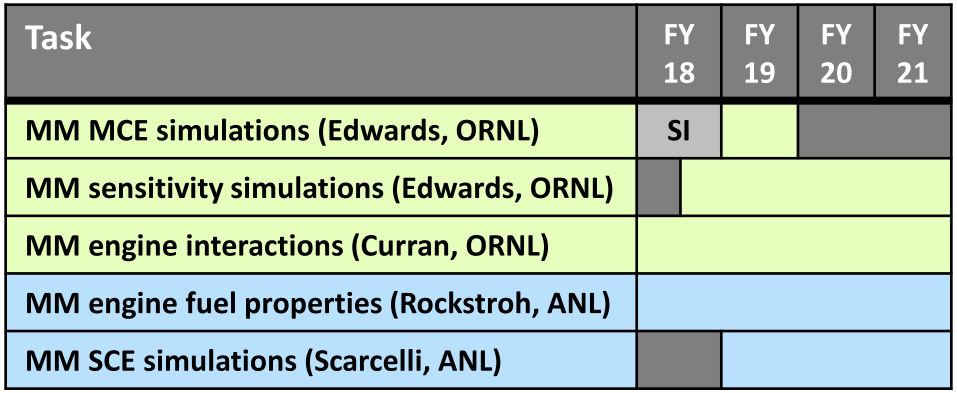


FY19 DOE Vehicle Technologies Office
Annual Merit Review
better fuels | better vehicles | sooner

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

Overview

Timeline



Task	FY 18	FY 19	FY 20	FY 21
MM MCE simulations (Edwards, ORNL)	SI	🟩	⬛	⬛
MM sensitivity simulations (Edwards, ORNL)	⬛🟩	🟩	🟩	🟩
MM engine interactions (Curran, ORNL)	🟩	🟩	🟩	🟩
MM engine fuel properties (Rockstroh, ANL)	🟦	🟦	🟦	🟦
MM SCE simulations (Scarcelli, ANL)	⬛	🟦	🟦	🟦

Barriers

- 2020/2025 Stretch Efficiency Goals for downsized boosted engines
- Determine the factors limiting range of LTC and develop methods for extending the limits
- Understanding impact of likely future fuels on LTC

Budget

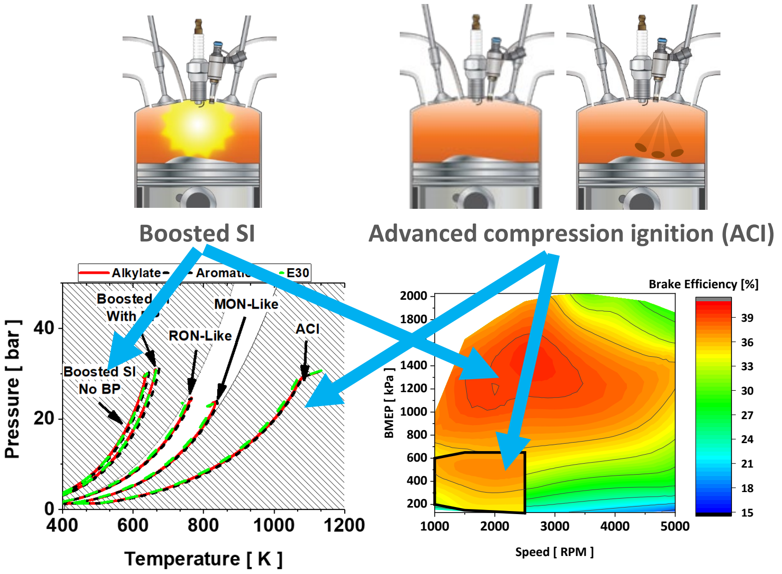
	FY2018	FY2019
MM MCE simulations	**($90k SI)**	**$100k**
MM sensitivity simulations	**$75k**	**$200k**
MM engine interactions	**$325k**	**$222k**
MM engine fuel properties	**$315k**	**$245k**
MM SCE simulations		**$175k**

Partners

- Co-Optima program includes research funded by 2 DOE Offices at 9 National Laboratories, 20+ universities, and 1 OEM with insight from external advisory board and 80+ stakeholders
- Task specific collaborations include…
  - Other National Laboratories (e.g., LLNL)
  - Universities (e.g., UConn)
  - Industry stakeholders (GM, Ford)
  - Software vendors (Convergent Science)

Overview of Multi-Mode Tasks

Multi-Mode (MM) operation

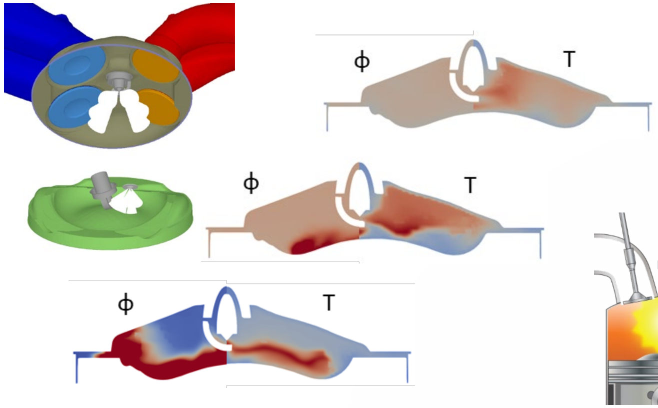


Boosted SI

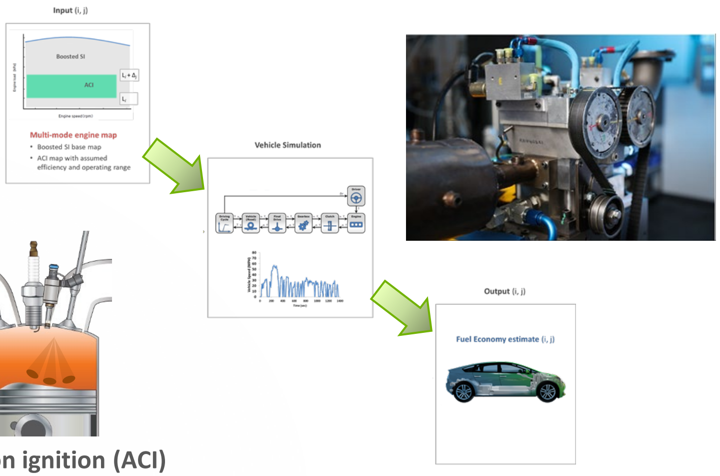
Advanced compression ignition (ACI)

Overview of Multi-Mode Tasks

MM sensitivity simulations (PI: Edwards, ORNL)



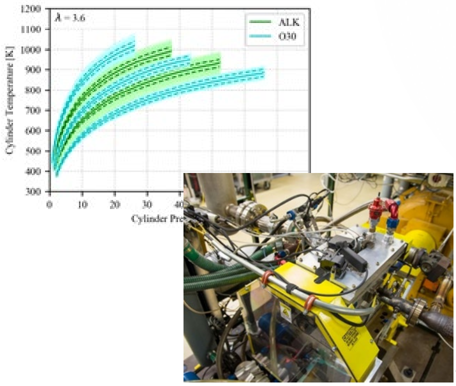
MM engine interactions (PI: Curran, ORNL)

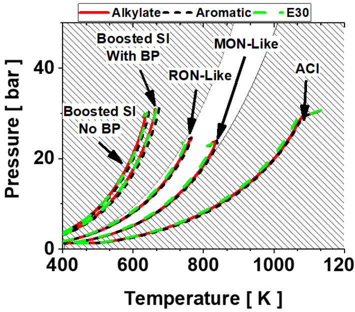


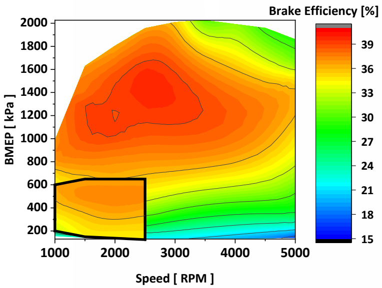
Multi-mode engine map

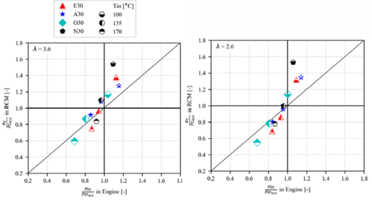
- Boosted SI base map
- ACI map with assumed efficiency and operating range

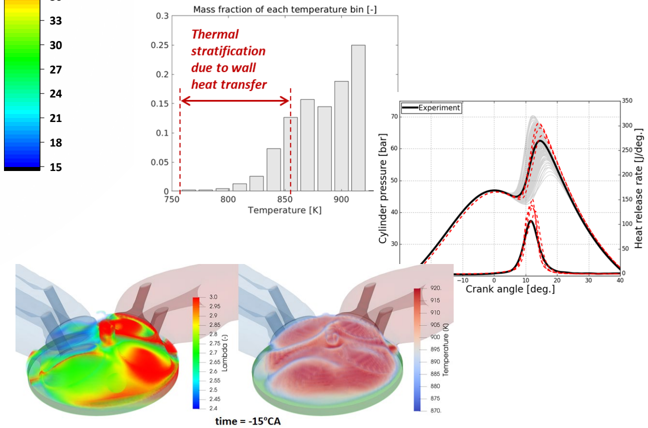
Boosted SI **Advanced compression ignition (ACI)**











time = -15°CA

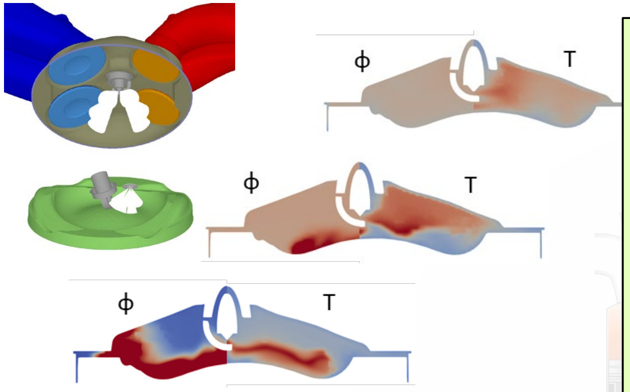
MM engine fuel properties (PI: Rockstroh, ANL)

MM SCE simulations (PI: Scarcelli, ANL)

Task *Relevance* and *Approach*

MM sensitivity simulations (PI: Edwards, ORNL)

MM engine interactions (PI: Curran, ORNL)



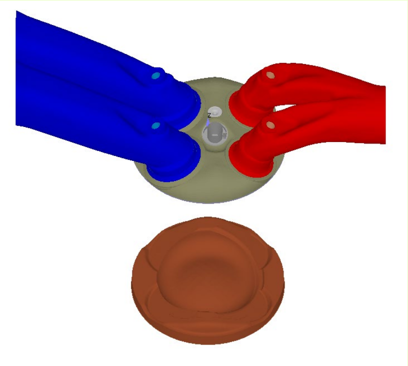
Objectives

- Develop flexible CFD engine models that capture *global trends* across *full ACI spectrum* and transitional spaces between modes
- *Explore sensitivity to fuel properties and engine parameters*
- Provide timely guidance and direction to experimental efforts and targeted simulation efforts

What is possible with ACI in an engine optimized for boosted SI?

Approach

- CFD engine model to fully explore ACI parameter space
  - Intake preparation: P-T-ϕ-EGR%
  - Charge stratification: HCCI –> PPCI –> MCCI
  - Engine geometry: variable CR
  - Fuel properties
- Engine architecture suitable for boosted SI operation
  - Maintain SI piston shapes and injector
  - High-RON, high-sensitivity fuels
- Simulations to explore global sensitivity of ACI performance



MM engine fuel properties (PI: Rockstroh, ANL)

MM SCE simulations (PI: Scarcelli, ANL)

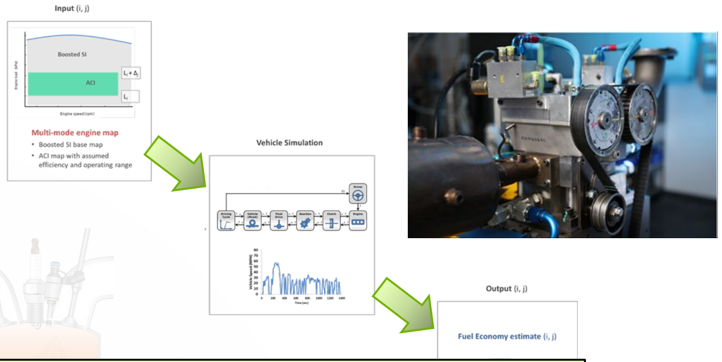
Task *Relevance* and *Approach*

MM sensitivity simulations (PI: Edwards, ORNL)

Objectives

- Characterize potential fuel-consumption benefits of various MM ACI modes for state-of-the-art SI engines
- Determine which fuel properties enable larger load ranges to maximize fuel-consumption improvements with MM operational constraints

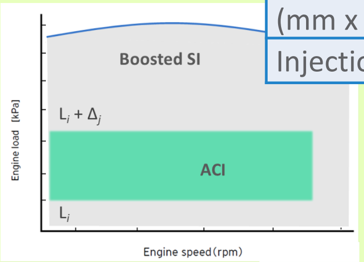
MM engine interactions (PI: Curran, ORNL)



Approach

- Metal engine experiments
  - GM SCE (SG2 head)* well-suited for MM
  - Advanced cam authority and ignition system
    - Trapped residuals, partial fuel stratification
- Better identify bookend P-T trajectories for ACI and opportunities with core fuels and custom blends
- Boundary-limit MM study across range of fuels
- Fuel economy estimates
  - Vehicle system simulation tools (Autonomie and Matlab Powertrain Blockset)
  - Study impact of ACI location and load range on estimated fuel economy

CR (-) - base	12.1:1
Disp. (L)	0.55
Bore x Stroke (mm x mm)	86 x 94.6
Injection	DI (central)



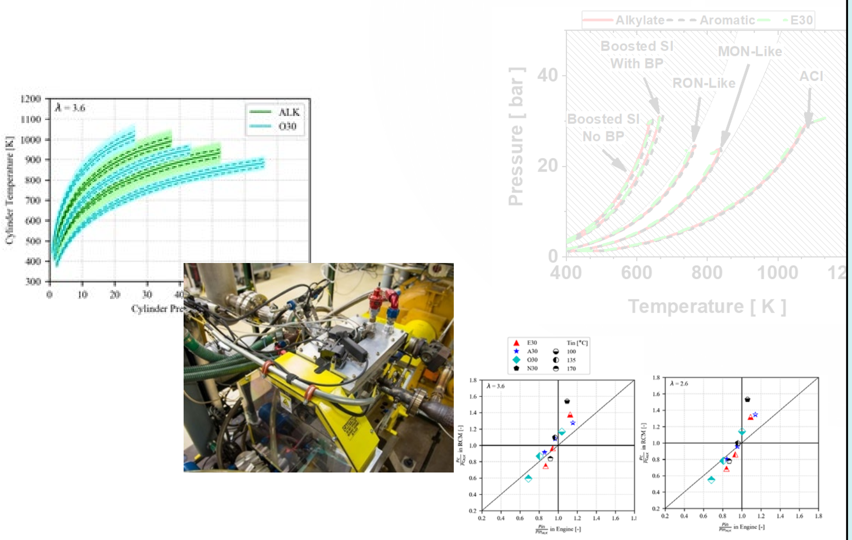
* Platform changed from 2018 - Ford 1.6L to GM SG2 (similar to optical SCE of Sjöberg at SNL)

lli, ANL)

Task *Relevance* and *Approach*

Objectives

- Characterize effects of octane sensitivity and fuel chemistry on MM operation in a light-duty SI engine
- Utilize engine compressed gas conditions and fundamental autoignition delay trajectory (P-T framework) to characterize the engine control parameters
- Identify constraints due to engine hardware and fuel properties



MM engine fuel properties (PI: Rockstroh, ANL)

Approach

- Low-load ACI experiments on a single-cylinder GDI engine with Co-Optima core fuels
  - Compression ratio (CR) of 15.3
  - Fixed combustion phasing of 12 dATDC
  - Sweep intake air temperature at two fuel loadings
  - No EGR
  - Intake boost pressure to control combustion phasing
  - Correlate ignition delay data at engine-relevant conditions from RCM experiments and chemical kinetic modeling (ANL – Goldsborough) to the engine cylinder / intake manifold conditions
- Three-level factorial experimental design
  - Establish geometric CR trade-offs between ACI and high-load SI
  - Assess fuel sensitivity to engine control parameters
    - RPM, intake T, boost P, EGR%, ϕ, SOI
- Establish mathematical correlations and generate an ACI operating map for each fuel

ANL Single-Cylinder Engine Geometry:

CR (-)	10.7 – 15.3:1*
Disp. (L)	0.63
Bore x Stroke (mm x mm)	89.04 x 100.6
Injection	PFI or DI (central)

*Fixed compression ratio (CR)

Task *Relevance* and *Approach*

MM sensitivity simulations (PI: Edwards, ORNL)

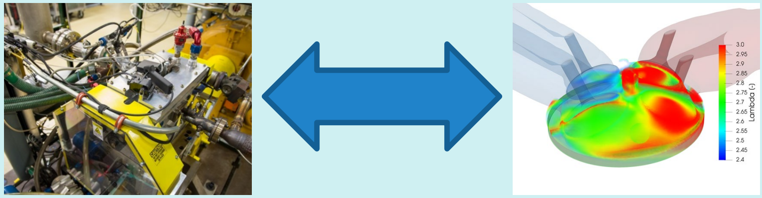
MM engine interactions (PI: Curran, ORNL)

Objectives

- Simulate MM ACI operation in a GDI engine platform
- Investigate impact of fuel properties on ACI and MM operation
- Use the validated numerical methodology to study the transition between ACI and SI modes and optimize MM operation

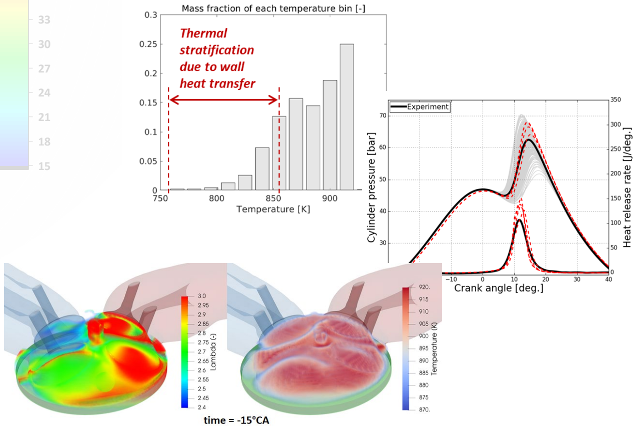
Approach

- MM CFD simulations of ANL single-cylinder engine (PI: Rockstroh)
  - Compression ratio of 15.3
  - 1500 RPM
  - Operating parameter sweeps:
    - Intake T, λ, load
  - Experimental data for validation



- Simulation efforts using Co-Optima core fuels
  - Initial validation and investigation with Alkylate core fuel
  - Extendi to other core fuels (E30, O30, A30, N30)
    - Dependent on availability of reduced mechanisms

MM engine fuel properties (PI: Rockstroh, ANL)



MM SCE simulations (PI: Scarcelli, ANL)

Milestones

Date	Lab, PI	Milestone	Status
FY2018 – Q4	ANL, Rockstroh	Evaluate relationship between fuel RON-MON sensitivity and temperature delta for ACI and SI	**MET**
FY2018 – Q4	ORNL, Curran	Make recommendation on viability of multi-mode strategy and report on potential for fuel economy	**MET**
FY2019 – Q2	ANL, Rockstroh	Preliminary evaluation of fuel autoignition characteristics on low load ACI engine operation and high load SI performance on a multi-mode SI-based engine architecture	**MET**
FY2019 – Q2	ANL, Scarcelli	Validate GDI engine simulations under multi-mode operation (ACI)	**MET**
FY2019 – Q3	ORNL, Edwards	Use LD CFD model to evaluate impact of fuel and operational parameters on MM strategies	**On track**
FY2019 – Q3	ANL, Scarcelli	Identify key fuel/engine effects on ACI combustion	**On track**
FY2019 – Q4	ORNL, Curran	Complete boundary-limit MM study across range of fuels	**On track**
FY2019 – Q4	ANL, Rockstroh	Identify fuel autoignition performance parameters to enable SI/ACI multi-mode operation	**On track**
FY2019 – Q4	ANL, Scarcelli	Explore transition strategies between ACI and SI modes	**On track**

Technical Accomplishments and Progress

MM sensitivity simulations (PI: Edwards, ORNL)

Completed development of flexible CFD model

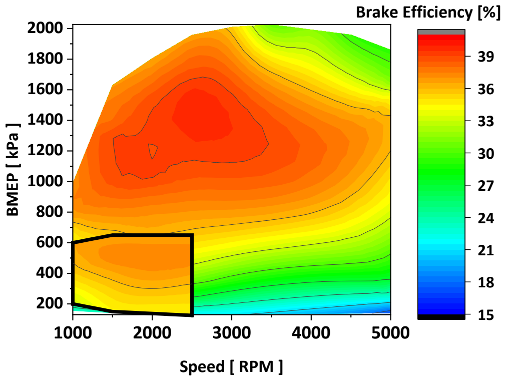
- Based on boosted SI architecture
  - Piston, head, injector (Ford 1.6-L GDI)
- Flexibility for ACI in boosted SI engine
  - Variable CR
  - Multiple DI injections for fuel stratification

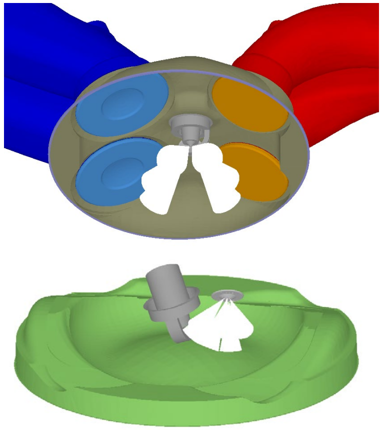
Approach allows for future refinement

- Initial parameter ranges chosen for wide coverage of ACI space
  - Ranges will be refined/expanded based on initial results
- Initial focus to expand in future efforts
  - E30 core fuel (future expansion to other fuels, parameterized fuel properties)
  - Positive valve overlap with EGR (NVO possible in future)
  - No spark (spark-assist possible in future)

Moderate detail to enable rapid simulations

- CONVERGE v2.4
- ~700k cells
- 8-species E30 fuel surrogate
- E30 mechanism (138 species, 623 reactions)
  - LLNL mechanism reduced by UConn
- Initial runs: ~18 hrs wall-time on 72 cores





Parameter	Initial Range
T intake	25 – 400+ °C
P intake	0.5 – 2 bar
EGR%	0 – 60%
IMEP target	Up to at least 6 bar
PM/DI ratio	HCCI (100% PM) PPCI (<100% to >0% PM) MCCI (0% PM)
DI SOI	-80 to +10 dATDC
CR	8 – 16

Technical Accomplishments and Progress

MM sensitivity simulations (PI: Edwards, ORNL)

Simulations underway for initial parameter sweeps to…

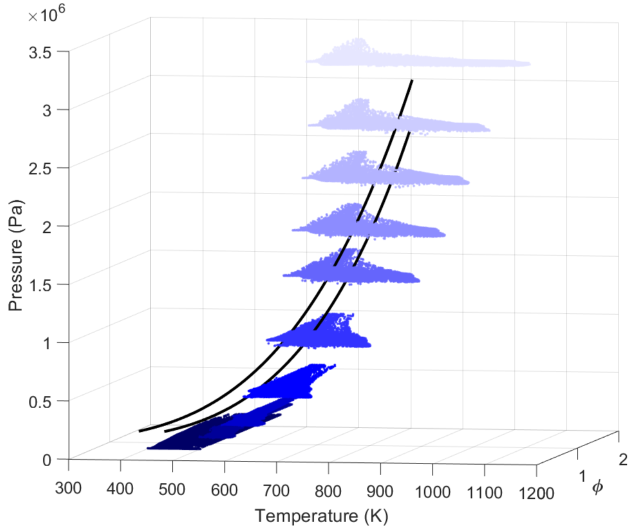
- Refine parameter ranges
- Evaluate parameter sensitivities and functionalities
- Evaluate parameter interactions

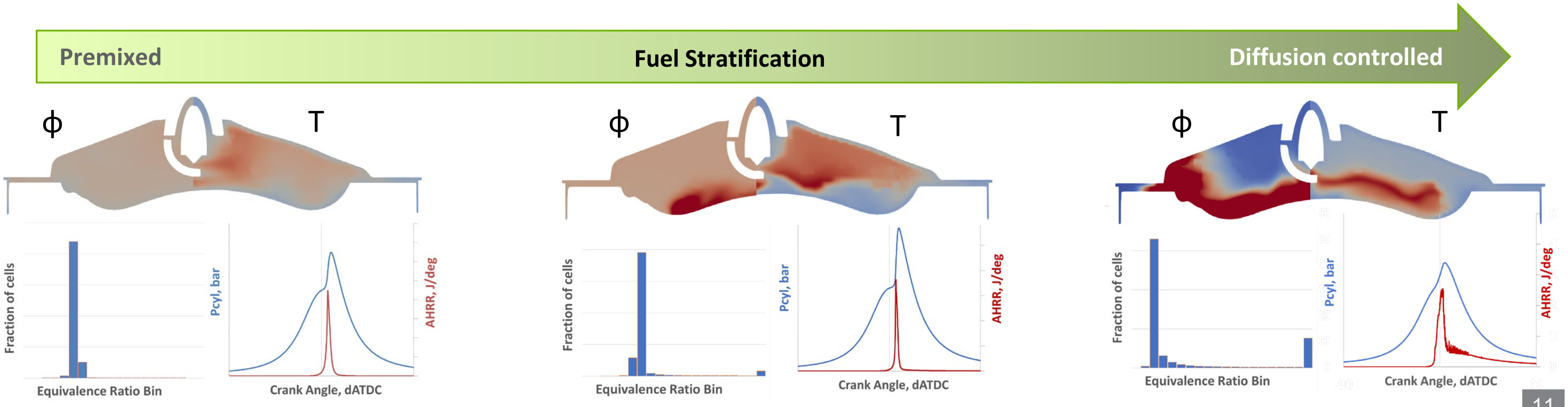
Production runs will cover the final parameter space using intelligent sampling strategies

- Denser sampling at regions of interest
    - Regions of high sensitivity/functionality
    - Regions with improved engine performance
    - Edges of ACI operating space

Apply TASMANIAN for low-order mapping of multi-dimensional parameter space

Fuel and temperature stratification during compression



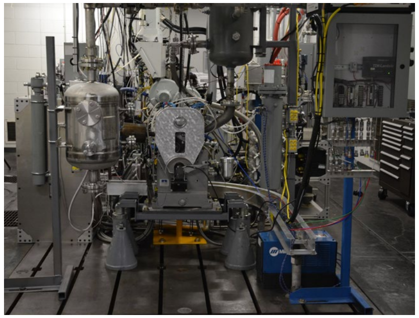


Technical Accomplishments and Progress

MM engine interactions (PI: Curran, ORNL)

Engine experiments underway with new SCE platform

- Bookend P-T trajectory study with new hardware over range of fuels
- Evaluate parameter sensitivities and functionalities
- Study effects of advanced boundary control for range of ACI stratifications with the different Co-Optima fuel blends

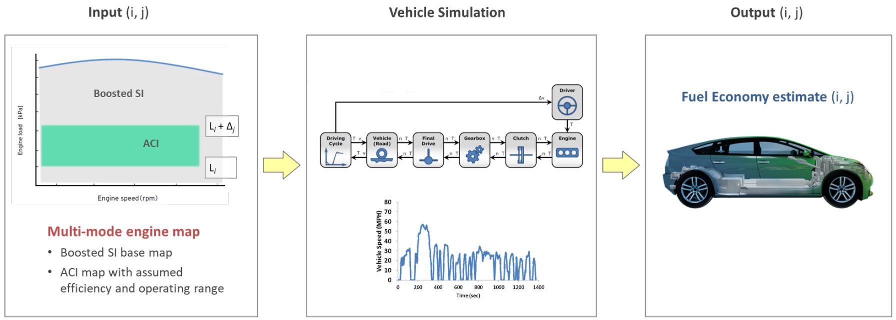


GM SCE with SG2 head (Similar to optical SCE of Sjoberg at SNL)

Performed study of potential impacts of ACI range & efficiency on urban fuel economy of LD vehicles

- Vehicle-systems simulations (Autonomie, Matlab Powertrain Blockset)
- Baseline engine map from a 2.2-L direct-injection SI engine
- Investigating effect of size and location of ACI region by manipulating engine map
- Systematically replaced BSFC values in ACI ranges with a new value (180 - 260 g/kWh)

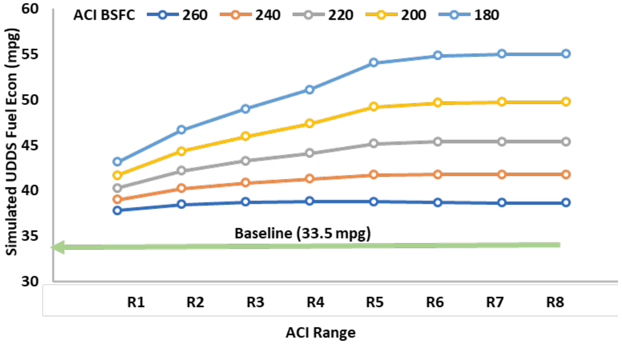
Substantial fuel economy gains even for slight efficiency increases and small ACI range



Multi-mode engine map

- Boosted SI base map
- ACI map with assumed efficiency and operating range

Engine map modification via vehicle system simulations



Technical Accomplishments and Progress

MM engine fuel properties (PI: Rockstroh, ANL)

Using RCM ignition delay experiments to provide guidance on intake boost requirements

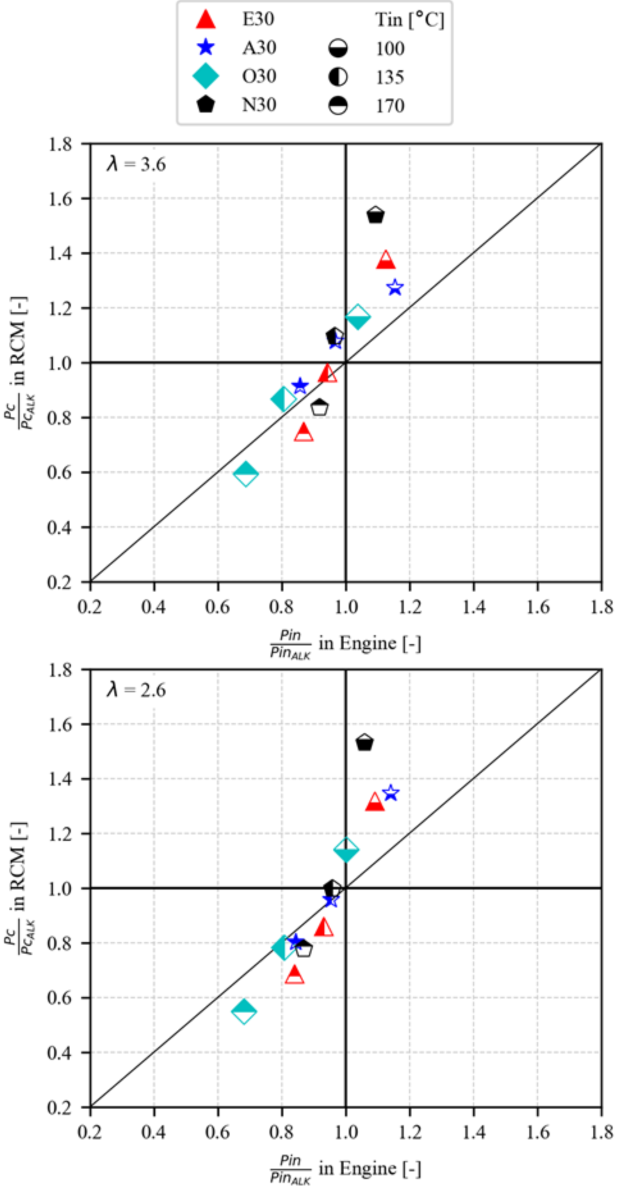
- Correlated engine boost requirements to RCM compressed pressure at constant 4-ms ignition delay over sweep of intake temperatures and fuels
  - Comparing relative rankings of the fuels from the turbulent engine to the static conditions in the RCM

Observed consistent trend relating boost requirements for the engine to compressed conditions in the RCM

Examining ACI reactivity of the Co-Optima core fuels

- Performed pressure – temperature analysis on engine data for each of the Co-Optima core fuels
- *Observed disparate auto-ignition characteristics between fuels despite similar RON and sensitivity*
- *Olefin fuel found to be the most reactive, requiring lower intake air boosting at same temperature*
- Behavior appears consistent for the two fuel loading conditions

RON and sensitivity do not fully capture fuel reactivity in ACI modes



Technical Accomplishments and Progress

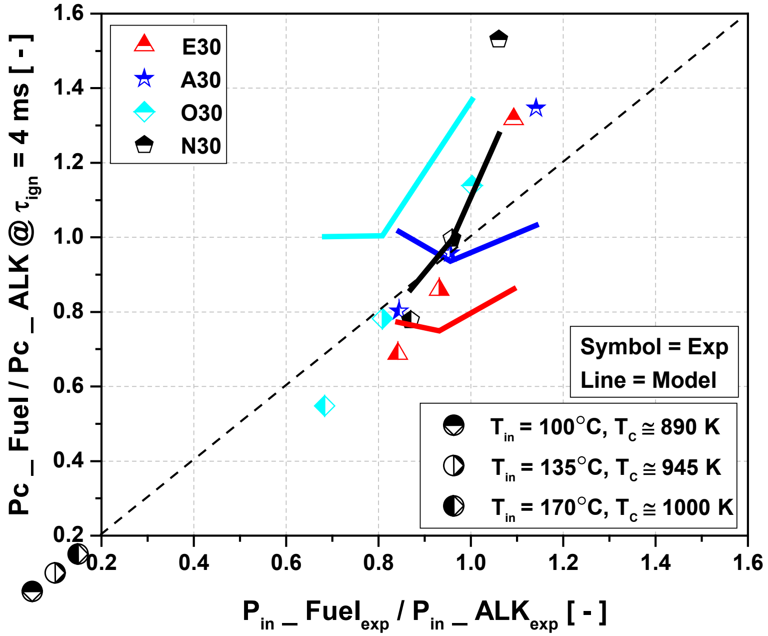
MM engine fuel properties (PI: Rockstroh, ANL)

Performed chemical kinetic simulations at RCM conditions

- Results using initial kinetic mechanism showed significant deviation from RCM measurements
- Recent updates to the kinetic mechanism more closely reflects the autoignition behavior in the RCM

Validated chemical kinetic mechanisms can be an efficient means to characterize fuel performance for ACI operation

Potentially useful to estimate the intake boost requirements for engine control strategies



Technical Accomplishments and Progress

MM engine fuel properties (PI: Rockstroh, ANL)

Design of Experiment – Taguchi Method

Goal: IMEP Control → Control Factor Selection → Design Array
L27 matrix
6 factors x 3 levels → Conduct Experiment → Statistical Data Analysis

Control Factors	**Levels**		
	1	**2**	**3**
Compression Ratio [-]	11.3	12	12.7
Engine Speed [RPM]	1000	1500	2000
Intake Air Temperature [°C]	180	230	280
Exhaust gas recirculation Rate [%]	0	20	40
Equivalence Ratio [-]	0.2	0.28	0.35
End of Injection [CAD bTDCf]	300	50	30
Independent Variable	**Intake Air Pressure**		
Operating target	**CA50% ~ 10 ± 2 CAD aTDCf**		
Response Variables	**IMEP / CoV IMEPn / Combustion Noise**		

Figure of merit – Signal to Noise ratio

“Larger the better” for IMEP

$$S/N = -10\log\left({}^{1}/_{n}\sum_{i=1}^{n} Y_i^2\right)$$

“Smaller the better” for CoV IMEP and combustion noise

$$S/N = -10\log\left({}^{1}/_{n}\sum_{i=1}^{n} 1/Y_i^2\right)$$

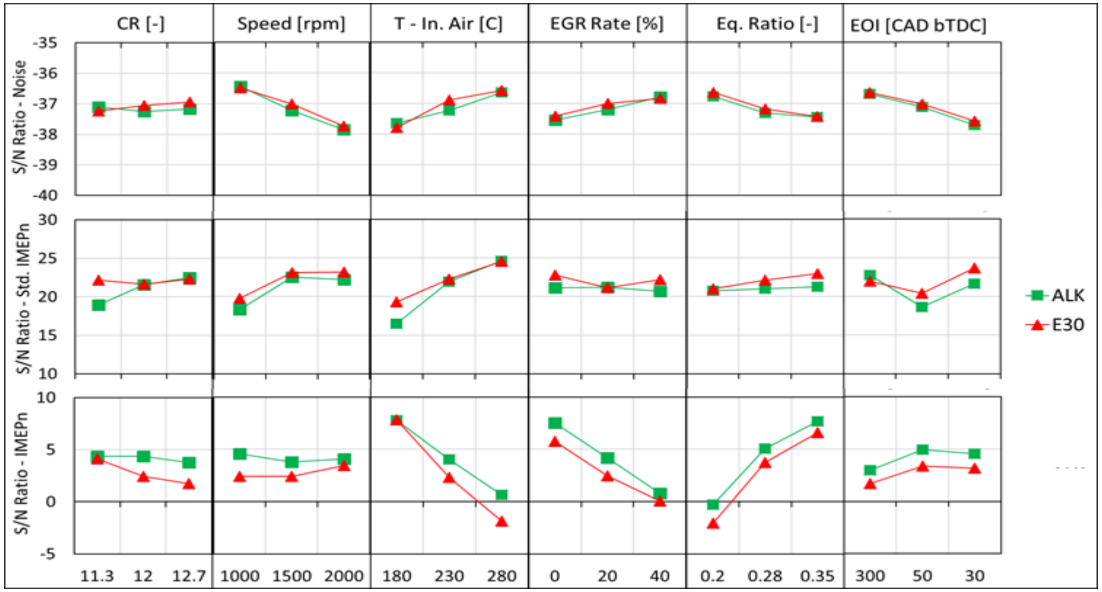
n = number of sample for each test
Yi = response variable

Technical Accomplishments and Progress

MM engine fuel properties (PI: Rockstroh, ANL)

Statistical Analysis

- Effect of control factors on the response variables (IMEP, combustion stability, and noise) are evident from the signal-to-noise-ratio plots
    - Overall similar responses for alkylate (ALK) and E30 fuels
- Analysis of variance (ANOVA) results show percent contribution to response variables
    - Contributions of the engine control parameters (Tin, EGR, phi) show slight differences for the two fuels



IMEP		
	ALK	E30
CR	2%	8%
N	3%	3%
Tin	28%	33%
EGR	27%	20%
Φ	32%	30%
SOI	8%	6%

Noise		
	ALK	E30
CR	3%	6%
N	28%	25%
Tin	20%	24%
EGR	15%	11%
Φ	14%	16%
SOI	20%	18%

Std. IMEPn		
	ALK	E30
CR	17%	4%
N	20%	21%
Tin	39%	32%
EGR	2%	10%
Φ	2%	12%
SOI	20%	20%

Next steps

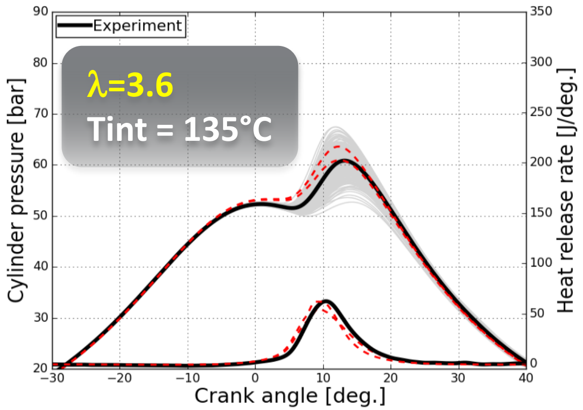
- Characterize remaining Co-Optima core fuels
- Use fuel-specific sensitivity to control parameters to establish ACI operating load range

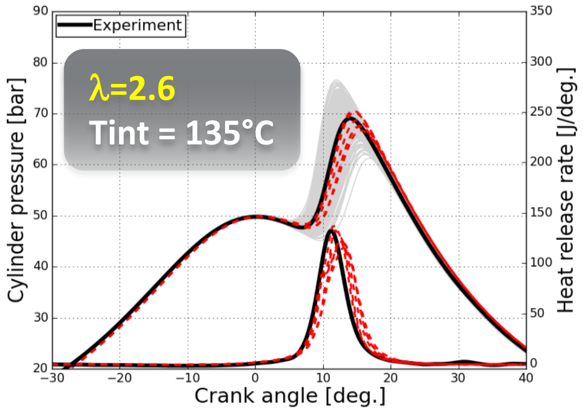
Technical Accomplishments and Progress

MM SCE simulations (PI: Scarcelli, ANL)

CFD simulations validated for ACI operation with Alkylate fuel

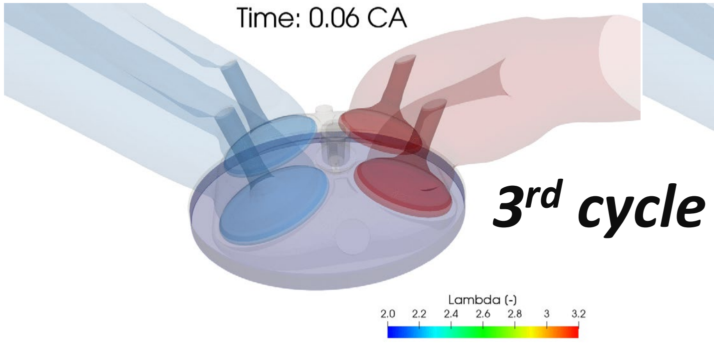
- Simulations capture experimental trends both qualitatively and quantitatively
  - RANS turbulence model
  - State-of-the-art spray and combustion model
  - No significant model tuning needed
- Cylinder pressure and HRR are extremely sensitive to in-cylinder temperature
  - *Wall temperature needs to be calibrated properly*
- At similar load, model captures different mixture properties without further tuning
- Multi-cycle simulations show little CCV
  - Consistent with CI combustion

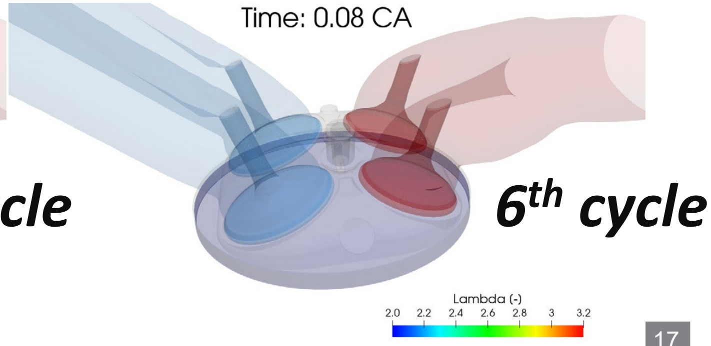




Cyclic variability
(λ=2.6, Tint = 135°C)

**** iso-Temp of T=1100 K colored by λ***



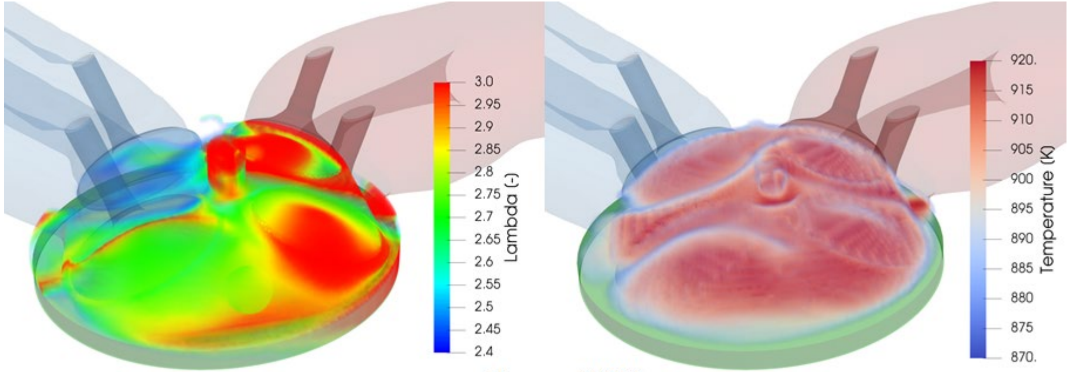


Technical Accomplishments and Progress

MM SCE simulations (PI: Scarcelli, ANL)

Identified impact of thermal/chemical stratification on ACI

- CFD analysis emphasizes impact of fuel and temperature stratification due to mixing and heat loss



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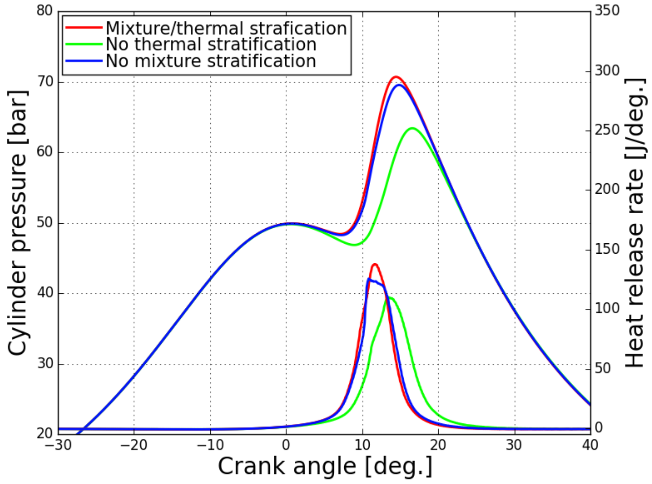
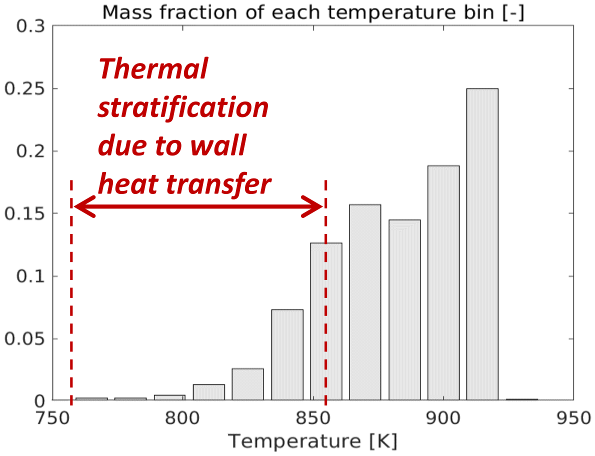


- While fuel stratification appears to be larger, *thermal stratification has greater impact on heat release and peak pressure*



Future ACI simulations need to…

- ***Improve characterization of thermal BCs***
- ***Further evaluate impact on thermal stratification and HRR***

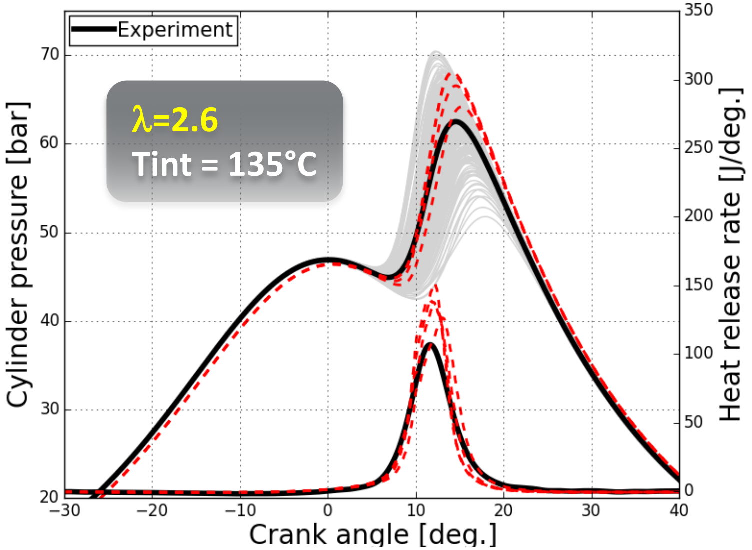
Technical Accomplishments and Progress

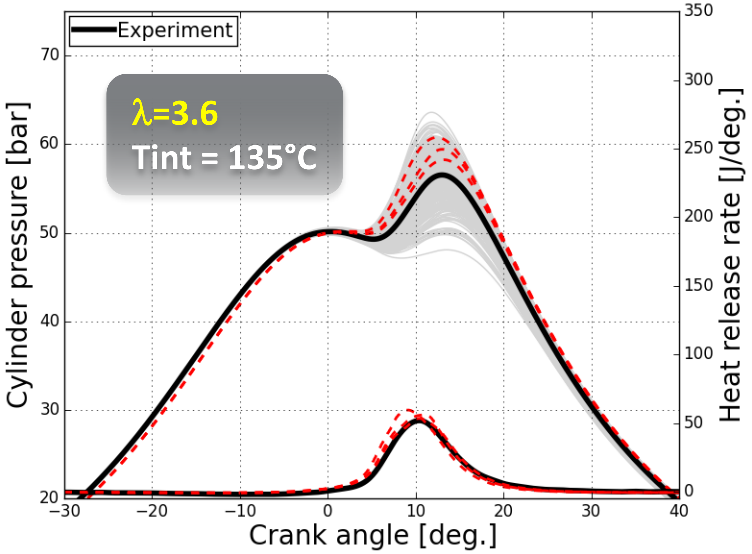
MM SCE simulations (PI: Scarcelli, ANL)

ACI simulations extended to other Co-Optima core fuels

- Repeated simulations for E30 core fuel at same conditions used for Alkylate
  - Updated fuel properties and kinetics
- E30 simulations match experimental data without substantial tuning
- After validation with different fuels, CFD will evaluate the impact of fuel properties on ACI operation and more actively support future experimental work

Solid CFD model available for studying fuel effects on ACI/MM with main uncertainty from wall-temperature BCs





Response to Previous Year Reviewers’ Comments

Two current tasks were reviewed in 2018:

- MM engine interactions (PI: Curran, ORNL)
- MM engine fuel properties (PI: Rockstroh, ANL)

Other tasks have either changed focus (e.g., MCE MM simulations, PI: Edwards, ORNL) or are new starts.

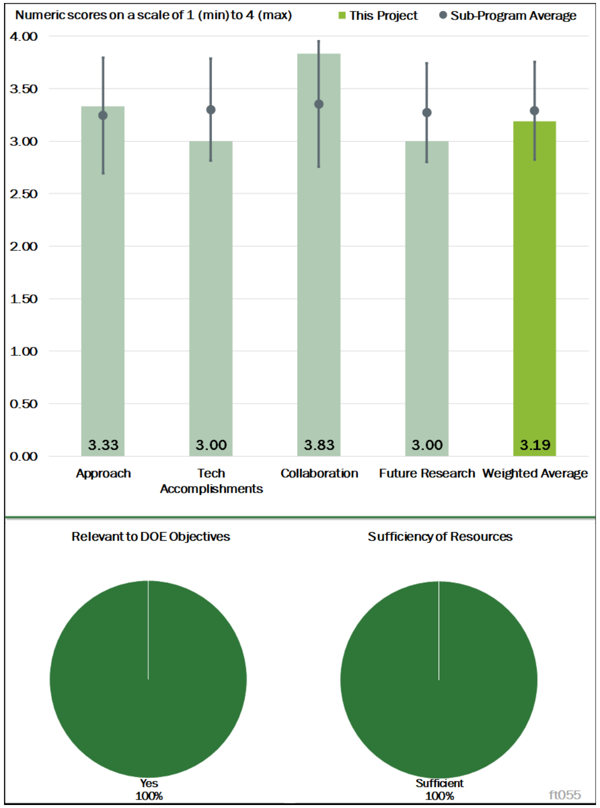
Reviewer: *“Achieving the tasks suggested for future research would definitely support the DOE objectives for several reasons: knowing ways to improve ACI operation model will be possible; developing optimal fuels for specific engine operation mode will be possible; and understanding what the major limiting factors/road blocks are in improving gasoline engine efficiency in ACI/SI mode will be possible.”*

Reviewer: *“…ACI modes that rely on high intake temperatures, there is a need to demonstrate that the high temperatures can be achieved using internal EGR/hot residuals. Alternatively, the team needs to account for the energy required to provide the hot air temperatures while estimating the efficiency of the ACI mode.*

Response: Reviewer makes a good point – the new MM SCE engine platform at ORNL provided by GM has advanced valve authority to study trapped residuals and will bound scope of study of what is realistic – advanced boundary control authority will allow for accounting of energy required for additional intake temperature requirements

Reviewer: *“For the Argonne National Laboratory (ANL) multimode work, the reviewer suggested that as new fuel properties are determined/defined that enable ACI operation, care should be taken that in a multimode engine, the same fuel needs to be used for high-load SI combustion as well.”*

Response: A parametric study using design of experiments is being conducted in FY19 in order to establish the geometric compression ratio trade-off for ACI, while maintaining high-load SI operation. In addition, engine combustion control parameters (intake air boosting and heating, equivalence ratio and exhaust gas recirculation) are being investigated to understand the fuel-specific characteristics in a multi-mode engine.

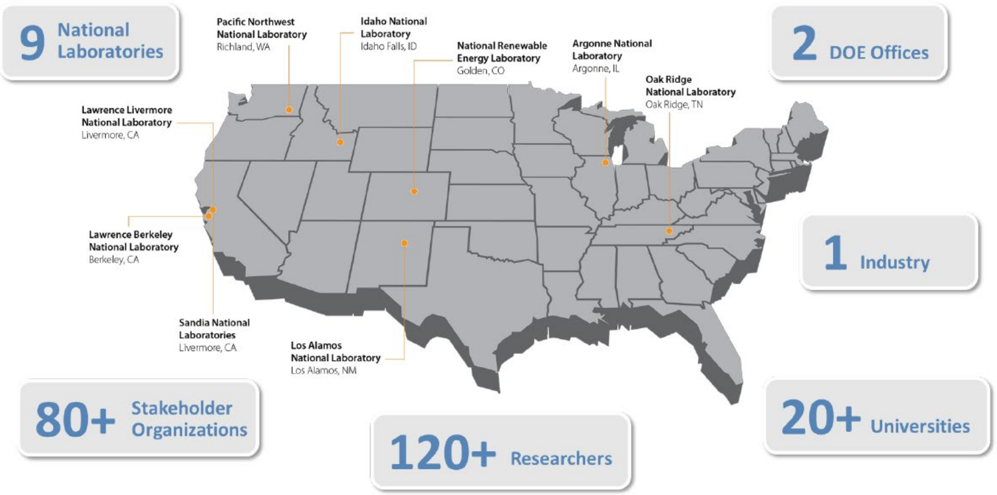


Scores and comments from 2018 Annual Merit Review Report
ft055 Co-Optima Boosted Spark-Ignition and Multimode Combustion, Part 3

Collaborations

Extensive, interdisciplinary collaboration exists across the Co-Optima program

- DOE-funded research at National Laboratories, universities, and industry
- Input from stakeholders and advisory board
- Regular program reviews (AMR, AEC MOU)



MM MCE and sensitivity simulations (PI: Edwards, ORNL)

- **Convergent Science, Inc.**
- **LLNL (Pitz, et al.) – Detailed kinetic mechanisms**
- **UConn (Lu) – Reduced kinetic mechanisms**
- ORNL (Sluder) – Complimentary boosted SI experiments on Ford GDI MCE
- ORNL (Curran) – Complimentary MM ACI experiments on GM SCE
- ANL (Som, et al.) – Integration of MCE, CFD, and vehicle systems modeling

MM engine interactions (PI: Curran, ORNL)

- **General Motors – support for SCE**
- ORNL (Edwards) – Complimentary MCE and CFD engine simulations
- ANL (Rockstroh) – Coordination of MM ACI experimental tasks
- ORNL (Curran) – Complimentary combustion program project on same engine

MM engine fuel properties (PI: Rockstroh, ANL)

- **Ford – Support for engine modifications**
- **ANL (Goldsborough, et al.) – Rapid compression machine (RCM) data**
- ANL (Scarcelli) – Complimentary CFD simulations
- ORNL (Curran) – Coordination of MM ACI experimental tasks

MM SCE simulations (PI: Scarcelli, ANL)

- **Convergent Science, Inc.**
- **LLNL (Pitz, et al.) – Detailed kinetic mechanisms**
- **UConn (Lu) – Reduced kinetic mechanisms**
- ANL (Rockstroh) – Complimentary experimental effort

Remaining Challenges and Barriers

Current efforts for these tasks address the following barriers and objectives outlined in the Co-Optima 3-year plan

- Determine quantitative relationships between critical fuel properties and important engine parameters (e.g., spray formation, mixing, retained residuals, operating constraints) for each combustion approach to achieve the multimode efficiency goal of +10%
- Determine target values of critical fuel properties and ranges for each combustion approach
- Assess fuel property impacts on engine efficiency and fuel economy and emissions

Proposed Future Research

MM MCE simulations (PI: Edwards, ORNL) – *remainder of FY2019*

- Examine impact of ACI fuels on boosted SI operation
- Explore SI operation approaches following mode transitions with residual high intake temperatures and EGR% (beyond-MON)

MM sensitivity simulations (PI: Edwards, ORNL)

- Complete mapping of ACI sensitivity to key engine parameters for E30 core fuel
- Expand sensitivity studies to include other core fuels and generalized fuel properties

MM engine interactions (PI: Curran, ORNL)

- Bookend P-T trajectory study with new engine platform and determine limits of hardware (both trapped residuals and amount of stratification)
- Complete boundary-limit MM study across range of fuels

MM engine fuel properties (PI: Rockstroh, ANL)

- Describe the effects of fuel octane and autoignition chemistry towards achieving stable part-load operation using a passive pre-chamber
- Implement an active pre-chamber system to characterize its potential to assist ACI operation

MM SCE simulations (PI: Scarcelli, ANL)

- Simulate the effect of conventional ignition and pre-chamber ignition on ACI operation, and validate simulations against engine data
- Identify the impact of fuel properties and chemistry on passive and active types of pre-chamber ignition, for both ACI and SI operation

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

Summary

Relevance

- Delivering foundational science to understand fuel properties impacts on multi-mode operation
- Longer-term opportunity for improved efficiency across drive-cycle with multi-mode combustion

Approach

- Multi-lab collaborations, 2 metal single-cylinder engines, CFD and vehicle system simulations

Technical Accomplishments

- Initiated simulation study of global sensitivity for ACI modes
- Observed substantial fuel economy gains even for slight efficiency increases and small ACI range
- Observed consistent trend relating boost requirements to RCM compressed conditions
- Demonstrated RON and sensitivity do not fully capture fuel reactivity in ACI modes
- Observed that thermal stratification has considerable impact on combustion performance of ACI
- Validated CFD model for future studies on the impact of fuel properties on ACI operation

Collaboration and Coordination

- Co-Optima includes collaborative research funded by 2 DOE offices at 9 NLs, 20+ universities, and 1 OEM with strong industry engagement from external advisory board and 80+ stakeholders
- For specific tasks: strong collaboration between lab teams and with industry and academia

Proposed Future Research*

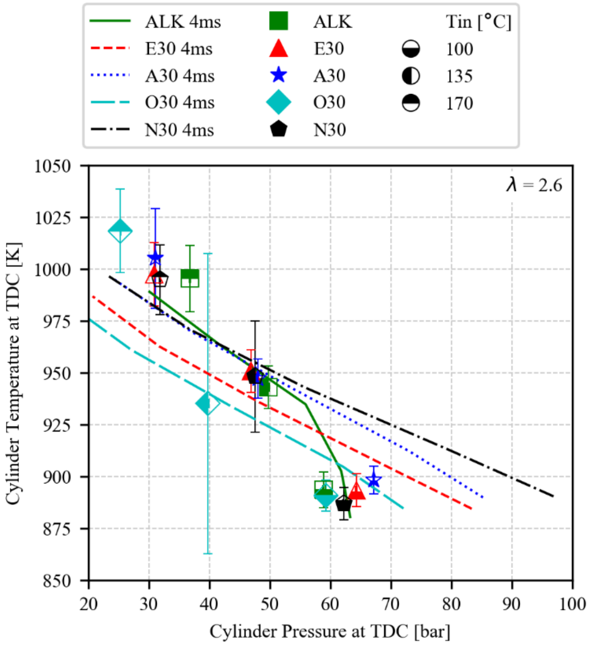
- Continuation of collaborative experimental and numerical efforts to understand sensitivity of ACI modes to fuel properties and engine parameters and limits of ACI operation

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

Technical Back-Up Slides

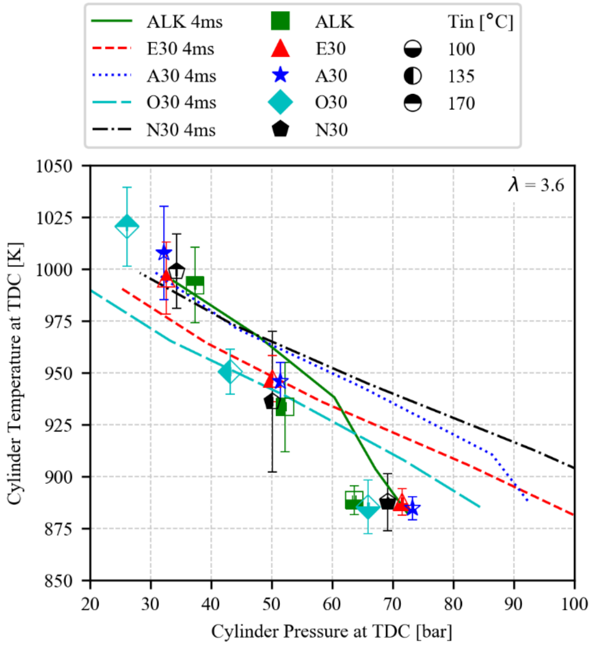
Technical Backup Slides
Mapping compression P-T between engine and RCM

MM engine fuel properties (PI: Rockstroh, ANL)



Intake manifold pressure [bar-a]

Fuels	Intake air temperature [°C]		
	100	135	170
ALK	1.64	1.45	1.11
E30	1.80	1.35	0.93
A30	1.88	1.39	0.94
O30	1.65	1.17	0.76
N30	1.74	1.39	0.97



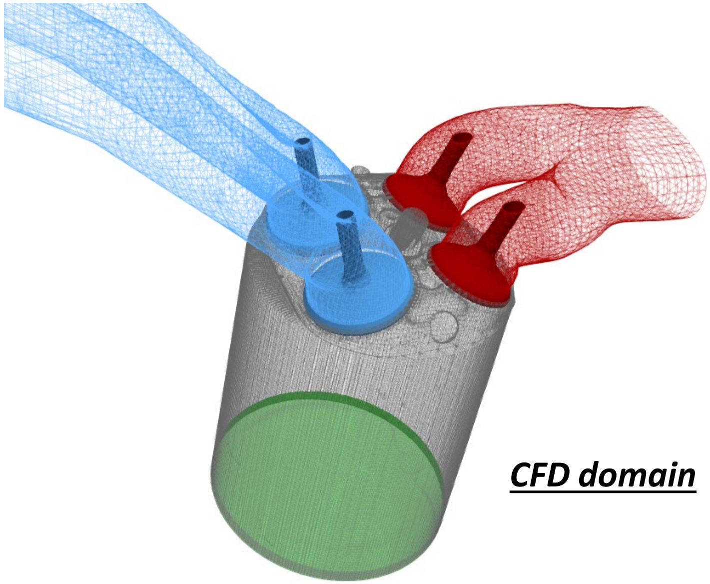
Intake manifold pressure [bar-a]

Fuels	Intake air temperature [°C]		
	100	135	170
ALK	1.76	1.52	1.12
E30	1.98	1.43	0.97
A30	2.03	1.47	0.96
O30	1.83	1.22	0.77
N30	1.93	1.47	1.03

Technical Backup Slides
CFD model and operating conditions (ANL GDI SCE)

MM SCE simulations (PI: Scarcelli, ANL)

Engine	Ford single-cylinder GDI engine
Displacement	0.626 L
Compression ratio	15.3
Speed	1500 rpm
Intake air temperature	100°C - 170°C
Excess-air ratio (λ)	2.6 - 3.6
Load	1.2 – 9.2 bar [NMEP]
Injection timing	-300° CA aTDC
CA50	12 CA aTDC
Fuel	Alkylate and E30



CFD domain

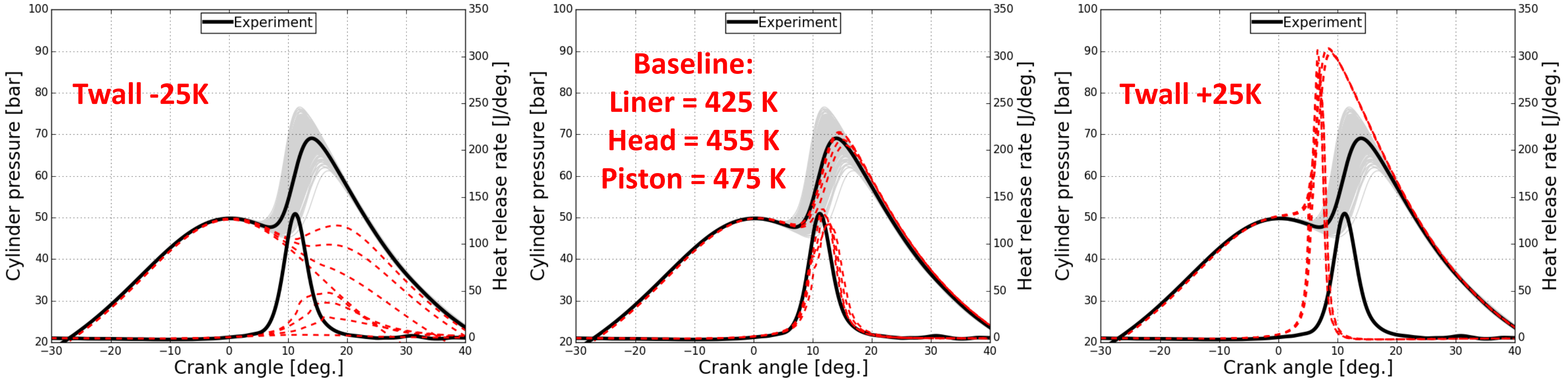
CFD setup (CONVERGE CFD)

Combustion	CONVERGE SAGE model (well mixed reactor) with multi-zone model
Turbulence	Reynolds-Averaged Navier-Stokes (RANS) RNG k-e model
Pressure-velocity coupling method	PISO integration (2nd order space and fully implicit time integration)
Mesh resolution	• 4 mm (base) through 0.5 mm by AMR (Adaptive Mesh Refinement) • Fixed embedding (0.5 mm) in injector and valve seat regions.
Discrete phase	• Euler-Lagrangian two-way coupling • Composite species evaporation (Co-Optima fuel surrogates)

Technical Backup Slides
Combustion phasing sensitivity to wall temperatures

MM SCE simulations (PI: Scarcelli, ANL)

λ=2.6 Tint = 135°C, Alkylate



- ACI combustion calculations showed large sensitivity to the thermal stratification inside the cylinder.
- Cylinder wall temperature becomes a calibration parameter (challenging to measure), as it can significantly affect thermal stratification.
- 25K difference in cylinder wall temperature can significantly impact CFD results.
- Future simulations must accurately update the T_{WALL} BCs at changing load/speed.