

2021 DOE Vehicle Technologies Office
Annual Merit Review

Fuel Effects in Boosted, Spark-Ignition Combustion

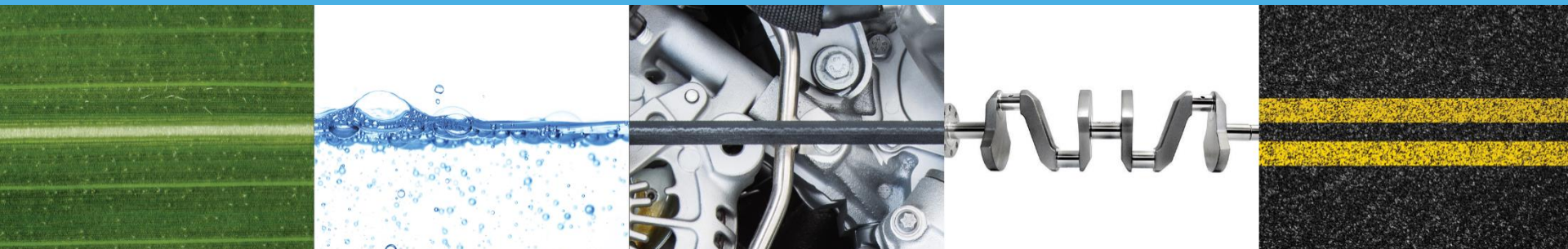
Presenter: James Szybist (ORNL)
Project ID #FT091

June 24, 2021



CO-OPTIMIZATION OF
FUELS & ENGINES

better fuels | better vehicles | sooner



Acknowledgements



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Sibendu Som – Argonne National Laboratory
Hengjie Guo – Argonne National Laboratory
Roberto Torelli – Argonne National Laboratory
Zongyu Yue – Argonne National Laboratory
Many others on the Co-Optima Team



The purpose of this presentation is to provide a multi-year overview of the boosted spark-ignition research rather than a 1-year progress update. As a result, this presentation does not adhere to the typical AMR template.



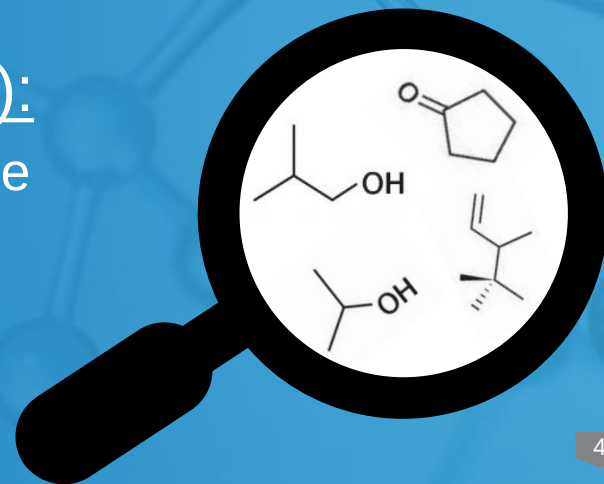
Central Engine Hypothesis:

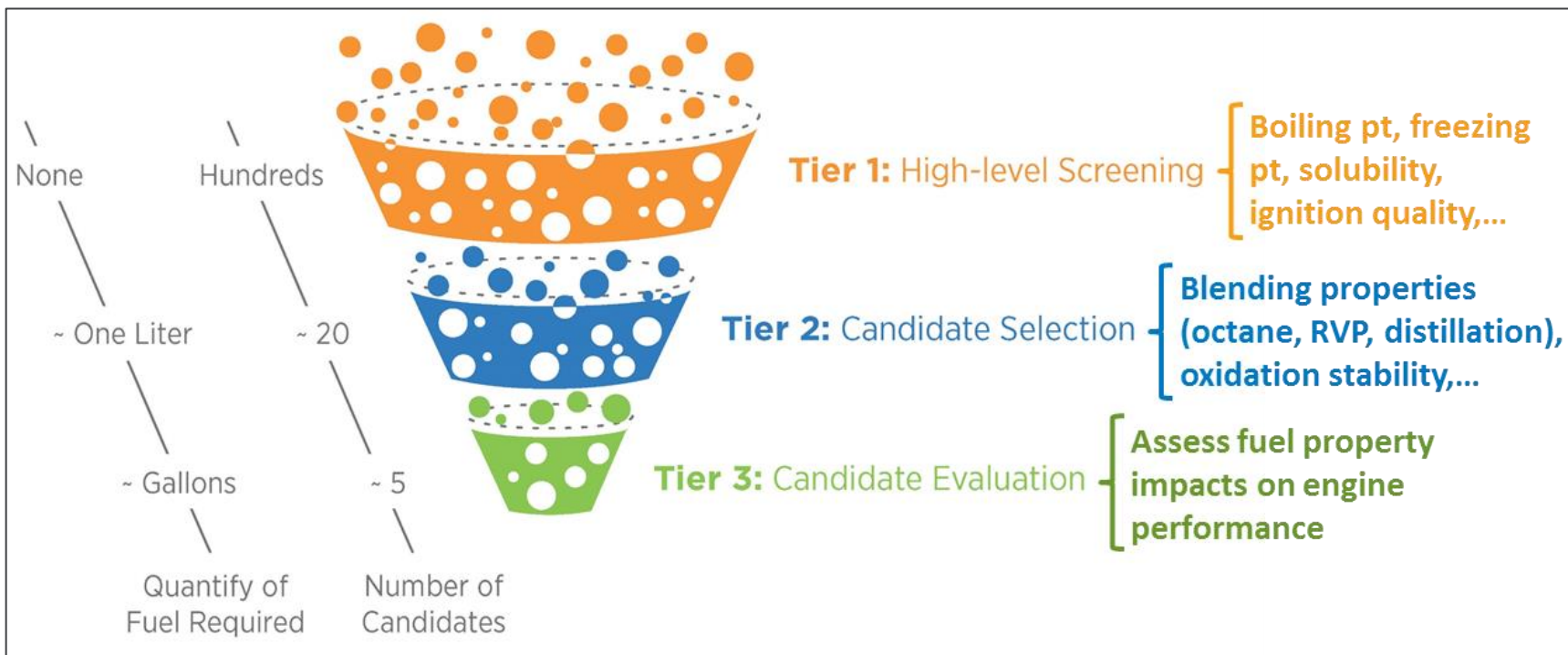
There are engine designs and operating strategies that can improve efficiency. Improved fuels can enable the use of these designs and operating strategies.



Central Fuel Property Hypothesis (CFPH):

Equivalent fuel properties will result in equivalence performance, regardless of the composition







Co-Optimization of Fuels & Engines
Properties of Co-Optima Core Research Gasolines

August 2018



Table 1. Fuel Properties of Co-Optima Core Research Gasolines

		Olefinic	E30	Aromatic	Alkylate	High cycloalkane
Specific gravity	D4052	0.7231	0.7529	0.7575	0.6969	0.7557
Density @ 15°C (g/mL)	D4052	0.7229	0.7527	0.7572	0.6968	0.7555
Index of refraction @ 20°C [4]		1.409	1.401	1.431	1.391	1.426
RON (R)	D2699	98.2	97.4	98.1	98.0	98.0
MON (M)	D2700	88.0	86.6	87.8	96.6	87.1
Octane rating	R+M/2	93.1	92.0	93.0	97.3	92.6
Octane sensitivity	R-M	10.2	10.8	10.3	1.4	10.9
Reid vapor pressure (psi)	D5191	6.10	7.66	7.17	4.15	8.00
Gross heating value (MJ/kg)	D4809	47.148	41.096	45.735	47.877	46.018
Net heating value (MJ/kg)	D4809	44.071	38.170	42.952	44.524	43.208
HOV (measured) (kJ/kg)		337	565	412	309	393
HOV (calc. from DHA) (kJ/kg)		330	532	361	308	370
PMI		1.004	1.275	1.803	0.221	1.491
Yield sooting index [11]		80.95	47.86	114.9	60.91	97.92

- Core fuels represent the major chemical families of fuel candidates

Alkane

Aromatic

Alcohol

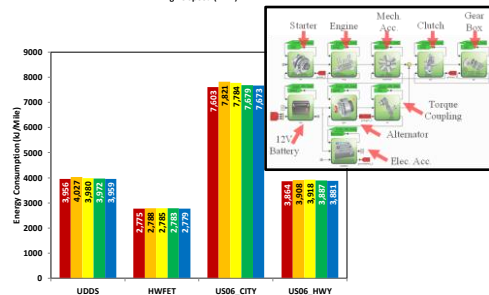
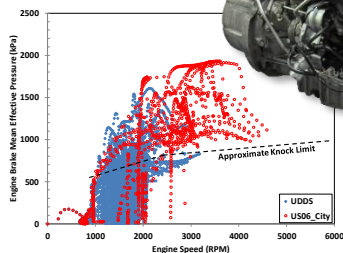
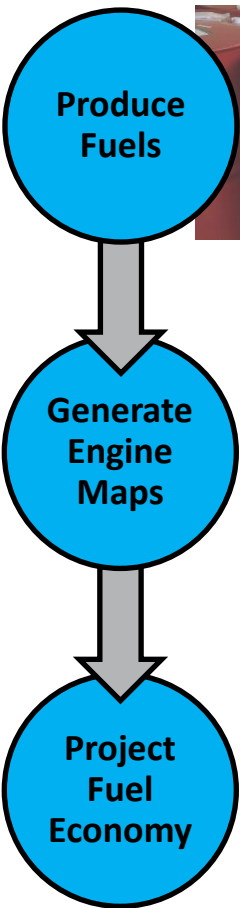
Olefin

Naphthene

- Same nominal research octane number (RON): 98
- Four fuels with same nominal octane sensitivity (S_{octane}): 10.5
- Range of heat of vaporization (HoV)
- Range of particulate matter index (PMI)

- Heavily used throughout Co-Optima initiative

- Used at 6 national labs, numerous universities
- LLNL developed a kinetic model and surrogate formulations for each core fuel
- >20 publications



- Quantified efficiency benefits of up to 9.9% in collaboration with industry
 - Affirmed central engine hypothesis
 - Affirmed CFPH

		Projected Engine Efficiency Increase (%)					
		Ethanol	n-Propanol	Isopropanol	Isobutanol	Diisobutylene	Bioref. Sur.
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	3.3
97 RON							
Leone et al.	4.6	4.3	4.3	4.1	3.6	3.6	3.6
Co-optima Merit	5.6	6.1	4.4	6.0	5.4	5.2	5.2
100 RON							
Leone et al.	6.4	6.1	6.0	5.8	5.0	5.0	5.0
Co-optima Merit	9.3	9.9	7.1	9.6	8.7	7.8	7.8
		Projected Volumetric Fuel Economy Increase (%)					
		Ethanol	n-Propanol	Isopropanol	Isobutanol	Diisobutylene	Bioref. Sur.
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. Sur.
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	



Well-to-Wheels Energy and Greenhouse Gas Emission Analysis of Bio-Blended High-Octane Fuels for High-Efficiency Engines



Potential Impacts of Increased Ethanol Blend-Level in Gasoline on Distribution and Retail Infrastructure



U.S. DRIVE Fuels Working Group Engine and Vehicle Modeling Study to Support Life-Cycle Analysis of High-Octane Fuels

By: C. Scott Stulen, David E. Smith, Oak Ridge National Laboratory
James E. Anderson, Thomas G. Leone, Michael H. Shelby, Ford Motor Company



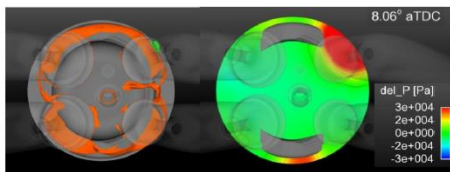
<https://www.energy.gov/eere/vehicles/downloads/us-drive-fuels-working-group-high-octane-reports>



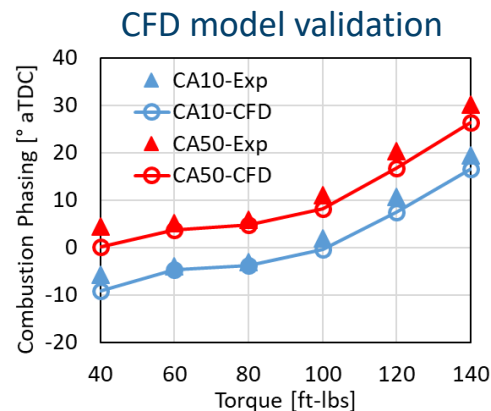
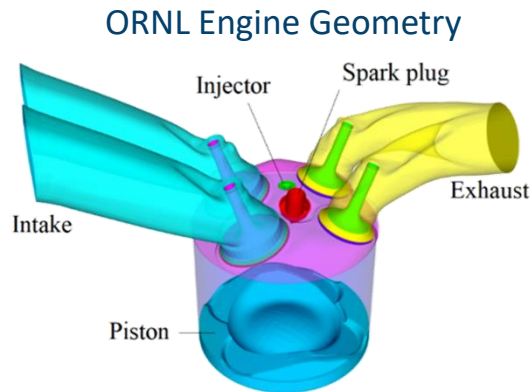
An accurate and low-cost CFD modeling approach developed for KLSA prediction

- G-equation for efficient combustion modeling
- Transported Livengood-Wu (LW) integral for knock modeling
- Automatically switch between single- and two-stage LW integrals for fuels with simple and complex ignition behaviors
- Key advantage:** no detailed chemistry or Mach CFL constraint are needed → Low computational cost

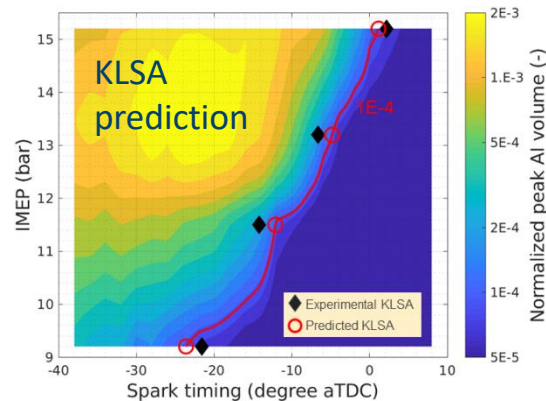
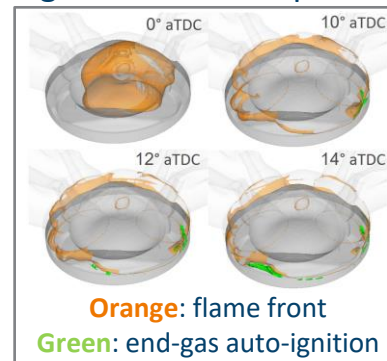
Knock detected in end-gas with detailed chemistry



Spark-ignited flame (orange iso-surface) and end-gas ignition (green iso-surface)



Livengood-Wu model predictions



Yue et al, *J. Energy Resour. Technol.*, 2019, doi:10.1115/1.4043393
 Yue & Som, *Applied Energy*, 2021, doi:10.1016/j.apenergy.2019.114221
 Yue et al., *J. Eng. Gas Turbines Power*, 2021, doi:10.1115/1.4050583

Accomplishment

Attributing Efficiency Potential of Individual Fuel Properties using Merit Function

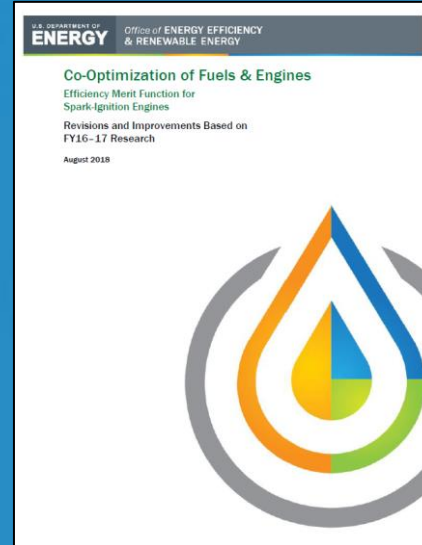


Fuel Properties Quantified for Efficiency

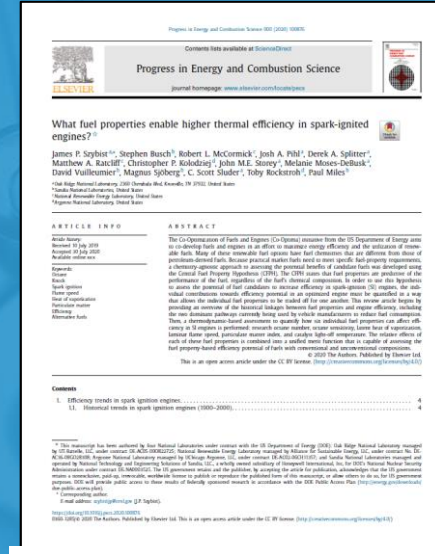
- Research octane number (RON)
- Octane sensitivity (S_{octane})
- Heat of vaporization (HoV)
- Laminar flame speed
- Catalyst light-off temperature
- Particulate matter index (PMI)

Basis for Fuel Property Effects

- Increased compression ratio (r_c)
- Downsizing and downspeeding
- Dilute combustion
- Cold start emissions compliance
- Particulate emissions compliance



<https://www.nrel.gov/docs/fy18osti/67584.pdf>



[10.1016/j.pecs.2020.100876](https://doi.org/10.1016/j.pecs.2020.100876)

Accomplishment Octane Index Found to Correlate to Knock



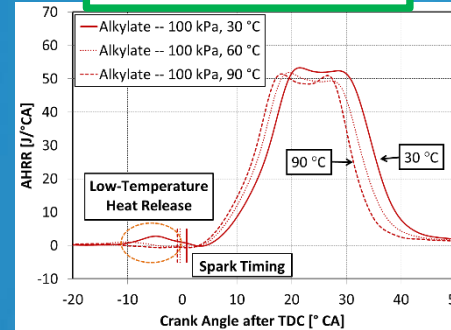
- RON and motor octane number (MON) are not predictive of knock in modern engines
- RON and S_{octane} are combined in the octane index* (OI) to predict knock

$$\text{OI} = \text{RON} - K * S_{\text{octane}}$$

- K is determined through multi-variable linear regression analysis
 - K is physically significant due to low temperature heat release
 - $K < 0$ corresponds to pressure-temperature conditions kinetically conducive to LTHR
 - S_{octane} indicates fuel-specific propensity to producing LTHR
- Boosted SI engines operate at negative K, making OI and K determination important

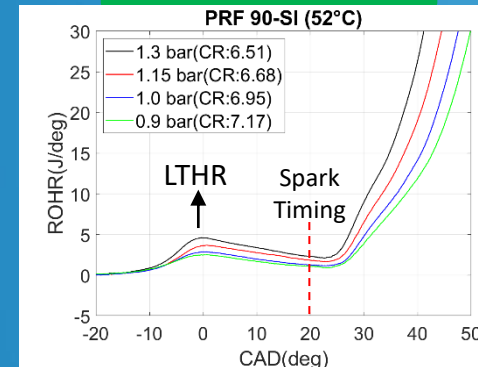
*OI developed by Kalghatgi (SAE 2001-01-3584, 2001-01-3585)

SNL LTHR Data



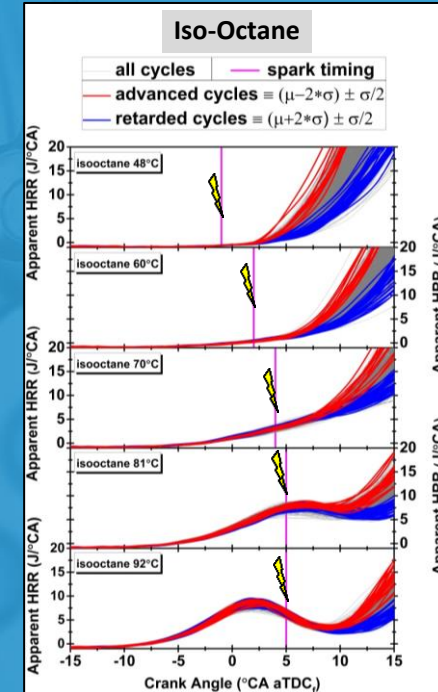
Vuilleumier and Sjöberg, DOI: [10.4271/2017-01-0662](https://doi.org/10.4271/2017-01-0662)

ANL LTHR Data



Waqas et al., DOI: [10.1016/j.fuel.2019.115745](https://doi.org/10.1016/j.fuel.2019.115745)

ORNL LTHR Data



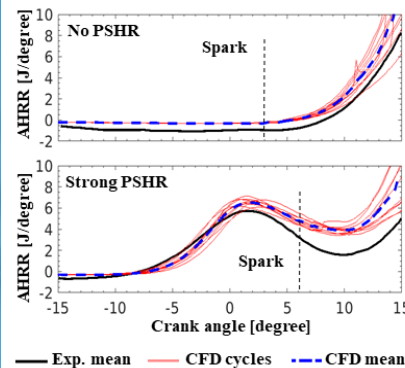
Szybist and Splitter,
DOI: [10.1016/j.combustflame.2016.12.002](https://doi.org/10.1016/j.combustflame.2016.12.002)



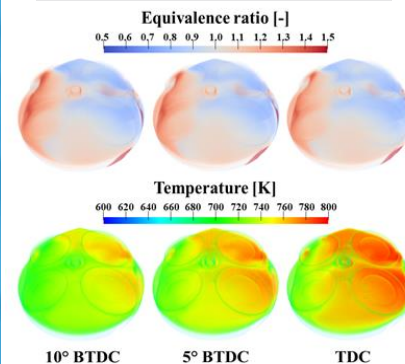
First-of-its-kind study on characterizing low-temperature, pre-spark heat release (PSHR) using 3-D CFD tools

- Developed combustion model best practices to capture the onset of PSHR accurately: the chemistry solver must be kept active during gas exchange.
 - ✓ Previous-cycle residuals are key to the occurrence of PSHR
 - ✓ Simulations integrate chemistry mechanisms by LLNL
- 3-D analyses revealed PSHR begins in the fuel-lean region near the intake, but its effect becomes more significant in the fuel-rich region as time progresses
- P-T trajectories provided further insights in the trends observed for the different levels of PSHR intensity
- Fuel property effects were also examined: heat of vaporization (HoV), laminar flame speed, saturation pressure, liquid specific heat

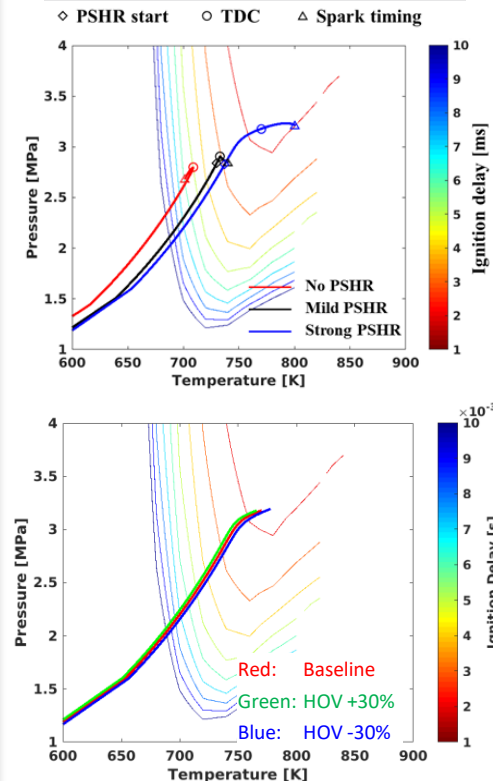
Model validation



Dynamics of PSHR

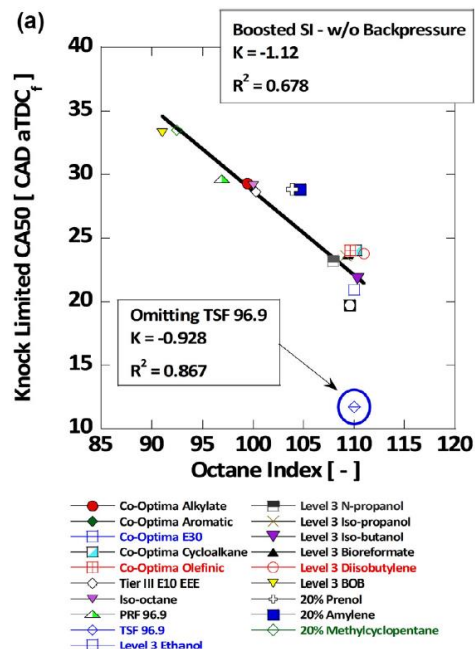


P-T trajectory analysis



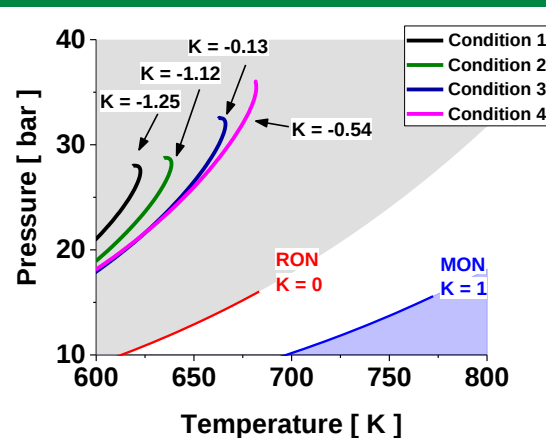


Outlier Behavior of Fuel Under Boosted Operation



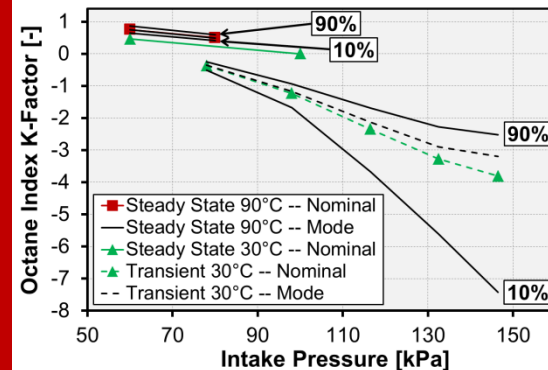
Non-Monotonic Behavior of K in Pressure-Temperature Domain

Maximum K Value Does Not Correspond to Highest Temperature Condition



K-Factor Uncertainty Increases with Intake Pressure

K-Factor is Lower Under Transient Conditions Due to Lower Surface T

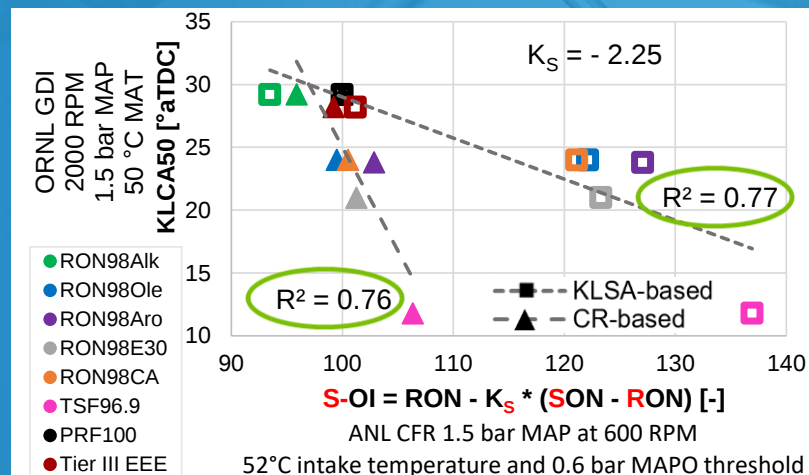
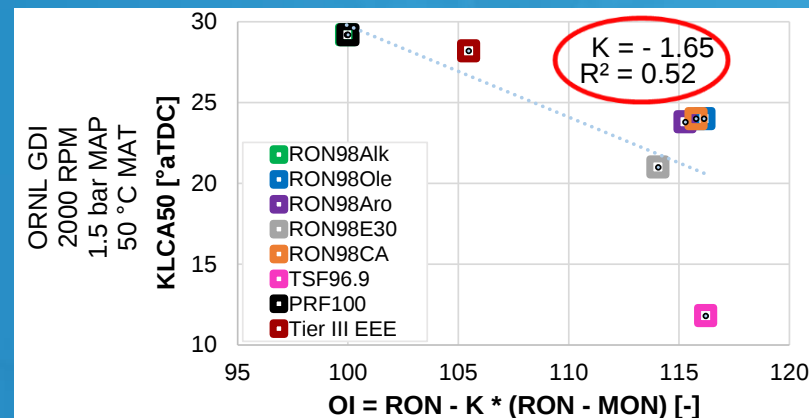


Accomplishment

Supercharged Octane Index (S-OI) improves correlation over Octane Index



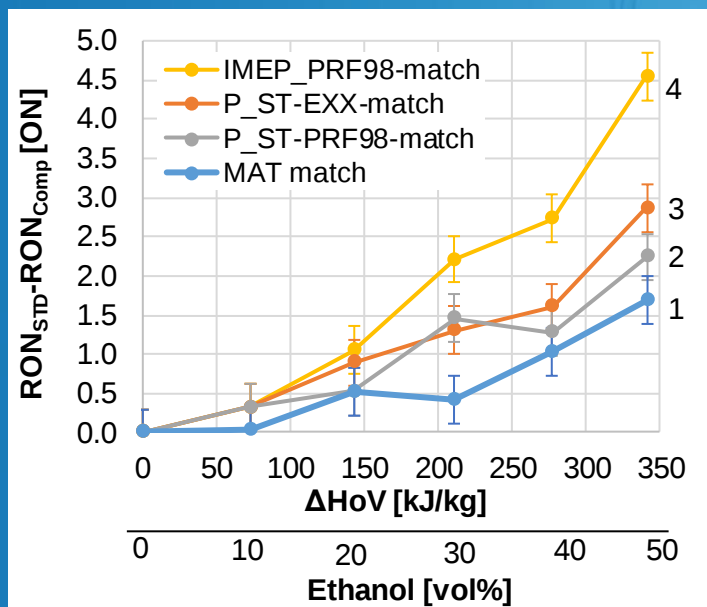
- Determination of K values based on RON and MON may have intrinsic uncertainties
- Supercharged octane number (SON), developed under Co-Optima, is more relevant to modern boosted engines
- OI based on RON and SON produces much stronger correlation
- Thus, new fuel property measurements, such as SON, can enable more predictive performance determination





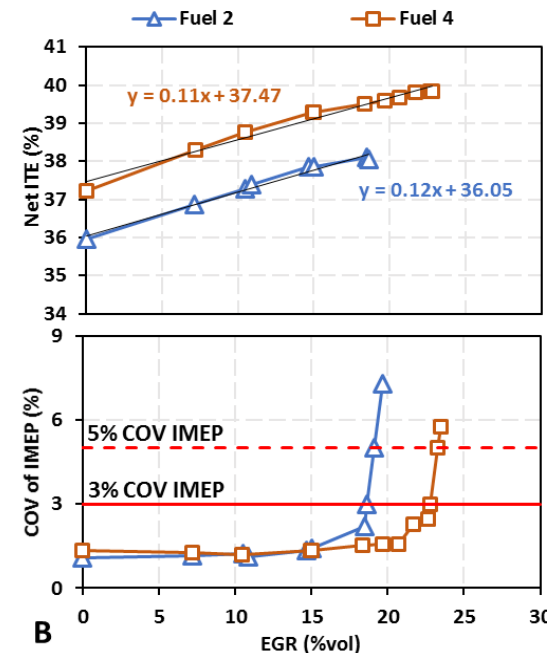
HoV Reduces Knock Propensity

- Only partially accounted for in RON test
- HoV also increases downsizing potential



Flame Speed Increased Dilution Tolerance

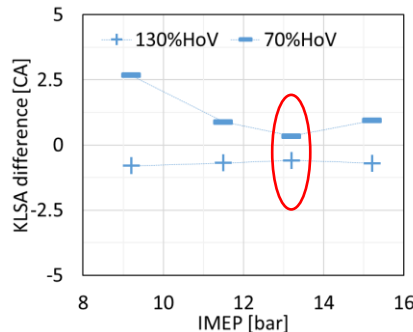
- Reduced cycle-to cycle variations
- Higher efficiency through increased dilution



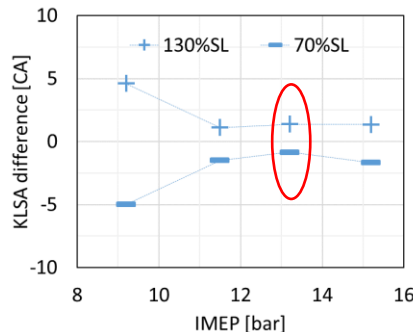


- HOV affects KLSA and knock tendency through its cooling effect in the end-gas region
- S_L has significant impact on combustion phasing, which in turn affects end-gas auto-ignition and knock onset
- HOV and SL also impact ITE by affecting heat loss and combustion duration, respectively

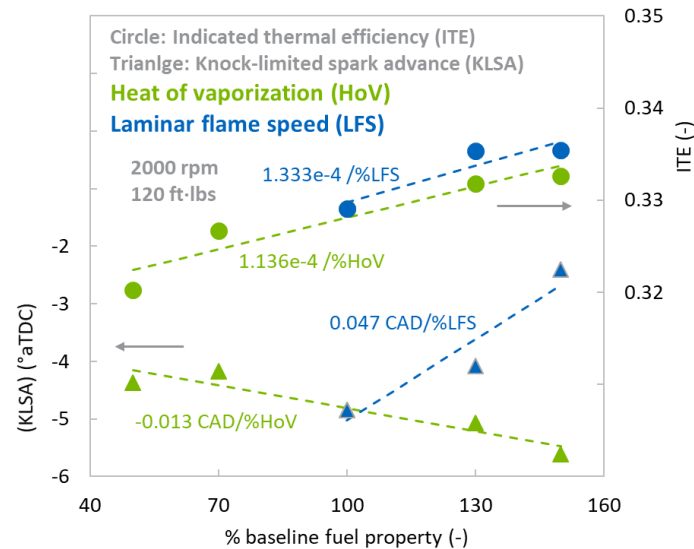
Heat of vaporization (HOV)



Laminar flame speed (S_L)



Effect of HOV and S_L on KLSA and ITE

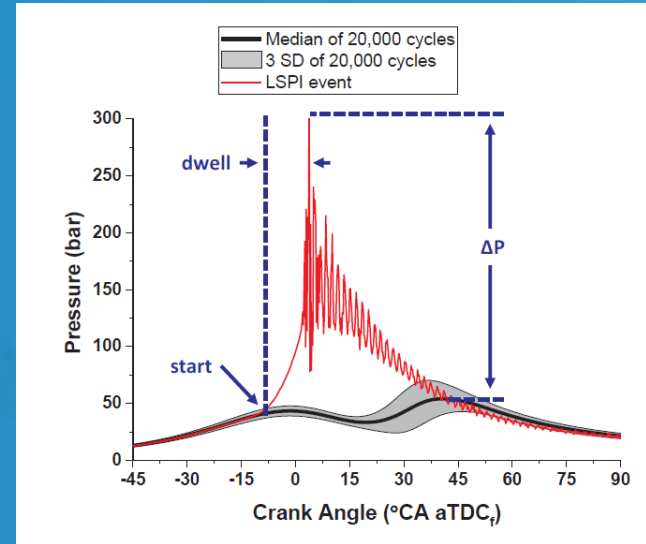


Yue & Som, *Applied Energy*, 2021, doi:10.1016/j.apenergy.2019.114221

IMEP = indicated mean effective pressure, a measure of load



- There is a multi-step process that leads to damaging superknock
 - Initiation → flame establishment → autoignition → superknock
 - Fuels can effect likelihood and severity of superknock at multiple steps
 - Present analysis focuses on initiation
- Well-established that preignition propensity increases with retained fuel in top ring zone
 - Proportional with increased high boiling point components, particulate matter index (PMI)
 - PMI increases with lower volatility higher double bonds equivalent (DBE)
 - Consistent with recent study by Swartz et al. (SAE 2020-01-0612)



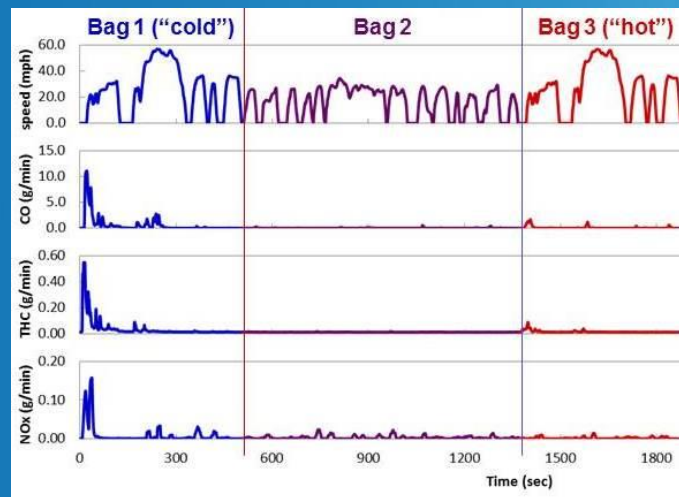
Jatana et al., *Fuel*. 2018;230:474-82.

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

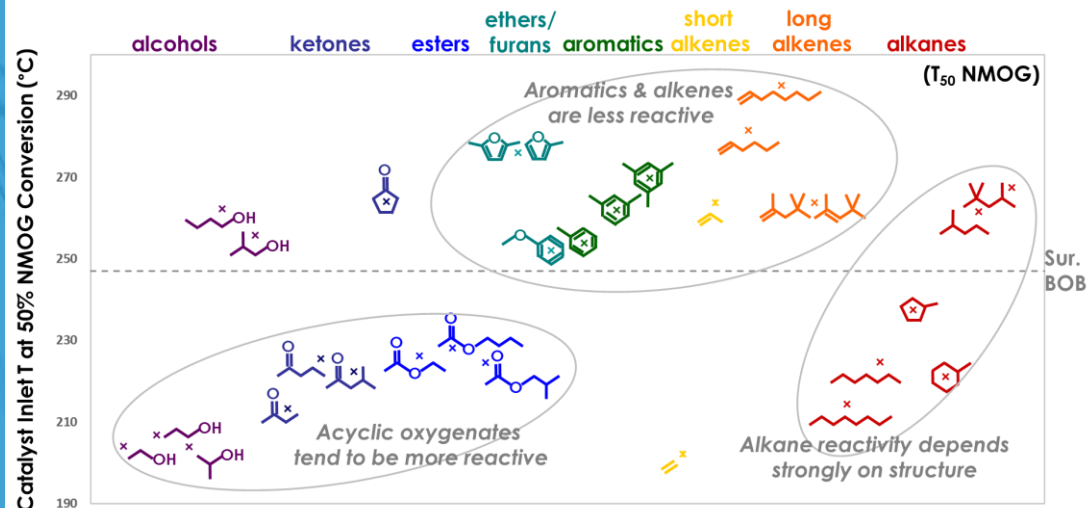
Aikawa et al., *SAE Int. J. Fuels and Lubes*. 2010;3:610-22.



- Cold-start represents a 2-3% fuel consumption penalty over the FTP cycle

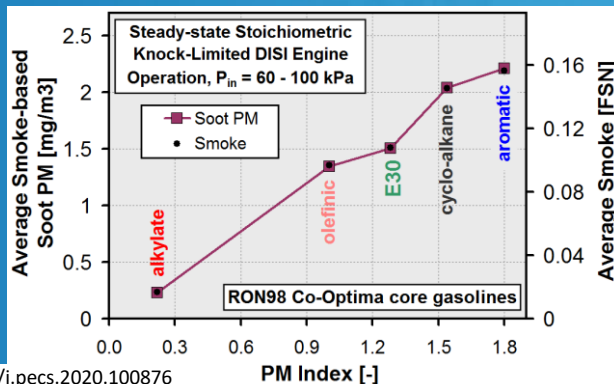


- Fuels with lower light-off temperatures can reduce the cold-start fuel penalty
- Many of the Co-Optima biofuel candidates exhibit reduced light-off temperature



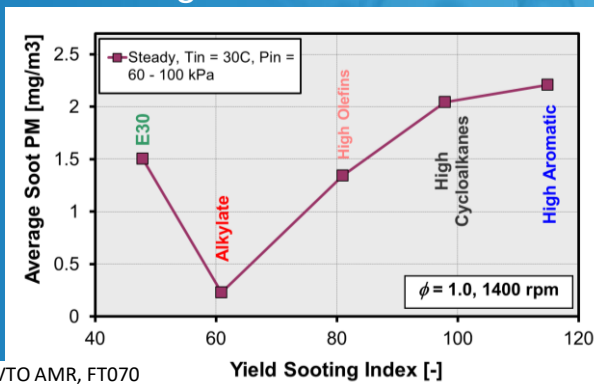


Steady-State Soot Emissions Correlate with PMI



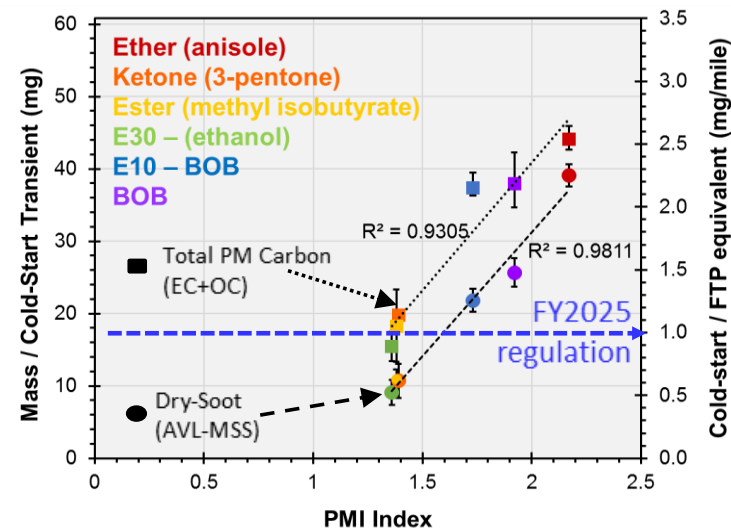
Szybist et al., DOI: [10.1016/j.pecs.2020.100876](https://doi.org/10.1016/j.pecs.2020.100876)

PMI is More Robust for Engine-Out than YSI



Sjöberg et al., 2020 DOE VTO AMR, FT070

Soot Emissions Correlate with PMI under 90s Transient Cold-Start Idle Conditions



BOB from Co-Optima E30 was splash blended with 4 oxygenated bio-fuels and EtOH resulting in 70%BOB + 20% bio-fuel +10%EtOH. Also shown was an E10 and the BOB. 4 bio-fuels were an ether, ketone, ester and alcohol.



$$\text{Efficiency} = 100 * \frac{\eta - \eta_{ref}}{\eta_{ref}}$$

$$= \frac{(RON[-] - 91)}{1.6 + 0.3 * H(PMI - PMI_{LSPi,crit})} - K[-] \frac{(S_{Octane} [-] - 8)}{1.6 + 0.3 * H(PMI - PMI_{LSPi,crit})}$$

Octane Index Terms

$$+ \frac{0.085 \left[\frac{kJ}{kg} \right]^{-1} \cdot \left(\frac{HoV \left[\frac{kJ}{kg} \right] / (AFR[-] + 1) - 415 [kJ/kg]}{14.0[-] + 1} \right)}{1.6 + 0.3 * H(PMI - PMI_{LSPi,crit})}$$

Heat of Vaporization on Knock Mitigation

$$+ \frac{HoV[kJ/kg] / (AFR[-] + 1) - (415 \left[\frac{kJ}{kg} \right] / 14.0[-] + 1)}{15.3 \left[\frac{kJ}{kg} \right]}$$

Other Combined Heat of Vaporization

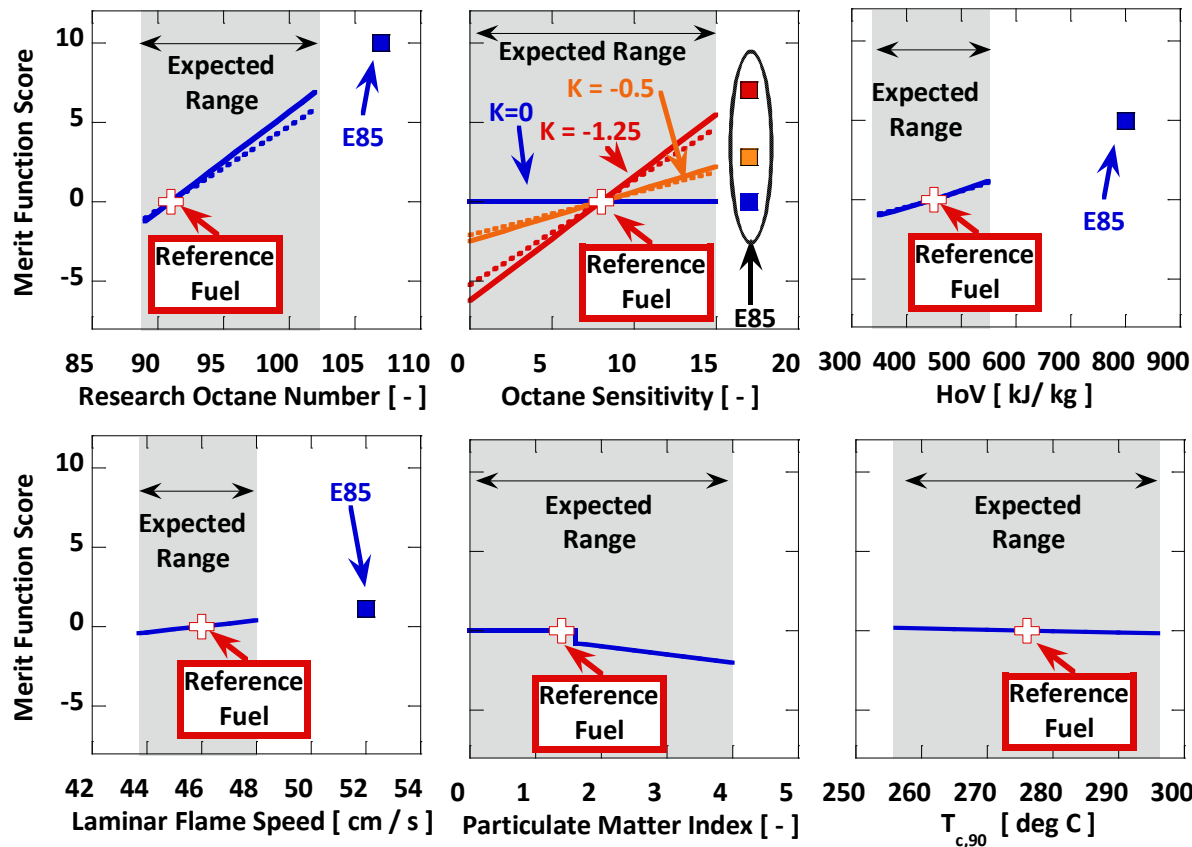
Flame Speed

$$+ \frac{(S_L [cm/s] - 46 [cm/s])}{5.4 \left[\frac{cm}{s} \right]} - H(PMI - 1.6) [0.7 + 0.5(PMI - 1.4)]$$

Particulate Emissions

$$+ 0.008 [^{\circ}C]^{-1} (T_{c,90,conv} [^{\circ}C] - T_{c,90,mix} [^{\circ}C])$$

Catalyst Light-Off



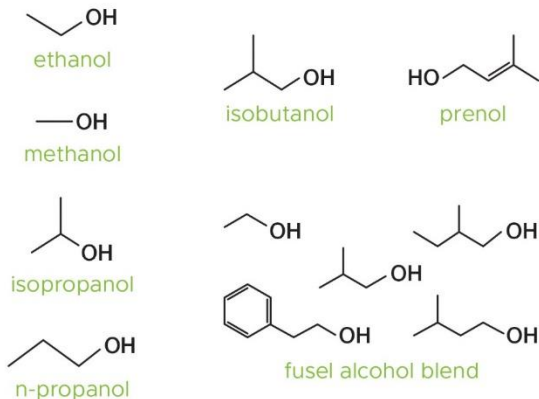
Realistic Ranges of Fuel Properties

	Realistic Low Value	Realistic High Value	E85 value
RON [-]	89	102	107
S [-]	0	15	17
HoV [kJ/kg]	350	550	800
SL [cm/s]	43.7	48	52
PMI [-]	0.0	4.0	N/A
TC ₉₀ [°C]	261	291	N/A

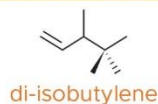
Note: Merit function calculations assume that engine changes, such as increased compression ratio, are made to take advantage of the fuel potential.



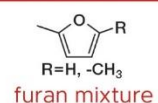
Alcohols



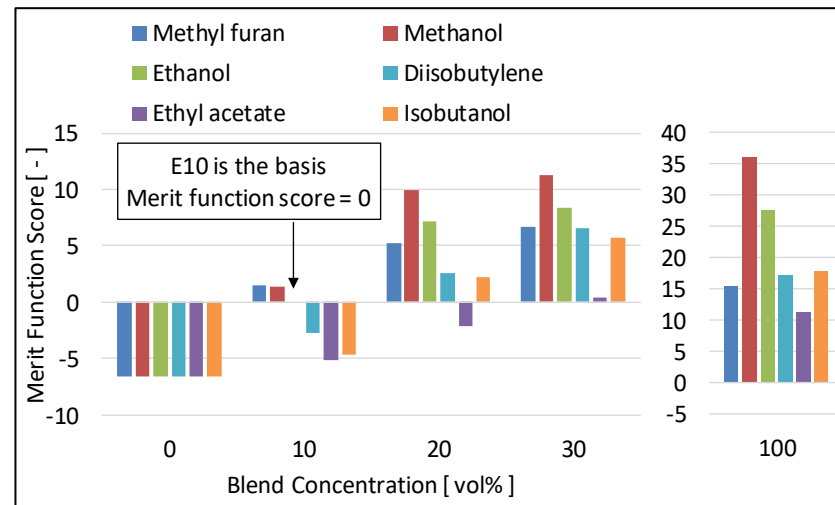
Olefins



Furans



Ketones



- Co-Optima has been focused on blends with petroleum (BOB) up to 30 vol%
- Fuel properties of the blends are used as input for the merit function
- Many fuel properties, including RON and S_{octane} , blend non-linearly
 - Fuels with synergistic blending show good performance (methyl furan, ethanol, methanol)
 - Fuels with antagonistic blending show poor performance (ethyl acetate)



- Central engine and central fuel property hypotheses set baseline expectations, allowing research to proceed in a fuel-agnostic manner
 - Thermodynamic basis for fuel property-based efficiency increases
 - Requires engine optimization for full benefit (r_c , EGR dilution, degree of downsizing, etc.)
- Knock mitigation, quantified by OI, was the most impactful
 - OI correlates to LTHR from the fuel, which is prominent for boosted engines
 - Determination of K for accurate OI remains challenging
- Additional fuel properties considered include HoV, flame speed, catalyst light-off temperature, and two mechanisms for PMI: LSPI and particulate mitigation
- Accurate high-fidelity modeling tools developed to accurately predict fuel effects
- Merit function provides a tool to compare the potential of alternative fuel candidates for both naturally aspirated and boosted SI engines



For a complete record of publications:

<https://www.energy.gov/eere/bioenergy/co-optima-publications-library>

Select publications on the merit function:

- Szybist, J.P., Busch, S., McCormick, R.L., Pihl, J.A., et al., "What Fuel Properties Enable Higher Thermal Efficiency in Spark-ignited Engines?", Progress in Energy and Combustion Science, 82, 2021, 100876. <https://doi.org/10.1016/j.pecs.2020.100876>
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- Gaspar, D., "Ten Blendstocks For Turbocharged Gasoline Engines: Bioblendstocks With Potential to Deliver the for Highest Engine Efficiency," PNNL-28713, 2019, Pacific Northwest National Laboratory.

Select publications on octane index and LTHR:

- Szybist, J.P., Splitter, D.A., "Impact of Engine Pressure-Temperature Trajectory on Autoignition for Varying Fuel Properties," Applications in Energy and Combustion Science, 1, 2020, 100003. <https://doi.org/10.1016/j.jaecs.2020.100003>
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Select publications on PMI

- Ratcliff, M.A., Windom, B., Fioroni, G.M., St. John, P., et al., "Impact of ethanol blending into gasoline on aromatic compound evaporation and particle emissions from a gasoline direct injection engine." Appl Energy, 250, 2019, 1618–31. <https://doi.org/10.1016/j.apenergy.2019.05.030>



Select publications on heat of vaporization

- Sluder, C., Szybist, J., McCormick, R., Ratcliff, M., Zigler, B., "Exploring the Relationship Between Octane Sensitivity and Heat-of-Vaporization," SAE Int. J. Fuels Lubr., 9, 2016, pp 80-90. <https://doi.org/10.4271/2016-01-0836>

Select publications on flame speed

- Szybist, J. and Splitter, D., "Effects of Fuel Composition on EGR Dilution Tolerance in Spark Ignited Engines," SAE Int. J. Engines, 9, 2016, pp 819-831. <https://doi.org/10.4271/2016-01-0715>
- Kolodziej, C., Pamminger, M., Sevik, J., Wallner, T. et al., "Effects of Fuel Laminar Flame Speed Compared to Engine Tumble Ratio, Ignition Energy, and Injection Strategy on Lean and EGR Dilute Spark Ignition Combustion," SAE Int. J. Fuels Lubr., 10, 2017, pp 82-94. <https://doi.org/10.4271/2017-01-0671>

Select publications on catalyst light-off

- Pihl, J.A., Thomas, J., Sinha Majumdar, S., Huff, S. et al., "Development of a Cold Start Fuel Penalty Metric for Evaluating the Impact of Fuel Composition Changes on SI Engine Emissions Control", SAE Technical Paper 2018-01-1264, 2018, <https://doi.org/10.4271/2018-01-1264>
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Select publications on modeling

- Yue, Z., Edwards, K.D., Sluder, C.S., and Som S., "Prediction of Cyclic Variability and Knock-Limited Spark Advance in a Spark-Ignition Engine," J. Energy Resour. Technol. 141, 2019, 102201. <https://doi.org/10.1115/1.4043393>
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