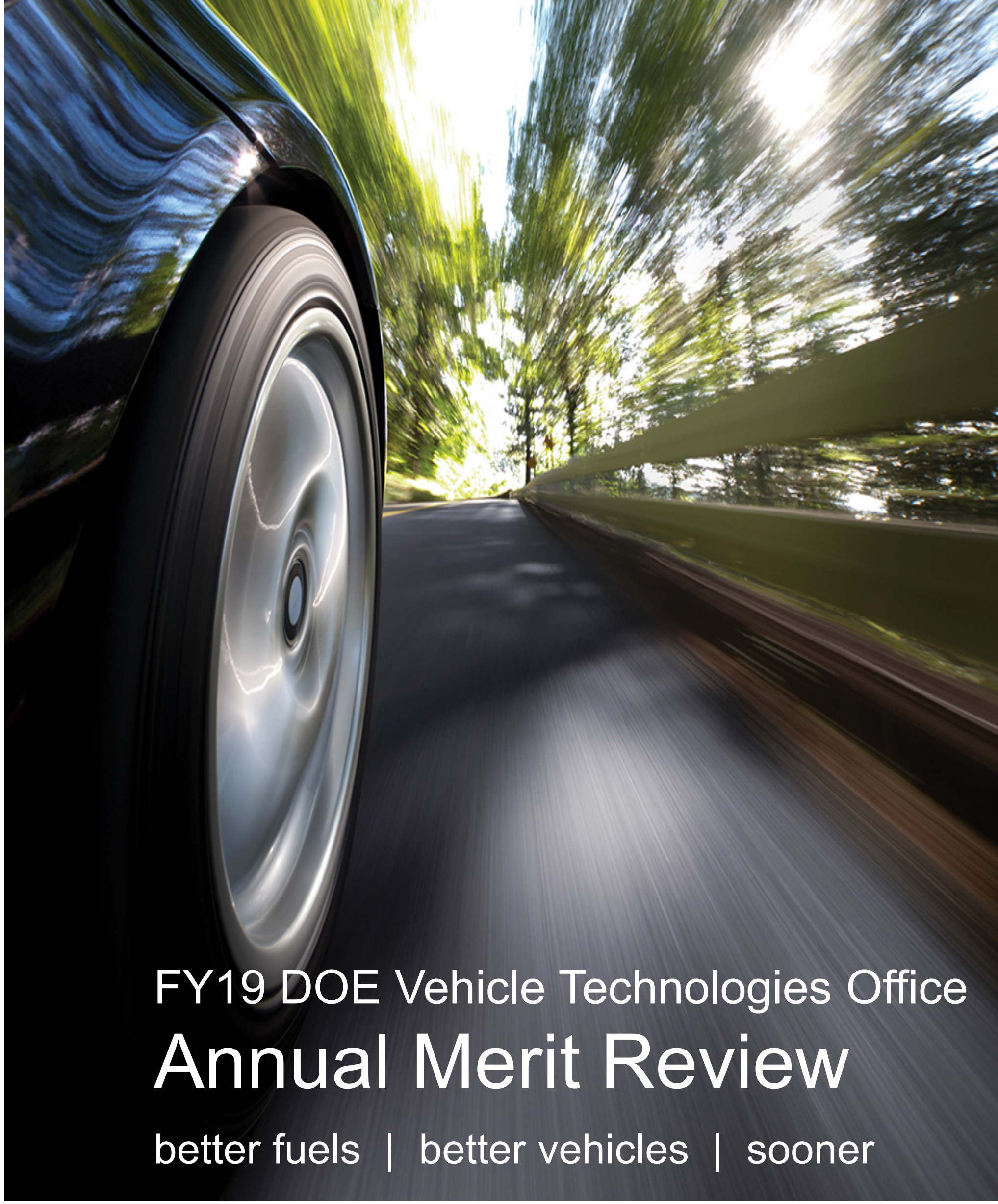
Co-Optimization of
Fuels & Engines

MM: Fuel Property Impacts and Limitations on Combustion – Spark Ignition Focus

James Szybist and Scott Sluder (ORNL)
Zongyu Yue and Sibendu Som (ANL)

June 10, 2019
Project # ft069



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

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Overview

Timeline* Phase 1 Phase 2

Task	FY16	FY17	FY18	FY19	FY20	FY21
E.1.1.2	Start		End	Re-Start		End
F.1.7.1	Start		End			
F.1.8.1			Start	Re-Start		End
G.1.10				Start		End
G.2.2	Start		End			

Budget

Task	FY18	FY19
E.1.1.2: ORNL, Multicylinder Multimode SI/ACI Autoignition Impacts on Operability and Efficiency	$440k	$376k
F.1.7.1: ORNL, Developing a Better Understanding of Octane Index	$280k	$0k
F.1.8.1: ORNL, Characterizing BOB Impacts and Limits within OI	$200k	$375k
G.2.2: ANL, Multi-cylinder CFD Engine Simulations	$175k	$0k
G.1.10: ANL, CFD Simulation of Single-cylinder (Szybist) Engine under Multimode Operation	$0k	$145k

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

Barriers**

<u>USCAR Priority 1: Dilute SI Combustion</u>

- Knock Mitigation

→ *Developing a better understanding of how fuel properties can be predictive of knock*

<u>USCAR Priority 3: Multimode ACI</u>

- Increased tolerance to market fuel variability

→ *Developing a better understanding fuel autoignition under ACI conditions*

Partners

- Co-optima partners include nine national labs, one industry, 20+ universities, external advisory board, and stakeholders (80+ organizations)
- 15 Industry partners in the AEC MOU
- <u>Task specific partners</u>
- General Motors – Hardware
- Ford - Hardware
- LLNL (W. Pitz et al.) – Chemical kinetics
- Convergent Science Inc. - Software
- *+ Many more – details in later slides*

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

Relevance

Overarching Co-Optima Relevance

- Internal combustion engines and the use of liquid fuels will continue to dominate transportation for many years.
- Significant opportunities exist to further improve engine efficiency.
- Research into better integration of fuels and engines is critical to accelerating progress towards efficiency, environmental, and economic goals.

Presentation Specific Relevance

- Mitigation of knock is listed as a top priority research area in USDRIVE roadmap to attain higher efficiency for light-duty engines
- Increasing the tolerance to market fuel variation for ACI multimode combustion is also listed as a barrier in the USDRIVE roadmap
    - The work presented in this presentation informs our ability to predict knock for SI combustion and autoignition for ACI
    - Improved predictions are based on fuel properties, chemical kinetics, and CFD simulations

Resources

Task	FY18 Budget	FY19 Budget	PI, NL Researchers	Equipment / Tools
E. 1.1.2: ORNL, Multicylinder Multimode SI/ACI Autoignition Impacts on Operability and Efficiency	$440k	$346k	Scott Sluder	Multi-cylinder GDI engine supported by Ford, standard 5-gas emissions analyzer, AVL micro soot sensor. ORNL vehicle systems team supportion Autonomie modeling.
F.1.8.1: ORNL, Characterizing BOB Impacts and Limits within OI	$480k*	$375k	Jim Szybist	Single cylinder GDI engine, open controller, standard 5-gas emissions analyzer.
G.1.10.1: ANL, ANL, CFD Simulation of Single-cylinder (Szybist) Engine under Multimode Operation	$175k**	$145k	Zongyu Yue, Sibendu Som	Laboratory computing resource center for HPC. CONVERGE CFD tools. In-house codes.

*FY18 Funding combines tasks F.1.7.1 and F.1.8.1
** FY18 Funding if for task G.2.2

Milestones

Task	Funding	Description of Milestone or Go/No-Go Decision	Status
E.1.1.2 (ORNL, Sluder)	$346k	Investigate MON impacts on boosted SI efficiency at high speed and load for baseline compression ratio condition. (Increased compression ratio is anticipated future work for next year.)	On Track
F.1.8.1 (ORNL, Szybist)	$375k	F.1.8.1 (Szybist) - Quantify autoignition propensity, load range, and stability of olefinic fuel under ACI conditions relative to Co- Optima alkylate and aromatic fuels.	On Track
G.1.10 (ANL, Yue)	$145k	Impact of fuel properties on fuel/air mixture preparation and pre-spark heat release under multimode operation characterized	On Track

Multi-cylinder engine studies used to estimate potential vehicle-level impact of engine efficiency improvements

ORNL, Sluder: Approach

Objective:

Develop estimates of vehicle fuel economy, energy use, and tailpipe CO_2 emissions to inform technoeconomic and life cycle analyses of co-optima blendstocks and provide data to aid in predictive multi-mode engine model development and validation.

FY 19 Objectives (Ongoing investigations):

Determine minimum MON for efficient high-load SI operation.

- Supports multimode SI/ACI strategy for SI operation at high-load.
- Include increasing CR, elevated intake temperatures.

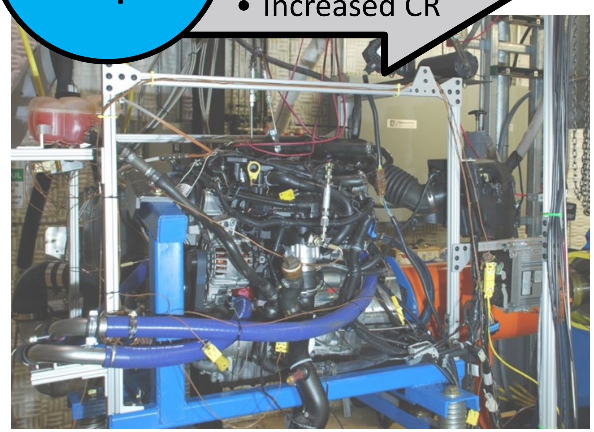
Approach: Engine and Vehicle Modeling Study

Produce Fuels

Biofuels
- High-octane
- Ethanol
- Non-ethanol

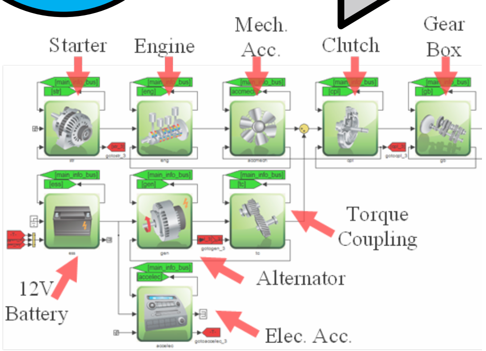
Generate Engine Maps

GTDI Engine
- Downsized, boosted
- Increased CR



Project Fuel Economy

Mid-size sedan
- Model using Autonomie



U.S. DRIVE Fuels Working Group High-Octane Study Reports completed and published

ORNL, Sluder: Accomplishments (1/2)

WTW Study (ANL)

Infrastructure Study (GM, Marathon, ORNL)

Engine and Vehicle Modeling Study (ORNL, Ford)

- Designed to inform LCA of high-octane fuel formulations.
- Ethanol, bioreformate surrogate, and wood-based biogasoline blends included.
- Parametric study of ON/CR effect on outcomes.
- **Projected vehicle efficiency improvements 1.5 – 6.0%.**
- **E30 blends projected to have fuel economy reduction; E20 and below can have improvement.**
- **Non-ethanol blends projected to cause higher tailpipe CO_2 emissions in some cases.**

Available to the public by download:
https://www.energy.gov/eere/vehicles/downloads/us-drive-fuels-working-group-high-octane-reports

Modeling assessment of Co-Optima Tier 3 blendstocks completed and published

ORNL, Sluder: Accomplishments (2/2)

- Blends formulated using a common "BOB", 97 RON target
- Blend level varied to meet target; 21 – 39%; ethanol was lowest
- Non-linear molar blend model informed by formulated fuels
- Leone et.al. is more conservative of the two models
- **Projected vehicle efficiency gains of up to 9.3% (at 100 RON)**
- **Fuel economy increase/decrease dependent upon heating value**
- **Bioreformate surrogate projected to increase tailpipe CO_2 emissions by up to 2.8%**

Projected Engine Efficiency Increase (%)	Ethanol	n-Propanol	Isopropanol	Isobutanol	Diisobutylene	Bioref. Surr.
95 RON						
Leone et al.	3.1	2.9	2.9	2.8	2.4	2.4
Co-optima Merit	3.3	3.7	2.6	3.7	3.3	3.3
97 RON						
Leone et al.	4.6	4.3	4.3	4.1	3.6	3.6
Co-optima Merit	5.6	6.1	4.4	6.0	5.4	5.2
100 RON						
Leone et al.	6.4	6.1	6.0	5.8	5.0	5.0
Co-optima Merit	9.3	9.9	7.1	9.6	8.7	7.8

Projected Volumetric Fuel Economy Increase (%)	Ethanol	n-Propanol	Isopropanol	Isobutanol	Diisobutylene	Bioref. Surr.
95 RON						
Leone et al.	1.9	2.7	1.8	2.7	6.0	9.9
Co-optima Merit	2.1	3.5	1.4	3.6	6.8	10.9
97 RON						
Leone et al.	1.5	2.7	1.4	2.7	7.2	12.4
Co-optima Merit	2.6	4.4	1.6	4.6	9.1	14.1
100 RON						
Leone et al.	0.0	1.4	-0.2	1.9	8.6	15.8
Co-optima Merit	2.7	5.0	0.8	5.6	12.4	19.0

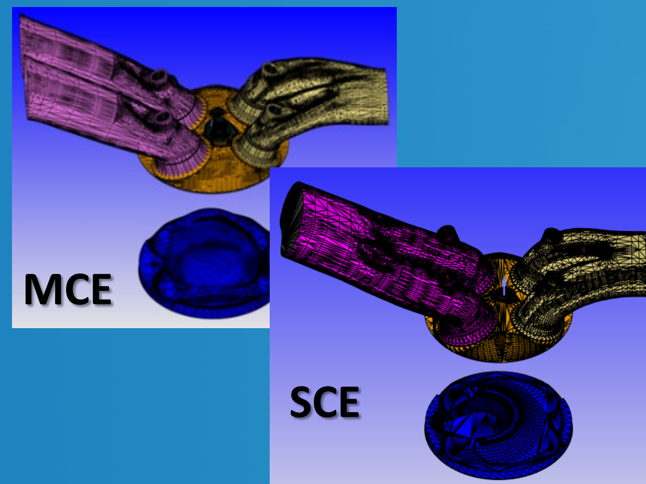
Projected Tailpipe CO_2 Emissions Decrease (%)	Ethanol	n-Propanol	Isopropanol	Isobutanol	Diisobutylene	Bioref. Surr.
95 RON						
Leone et al.	3.0	2.8	3.1	2.9	2.0	-2.0
Co-optima Merit	3.2	3.5	2.7	3.7	2.8	-1.1
97 RON						
Leone et al.	4.3	4.0	4.4	4.2	3.1	-2.1
Co-optima Merit	5.3	5.6	4.6	5.9	4.8	-0.5
100 RON						
Leone et al.	5.9	5.7	6.2	5.8	4.2	-2.8
Co-optima Merit	8.4	8.9	7.2	9.1	7.5	0.0

ANL developed CFD tools to investigate fuel effects on engine knock and pre-spark heat release

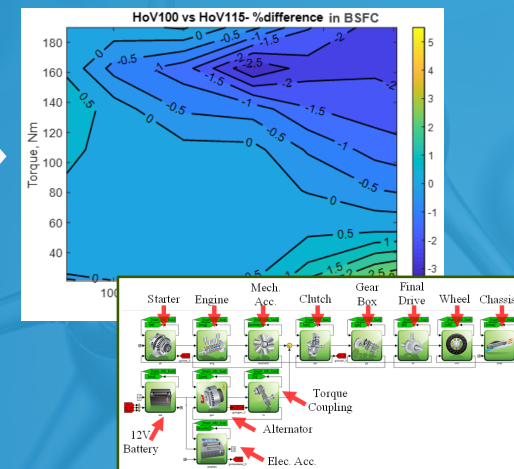
ANL, Yue: Approach

Engine experiments

CFD simulations



Vehicle-level simulations



- Multi-cylinder engine (MCE) and Single-cylinder engine (SCE) experiments at ORNL provide baseline and validation data
- ANL develop CFD models to predict SI combustion, end-gas auto-ignition and knock onset, and to investigate fuel property effects
- CFD-generated engine maps for candidate fuel to evaluate energy consumption and fuel economy benefits with Autonomie

CFD Model Incorporates KLSA Prediction and Has Been Validated on ORNL MCE

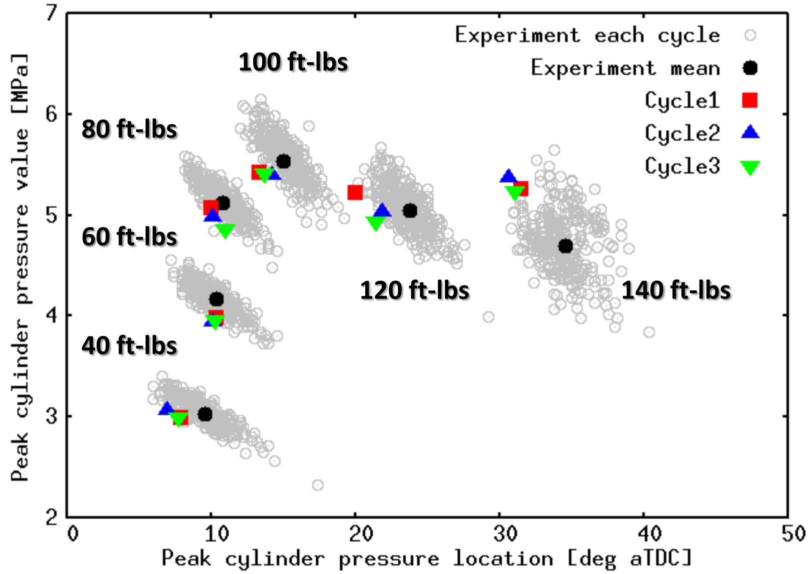
ANL, Yue: Accomplishments (1/3)

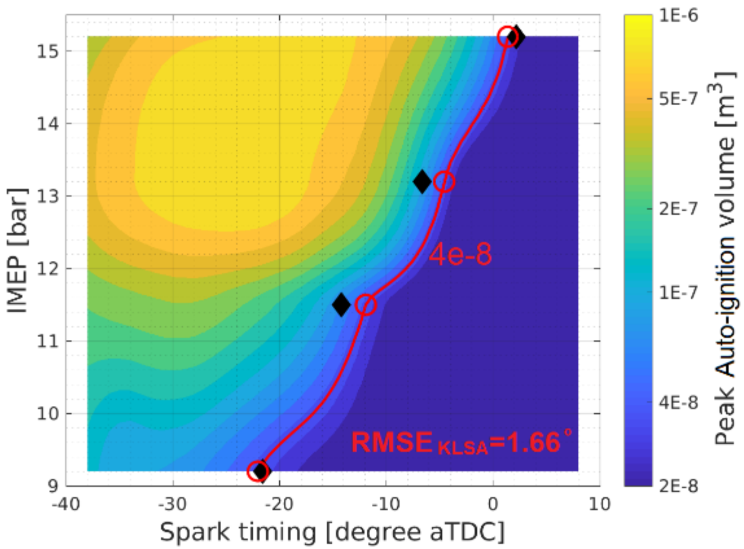
- Six operating loads at 2000 rpm, with three consecutive cycles simulation for each case
  - Maximum IMEP error is <5% (backup slide)
  - Maximum CA10&50 error <4°CA (backup slide)
- **~10 times speedup** in runtime than previous approach
- Transported Livengood-Wu integral for prediction of auto-ignition

$$\frac{\partial \rho \tilde{I}}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{I}}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D_T \frac{\partial \tilde{I}}{\partial x_i}\right) = \rho \dot{\omega}$$

$$\dot{\omega}_{PDF,avg}(P,T,\phi,\gamma) = \sum_{m=1}^{\phi_{tot}} \sum_{j=n}^{T_{tot}} P(\phi_m, T_n) \frac{1}{\tau(P,T_n,\phi_m,\gamma)} d\phi dT$$

- Knock model has been validated against engine knock sensor
- Important tool that now allows fuel property sensitivity to be investigated to vehicle level



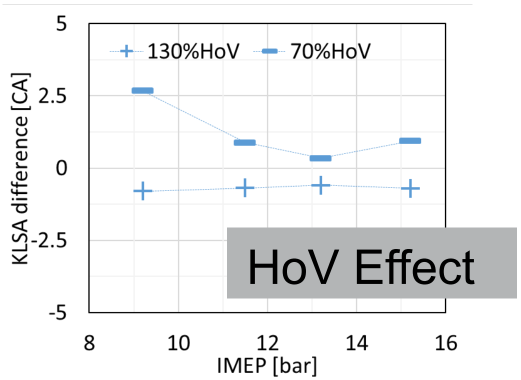


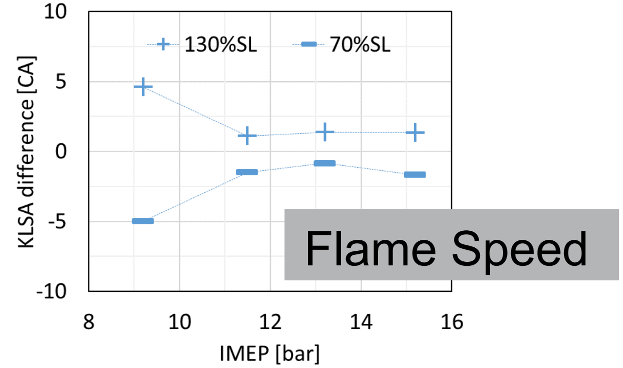
Validated Model Allows Study of Isolated Fuel Properties; Experiments Change Multiple Properties

ANL, Yue: Accomplishments (2/3)

Validated CFD model allows individual fuel properties to be investigated

1. Yue et al. ASME JERT 2019;
2. Yue et al. 11th US National Combustion Meeting.



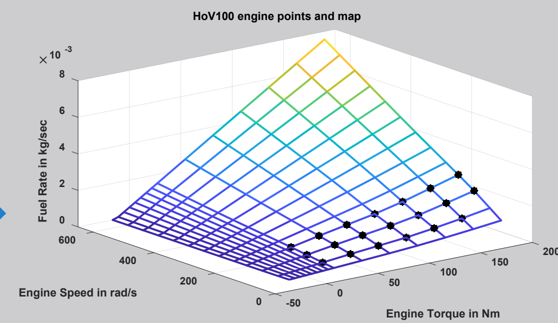


Individual fuel property effects extended to engine maps

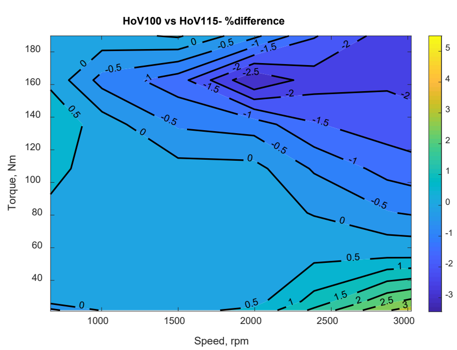
CFD generated data

Speed rad/s	Torque Nm	FC kg/s
209	27.1	0.00050594
209	54.2	0.00082492
209	81.3	0.00112178
209	108.5	0.00141174
209	135.6	0.00177447
209	162.7	0.00220708

Bi-linear fit



Maps used for vehicle system modeling to isolate effects of individual fuel properties on fuel economy



	UDDS (MPG)	HWFET (MPG)
Baseline	31.60	43.29
+15% HoV	31.70	43.20

Rousseau, ANL

Experiments and Kinetic Modeling Used to Develop an Understanding of Fundamentals of OI - Szybist

ORNL, Szybist: Approach

<u>Objective:</u>

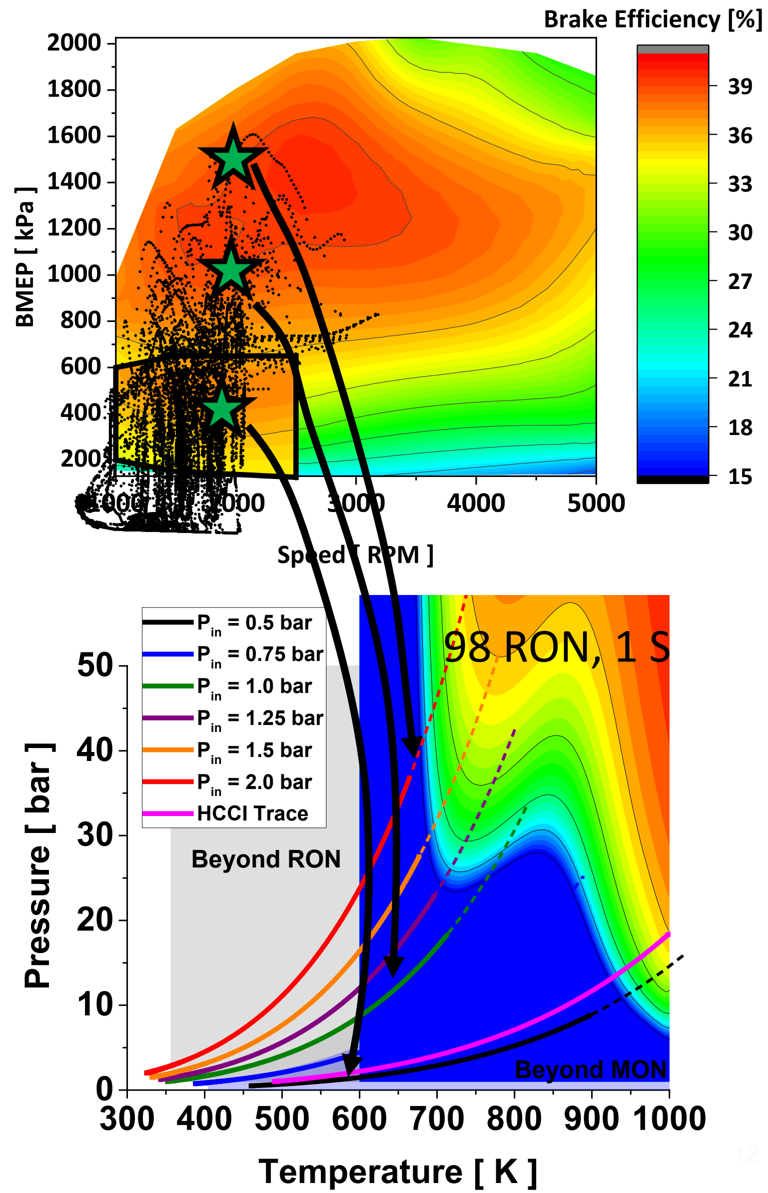
Determine the kinetic basis for octane index and whether or not it is sufficiently robust under all expected operating conditions.

<u>Approach:</u>

Develop an understanding of why the rank-ordering of fuel autoignition changes with operating condition, as predicted by OI, and determine if this will be reliable for SI and ACI components of multimode.

Study 1, Kinetic Modeling: In collaboration with LLNL, examine different PT trajectories kinetically.

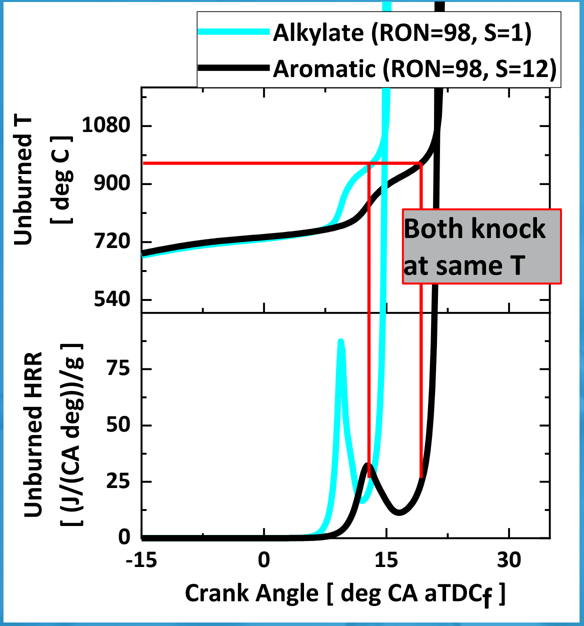
Study 2, Experimental: Examine 19 fuels at 5 different PT trajectories, including ACI, to assess OI and kinetic predictions.



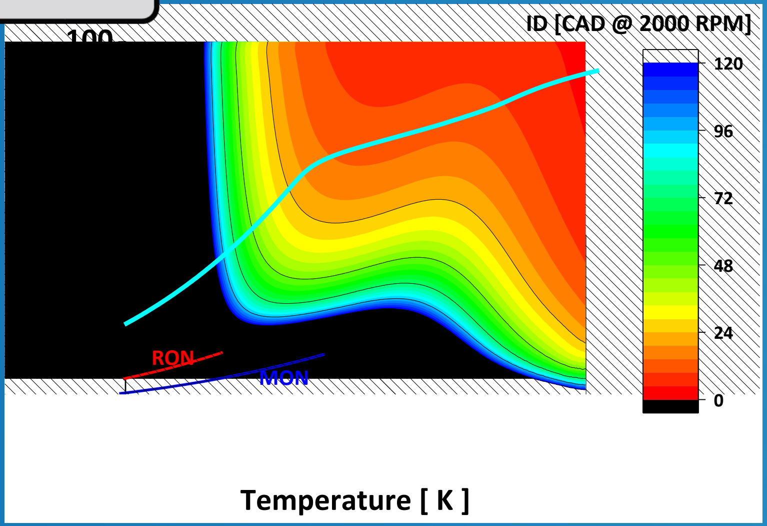
Kinetic Simulations Reveal Importance of LTHR for Boosted Operation

ORNL, Szybist: Accomplishments (1/5)

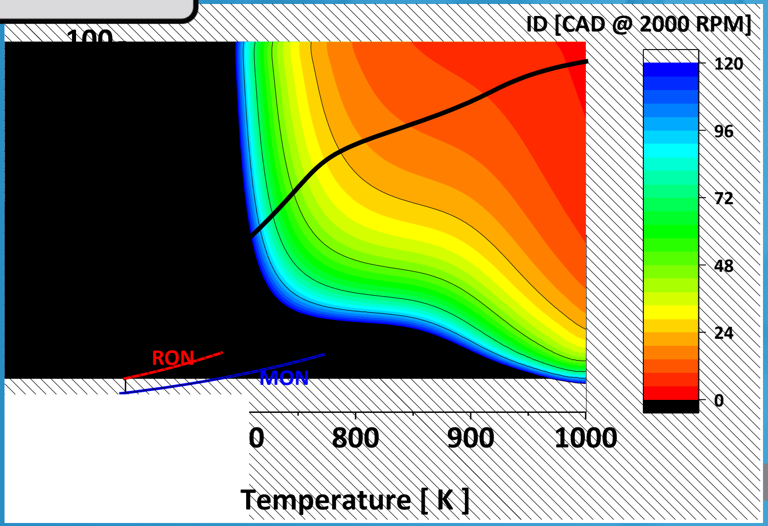
- Kinetic modeling predicts low S fuel (alkylate) is more prone to knock under boost
  - Agrees with OI predictions and experiments
  - Both fuels experience LTHR in unburned zone, but more for low S fuel
- Both fuels have similar temperature at time of knock
  - Knock is associated with HTHR, similar reactions for both fuels
  - Temperature increase from LTHR causes low S fuel to get to the temperature for HTHR (knock) sooner



Alkylate



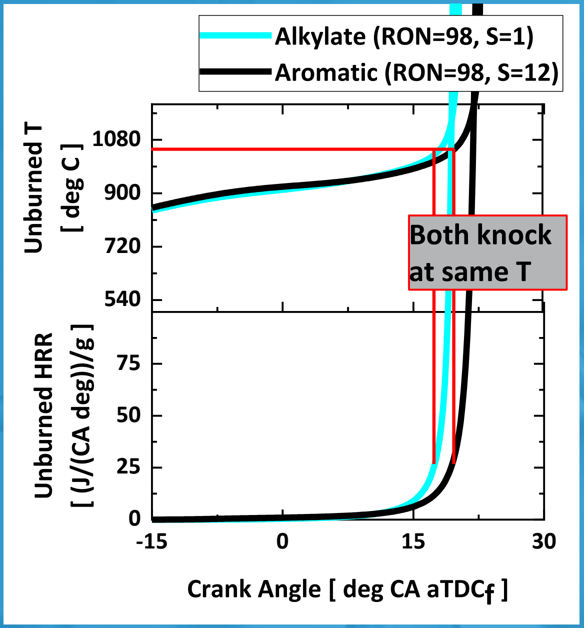
Aromatic



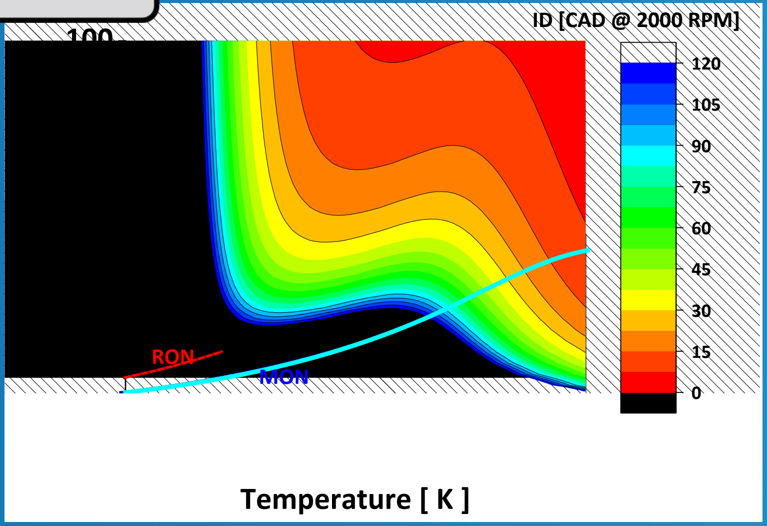
Kinetic Simulations Illustrate that LTHR is Not a Major Factor Under MON Conditions

ORNL, Szybist: Accomplishments (2/5)

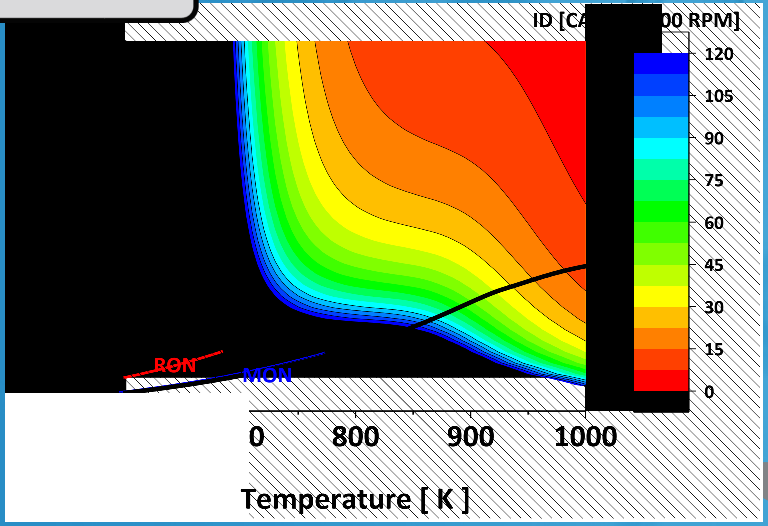
- For MON conditions, pressure is too low when T is between 650 K and 850 K for LTHR reactions
    - Minimal heat release occurs in end gas prior to HTHR
- Because LTHR is avoided, low At this condition, low S fuel (alkylate) is actually more resistant to knock
    - Reversal in rank ordering agrees with OI
- Similar lack of LTHR under ACI conditions, but lack of agreement with OI (see backup slide for more info)
    - E30 autoignites more readily than aromatic despite same RON and MON



Alkylate



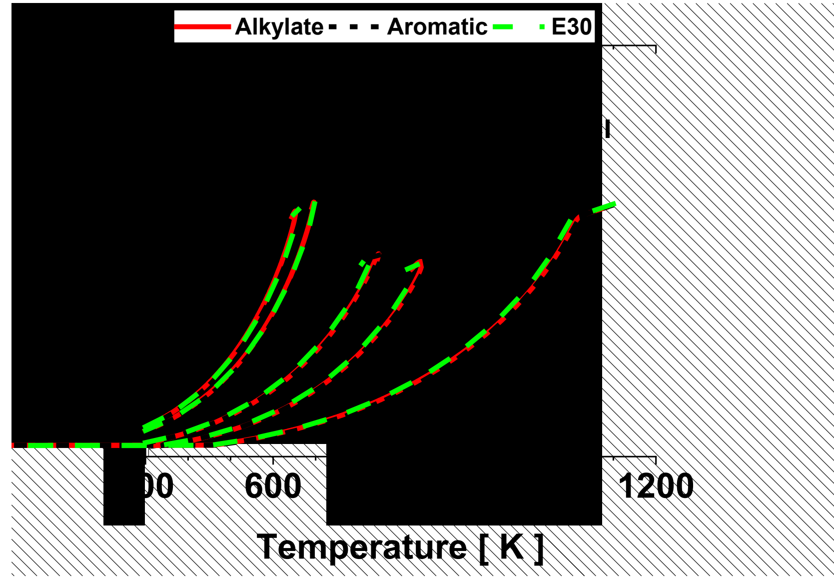
Aromatic



Experimentally, Autoignition Propensity Investigated for 19 Fuels Under 5 PT Trajectories in SCE at ORNL

ORNL, Szybist: Accomplishments (3/5)

	Boosted SI No Backpressure	Boosted SI With Backpressure	RON-like	MON-like	ACI
Compression Ratio	9.2:1	9.2:1	11.85:1	11.85:1	13.66:1
Engine Speed [RPM]	2000	2000	2000	2000	2000
Intake T [C]	50	50	50	150	240-300
Air Flow [g/min]	900	900	475	420	400
Intake Pressure [kPa absolute]	154-157	159-162	98-101	98-101	105-115
Exhaust Pressure [kPa absolute]	133-137	154-157	104-107	104-107	103-105
Engine Load [IMEPg, kPa]	1500-2000	1500-2000	800-1100	700-900	235
CA50 Phasing [CAD aTDC$_f$]	8-40	8-40	12-40	13-40	5-9
Equivalence Ratio	1.00	1.00	1.00	1.00	0.3



- **At a given condition, air flow held constant for all fuel**
  - **Fuel-specific variations in LHV per unit mass of air are small (~2%)**
  - **Engine load is primarily a function of combustion phasing**

Fuels

RON: 87-100

S: 0-11.7

HC Fuels: High alkylate, aromatic, olefinic)

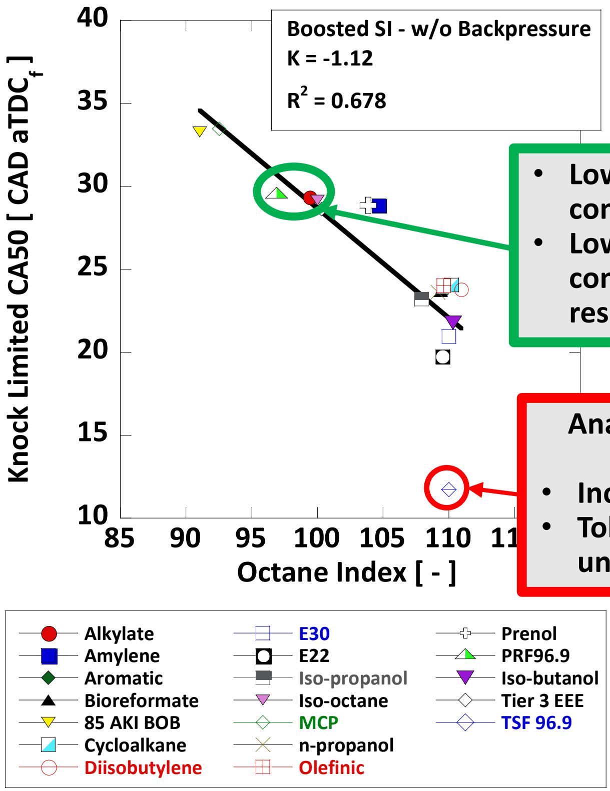
Oxygenates: ethanol, iso-propanol, n-propanol, iso-butanol, prenol

Under SI Conditions, OI Provides a Reasonable Correlation; Kinetic Modeling Agrees with Experiments, Provides Insights

ORNL, Szybist: Accomplishments (4/5)

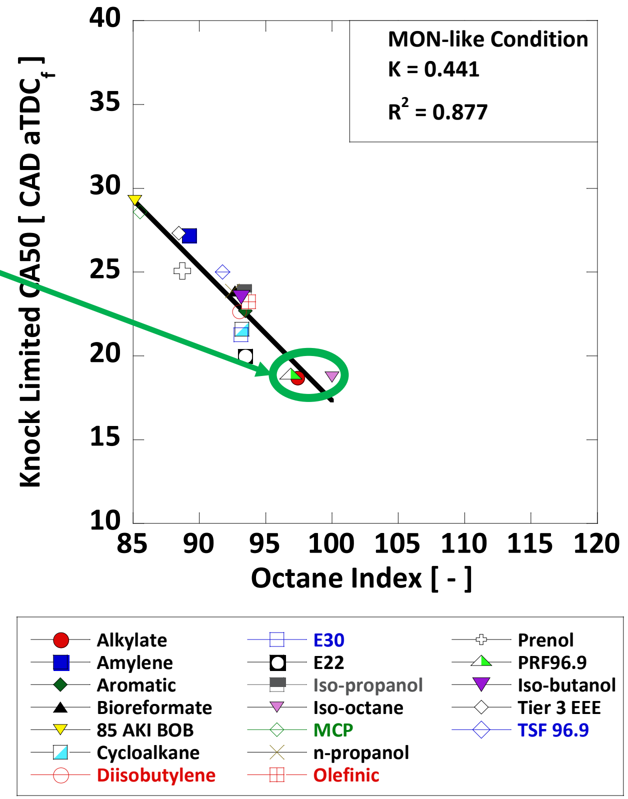
Boosted "Beyond RON" Condition
- Linear regression produces K<1
- Agrees with PT trajectory
- High S contributes significantly to improved knock resistance

MON-Like Condition
- Linear regression produces K>0
- Largely agrees with PT trajectory
- High S deteriorates knock resistance relative to low S fuels



- Low S fuels at boosted conditions are knock-prone
- Low S fuels at MON-like condition are knock-resistant

Analysis Excluding TSF96.9 Increases R^2 to 0.87.
- Includes 74% toluene
- Toluene is known to exhibit unique behavior

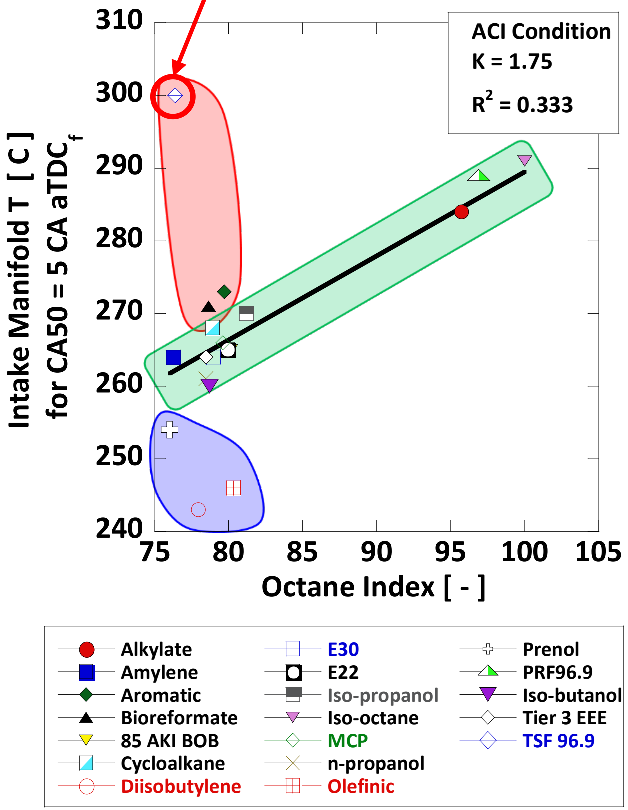


As with Kinetic Modeling, ACI Experiments Reveal Deviations from OI, Indicates Importance of Chemistry

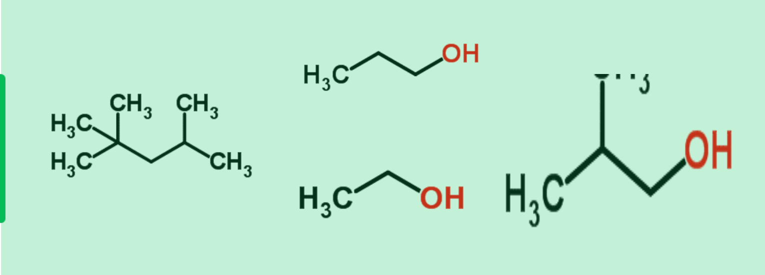
ORNL, Szybist: Accomplishments (5/5)

Reveals importance of chemistry/functional groups for ACI
- Is this attributable to single compounds (i.e., diisobutylene)?
- Do we find different fuel properties so that the central fuel property hypothesis still holds?

Analysis Excluding TSF96.9 Increases R^2 to 0.67.
- **Includes 74% toluene**
- **Toluene is known to exhibit unique behavior**

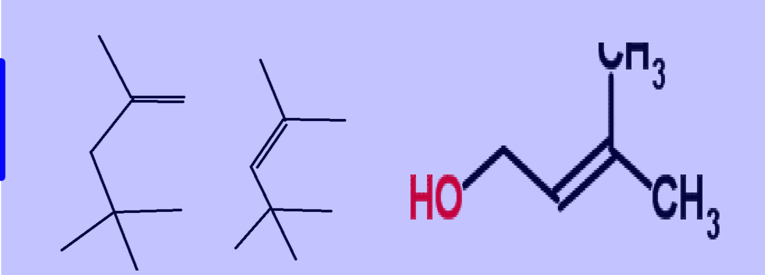


Performance of alkanes and alcohols aligned with octane index expectations



Aromatics require higher temperature than is predicted by octane index

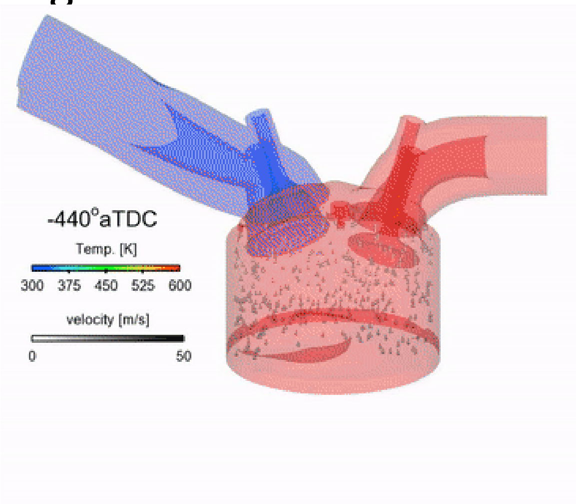
Olefins require lower temperature than is predicted by octane index

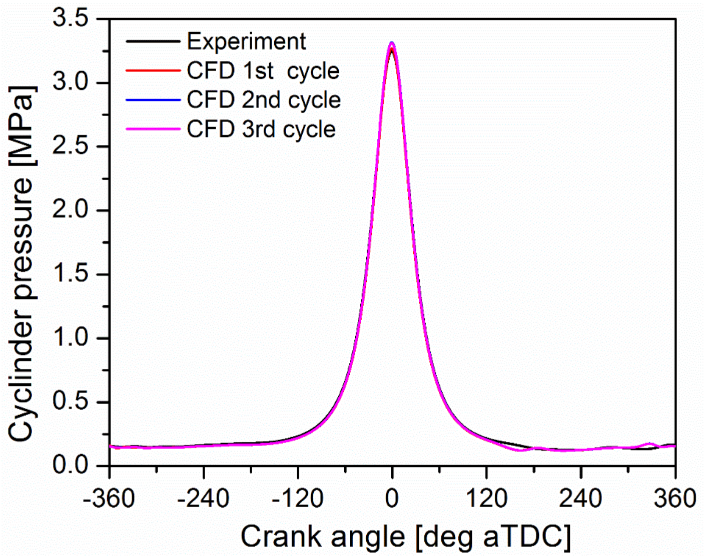


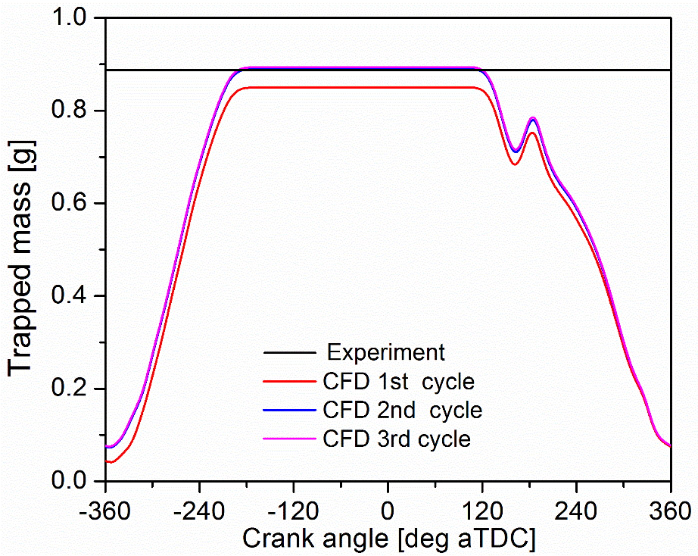
ANL Motored Model of ORNL SCE Validated; Moving Towards Simulations of Fired Cycles

ANL, Yue: Accomplishments (3/3)

- Model validation in the ORNL single-cylinder engine under motoring condition; validation under fired cycles is in-progress
  - Crank-angle resolved intake/exhaust pressures were provided from experimental measurements
  - Simulation results converge for the second and third cycle, with good accuracy in predictions of cylinder pressures (<2% error in peak pressure) and cylinder trapped mass (<1% error)
  - Fired cycle simulations will commence once GDI spray validation from SNL is complete







Response to Previous Year Reviewers' Comments Note: Most of FY18 Work Reviewed in FT053 in 2018

FT053: Co-Optima Boosted Spark-Ignition and Multimode Combustion, Part 1

Reviewer comments were mainly positive

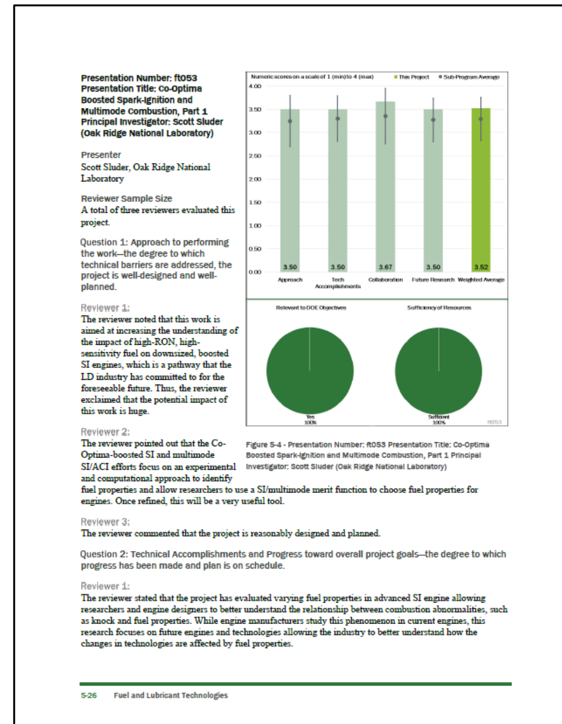
"…researchers have collaborated with OEMs, fuel manufacturers, academia, and national laboratories to perform this research. This work is a great example of how to collaborate with industry and national laboratories."

"…excellent progress and results have been achieved."

Reviewers also indicated room for improvement

"…the use of knock-intensity extrema in the knock model may be too conservative to be used in the design optimization, and it could lead to a design of less than the true optima."

Thank you for the input. The new model presented this year (L-W integral approach) has been calibrated against experimental KLSA measured by a knock meter under multiple conditions, so the current model actually considers the knock-sensor operation.



Presentation Number: ft053
Presentation Title: Co-Optima Boosted Spark-Ignition and Multimode Combustion, Part 1
Principal Investigator: Scott Sluder (Oak Ridge National Laboratory)

Presenter
Scott Sluder, Oak Ridge National Laboratory

Reviewer Sample Size
A total of three reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:
The reviewer noted that this work is aimed at increasing the understanding of the impact of high-RON, high-sensitivity fuel on downsized, boosted SI engines, which is a pathway that the LD industry has committed to for the foreseeable future. Thus, the reviewer exclaimed that the potential impact of this work is huge.

Figure 5-4 - Presentation Number: ft053 Presentation Title: Co-Optima Boosted Spark-Ignition and Multimode Combustion, Part 1 Principal Investigator: Scott Sluder (Oak Ridge National Laboratory)

Reviewer 2:
The reviewer pointed out that the Co-Optima-boosted SI and multimode SI/ACI efforts focus on an experimental and computational approach to identify fuel properties and allow researchers to use a SI/multimode merit function to choose fuel properties for engines. Once refined, this will be a very useful tool.

Reviewer 3:
The reviewer commented that the project is reasonably designed and planned.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer stated that the project has evaluated varying fuel properties in advanced SI engine allowing researchers and engine designers to better understand the relationship between combustion abnormalities, such as knock and fuel properties. While engine manufacturers study this phenomenon in current engines, this research focuses on future engines and technologies allowing the industry to better understand how the changes in technologies are affected by fuel properties.

5-26 Fuel and Lubricant Technologies

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]

ORNL - MCE
E.1.1.2

- Ford Motor Company
  - Hardware support
- Direct with ANL on CFD.
- USDRIVE Fuels Working Group
  - 14 member organizations
  - US OEMs, energy companies, US DOE, and National Labs (NREL, ANL, and ORNL)

ANL - CFD
G.1.10.1

- Direct collaborations with ORNL on MCE activities
- Direct collaborations with ORNL on SCE activities
- Convergent Science Inc. for software
- SNL for detailed spray data to validate model
- Autonomie group at ANL for vehicle system simulation

ORNL - SCE
F.1.8.1

- Direct collaborations with ANL for SCE modeling
- General Motor Company
  - Hardware support for future work to provide more realistic ACI strategy
- Shell Energy Company
  - Providing fuels for future work to provide more representative refinery streams

Remaining Challenges and Barriers

Progress is being made, but barriers discussed in the overview slide persist.

Barriers**

USCAR Priority 1: Dilute SI Combustion

- Knock Mitigation

→ *Developing a better understanding of how fuel properties can be predictive of knock*

- Progress on a predictive knock model that allowed CFD-to-fuel economy estimations
- Progress showing OI is a good framework for boosted conditions
- Work remains extending this to MON-relevant pressure-temperature conditions

USCAR Priority 3: Multimode ACI

- Increased tolerance to market fuel variability

→ *Developing a better understanding fuel autoignition under ACI conditions*

- Progress showing that fuel OI framework breaks down for ACI conditions, and that fuel chemistry may be important
- Work remains extending this to generalize observation
- Work remains getting to a fuel property for ACI conditions

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

Proposed Future Research

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

ORNL Multi-Cylinder

- Focus for remainder of FY19 and in FY20 will be on studying MON effects to assure reliable SI operation at high loads in a multimode SI/ACI strategy

ANL CFD Modeling:

- Study the auto-ignition process in SI/ACI multimode operation with focus on fuel properties and fuel-specific mixing process
- Extension of the P-T analysis framework to consider in-cylinder thermal/phi stratification and thermodynamic property effects such as heat of vaporization and heat capacity ratio

ORNL SCE:

- Pursue general applicability of finding that olefins autoignite more readily under ACI conditions
  - New experimental platform supported by GM for more realistic ACI operation
  - Use fuel blends provided by Shell with more refinery-relevant fuel streams (olefins, aromatics, ethanol)

Installation of GM SCE at ORNL capable of more production-relevant ACI

Summary

Relevance

- IC engines and the use of liquid fuels will continue to dominate transportation for many years
- Mitigation of knock is a key barrier to attaining higher efficiency for IC engines (USDRIVE roadmap)

Approach

- MCE experiments to quantify BTE improvements, feed into vehicle system, LCA, and other modeling
- Develop validated CFD models to enable investigations of isolated fuel properties in scalable manner
- SCE experiments with kinetic modeling to understand fuel properties and kinetics across PT domain

Accomplishments

- Provide foundational data and published series of octane studies with US DRIVE Fuel Working Group
- Demonstrated capability of tool to go from CFD to drive cycle to investigate isolated fuel properties
- Established kinetic basis for OI across PT domain, illustrating importance of LTHR activation under boost

Collaborations

- "Co-Optima" has 9 National Labs, stakeholder engagement, and external advisory board
- Projects presented at AEC semi-annual program review, engaged with ACEC TT
- Peer-to-peer collaborations across national labs to develop modeling support for experimental efforts
- Numerous project-level collaborations direct with industry and industry consortia for support and feedback

Future Work

Co-Optima has identified several areas where the fuel property approach falls short of fully describing behavior in the engine. Experimental and computation investigations will be conducted to elucidate the behavior of fuel properties as they relate to OI, HoV, and LSPI.

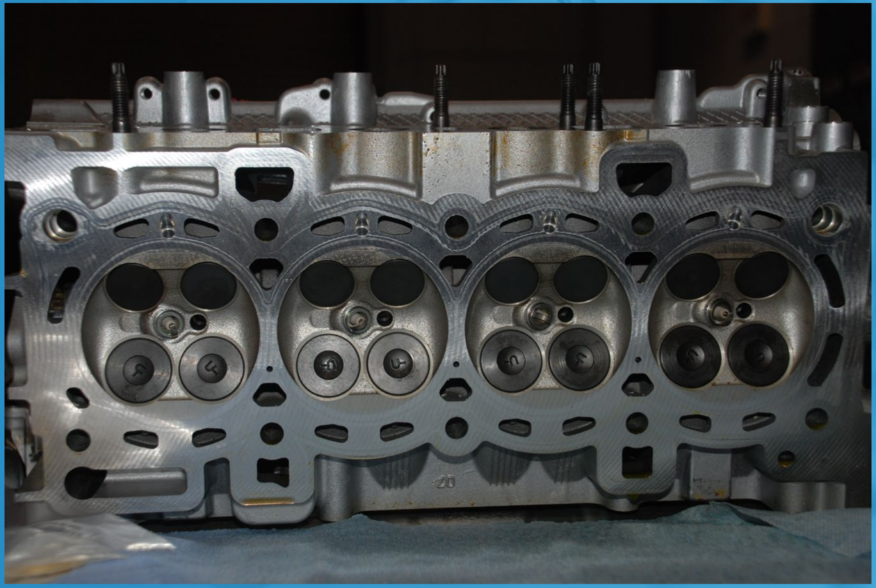
Any proposed future work is subject to change based on funding level

Technical Back-Up Slides

EcoBoost Engine At ORNL

Technical Backup Slide 1

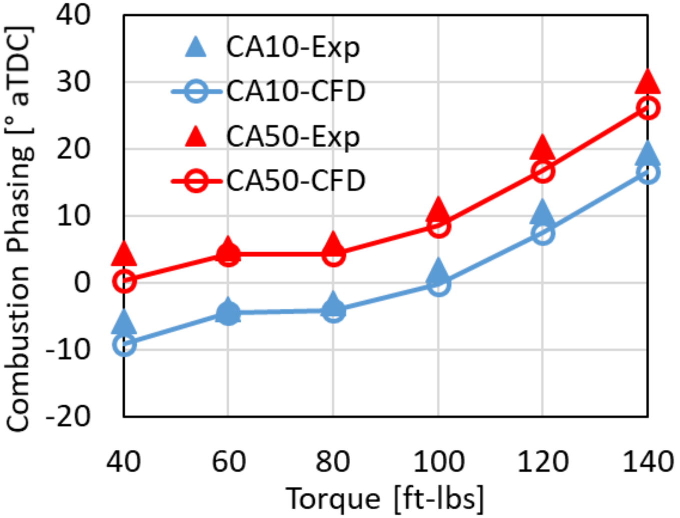
- Displacement 1.6 L
- 173 Hp @ 5,700 RPM
- 184 Ft-lbs @ 2,500 RPM
- 79mm x 81mm bore x stroke
- Compression Ratio 10.0
    - Modified pistons enable up to 13.2.
- Single Turbocharger
- Center-mount DI Fueling
- Twin-Independent Variable Cam Timing
- Open ECU

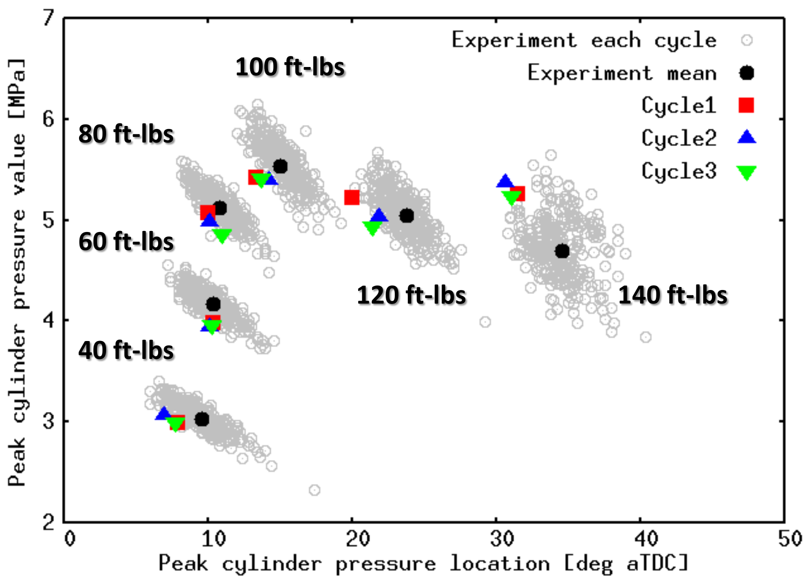


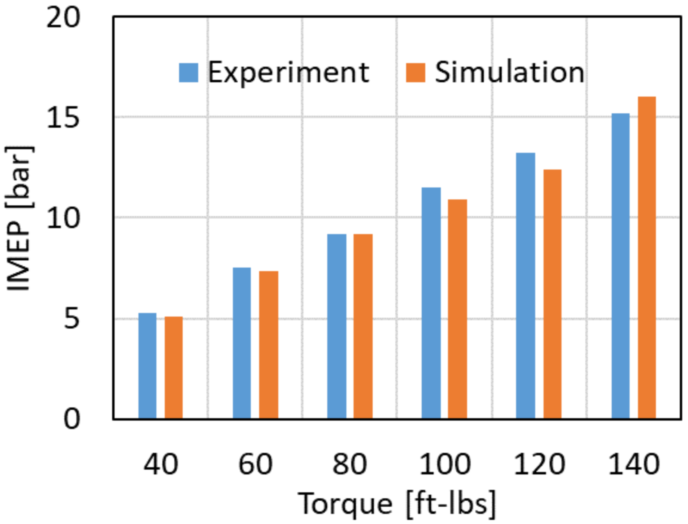
CFD Model Incorporates KLSA Prediction and Has Been Validated Validation on ORNL MCE

Technical Backup Slide 2

- Six operating loads at 2000 rpm, with three consecutive cycles simulation for each case;
- Maximum error in IMEP prediction is <5%; Maximum error in CA10&50 is <4°CA;
- **~10 times speedup** in runtime than previous approach.



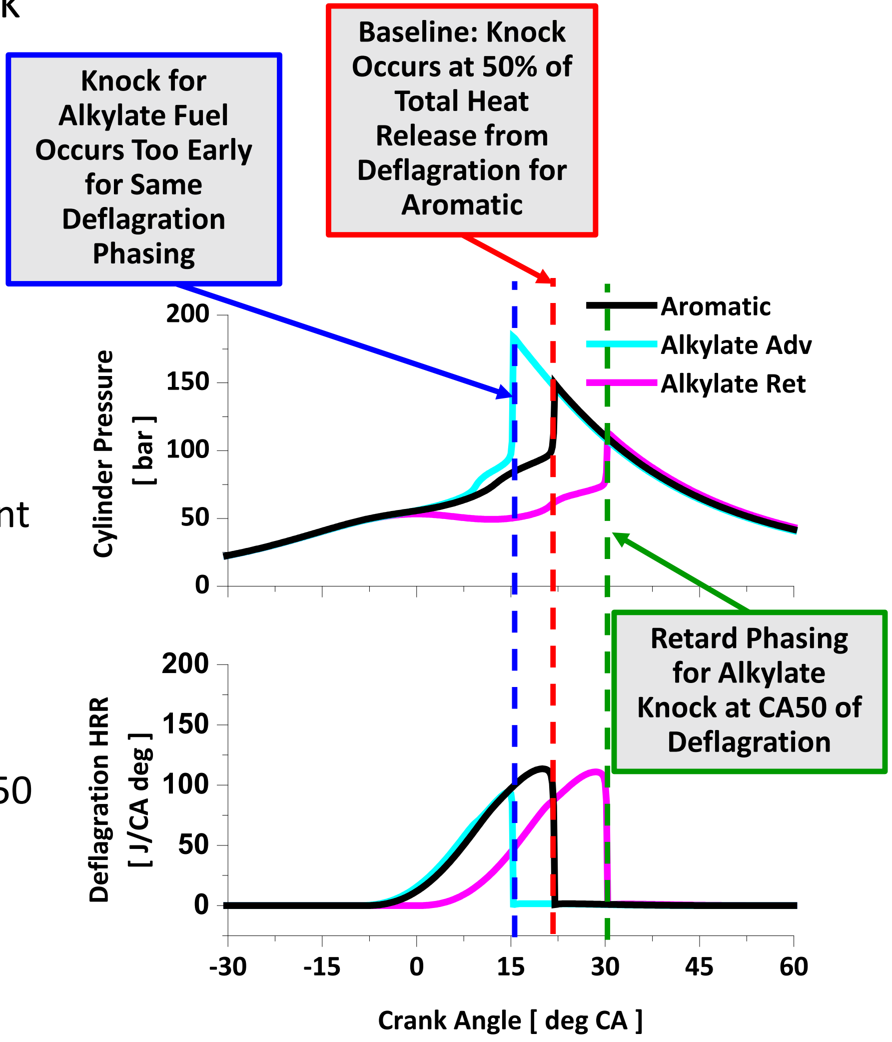




Kinetic Modeling Methodology for SI Combustion

Technical Backup Slide 3

- Chemkin-Pro Spark Ignition Zonal Model for Knock Assessment
  - 2-zone model, stoichiometric conditions, air and fuel only (no trapped residuals or minor species considered)
  - Adiabatic conditions (no heat transfer)
  - Mass moves from unburned zone to burned zone according to Weibe function (10-90% burn held constant at 26 CA deg)
  - Unburned zone kinetics calculated, taking into account compression heating from deflagration
  - Weibe function phasing adjusted through trial-and-error to achieve knock in unburned zone at CA50 of deflagration
  - Fuel quality, as predicted by kinetics, assessed by CA50 phasing
- Three operating conditions assessed
  1. Beyond RON: IVC T = 325 K, IVC P = 2 bar, CR = 12:1
  2. RON-like: IVC T = 355 K, IVC P = 1 bar, CR = 14:1
  3. MON-like: IVC T = 405 K, IVC P = 1 bar , CR = 14:1



Kinetic Modeling Reveals Inconsistencies with OI Under ACI Conditions, with E30 Fuel Most Prone to Autoigniton

Technical Backup Slide 4

Beyond RON-Relevant Condition

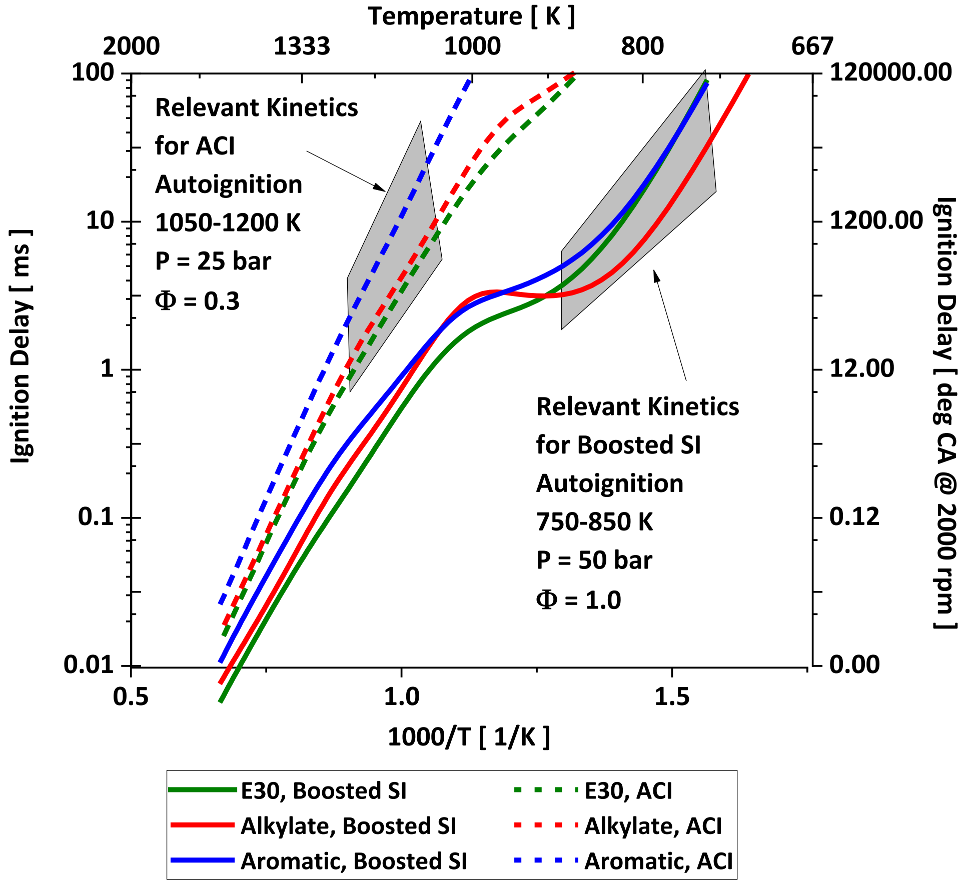
- Stoich, 50 bar, 750-850K
- Ethanol and aromatic fuel similar
- Alkylate fuel significantly more reactive
- Consistent with octane index

ACI-Relevant Conditions

Φ = 0.3, 30 bar, 1050-1200 K

E30 is slightly more reactive than alkylate (consistent with octane index)

Aromatic is least reactive (inconsistent with octane index)



19 Fuels Investigated Experimentally in ORNL SCE

Technical Backup Slide 5

Parameters	Units	Test method	Co-Optima "Core" Fuels					Regular Grade E10	Co-Optima LDSI Tier 3 Screening						BOB	Model Fuels			High S		
			Co-Optima alkylate	Co-Optima aromatic	Co-Optima E30	Co-Optima Cycloalkane	Co-Optima Olefinic	"Tier III" E10 EEE	Level 3 Ethanol	Level 3 n-propanol	Level 3 iso-propanol	Level 3 iso-butanol	Level 3 bioreformate	Level 3 Diisobutylene	Level 3 BOB	Iso-octane	PRF 96.9	TSF 96.9	20% Prenol	20% amylene	20% methyl-cyclopentane
Research Octane Number	—	ASTM D2699	98.0	98.1	97.9	98.0	98.2	91.8	98.0	97.2	97.5	98.0	97.4	98.1	86.8	100.0	96.9	96.9	93.0	93.6	87.5
Motor Octane Number	—	ASTM D2700	96.7	87.6	87.1	87.1	88.0	84.2	87.7	86.5	88.2	87.0	86.7	86.6	83.0	100.0	96.9	85.2	83.3	83.7	83.0
Octane Sensitivity	—	Calculated	1.3	10.5	10.8	10.9	10.2	7.6	10.3	10.7	9.3	11.0	10.7	11.5	3.8	0.0	0.0	11.7	9.7	9.9	4.5
Aromatics	vol %	ASTM D1319	0.0	35.8	8.1	28.2	10.6	22.6	15.3	14.9	15.5	14.1	50.5	13.5	19.4	‡	‡	‡	16.4	16.0	16.1
Saturates	vol %	ASTM D1319	100.0	65.0	57.1	70.3	58.1	71.2	58.9	57.4	59.1	53.3	45.8	52.5	75.7	‡	‡	‡	63.0	62.2	79.2
Olefins	vol %	ASTM D1319	0.0	4.2	5.0	1.5	31.3	5.2	2.9	2.7	2.6	2.6	2.2	33.1	3.7	‡	‡	‡	3.2	20.3	3.1
Ethanol	vol %	ASTM D4815mod	0.0	0.0	30.0	0.0	0.0	9.8	21.2	0.0	0.0	0.0	0.0	0.0	0.0	‡	‡	‡	0.0	0.0	0.0
iso-butanol	vol %	ASTM D4815mod	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	35.6	0.0	0.0	0.0	‡	‡	‡	0.0	0.0	0.0
iso-propanol	vol %	ASTM D4815mod	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	27.5	0.0	0.0	0.0	0.0	‡	‡	‡	0.0	0.0	0.0
n-propanol	vol %	ASTM D4815mod	0.0	0.0	0.0	0.0	0.0	0.0	0.0	27.7	0.0	0.0	0.0	0.0	0.0	‡	‡	‡	0.0	0.0	0.0
Initial boiling point	°C	ASTM D86	50.3	34.3	38.2	36.7	35.7	36.5	29.4	30.0	31.1	31.1	31.7	30.6	25.0	‡	‡	‡	26.1	25.6	28.3
T10[b]	°C	ASTM D86	93.1	59.4	60.7	55.7	77.1	54.6	48.9	54.4	55.0	60.0	50.6	62.2	44.4	‡	‡	‡	51.1	42.2	53.3
T50[b]	°C	ASTM D86	100.3	108.1	74.3	87.4	104.3	89.9	72.2	88.3	77.8	98.3	123.9	102.8	101.1	‡	‡	‡	106.1	86.7	192.2
T90[b]	°C	ASTM D86	105.9	157.9	155.2	142.7	136.2	157.9	131.7	131.1	130.0	107.7	169.4	126.7	140.6	‡	‡	‡	137.2	133.3	133.9
Final boiling point	°C	ASTM D86	161.3	204.4	204.1	203.5	197.7	195.0	193.3	195.6	192.2	187.7	196.1	191.1	197.8	‡	‡	‡	189.4	195.0	195.6
Carbon	wt %	ASTM D5291	83.75	87.22	74.78	87.08	85.40	82.63	77.78	78.32	77.64	77.28	88.16	85.88	85.72	84.21	84.20	89.95	82.50	86.09	85.79
Hydrogen	wt %	ASTM D5291	15.80	13.12	13.79	13.24	14.50	13.66	14.11	14.12	14.02	13.98	12.40	14.39	14.32	15.79	15.80	10.05	13.71	14.32	14.28
Oxygen	wt %	ASTM D5599	0.00	0.00	11.19	0.00	0.00	3.71	8.11	7.56	8.34	8.74	0.00	0.00	0.00	0.00	0.00	0.00	3.79	0.00	0.00
Density at 15°C	—	ASTM D4052	0.696	0.757	0.752	0.756	0.723	0.744	0.737	0.745	0.739	0.752	0.784	0.722	0.721	‡	‡	‡	0.746	0.712	0.727
Lower heating value (LHV)	MJ/kg	ASTM D4809	44.520	42.950	38.170	43.208	44.071	41.690	39.776	40.126	39.978	39.738	42.579	43.846	43.921	44.300	44.310	41.309	41.921	43.925	43.863
Stoichiometric air-fuel ratio	—	Calculated	15.17	14.52	12.92	14.55	14.85	14.07	13.48	13.57	13.42	13.35	14.35	14.82	14.81	15.15	15.15	13.83	14.07	14.80	14.80
LHV for stoichiometric mixture per kilogram air	MJ/kg air	Calculated	2.94	2.96	2.95	2.97	2.97	2.96	2.95	2.96	2.98	2.98	2.97	2.96	2.97	2.92	2.92	2.99	2.98	2.97	2.96

RON ≈ 98

Alkylate fuel has low S (1.3)

Other fuels have S ~ 10.7 with chemical source of S changing (aromatics, ethanol, olefins, cycloalkanes)

Blended to RON ≈ 98 in common BOB

- **Variable concentration of bioblendstock of interest**
  - **n-propanol**
  - **iso-propanol**
  - **ethanol**
  - **aromatics (bioreformate)**
  - **olefins (diisobutylene)**
  - **iso-butanol**

- **Contain up to 3 compounds**
- **PRF and TSF relevant to RON and MON tests**

3 fuel candidates with moderate RON and high S blended into BOB at 20 vol%