Co-Optimization of
Fuels & Engines

U.S. Department of Energy
Bioenergy Technologies Office
2019 Project Peer Review

Bio-Blendstock Fuel Property Characterization

Co-Optima Review Session
March 7, 2019

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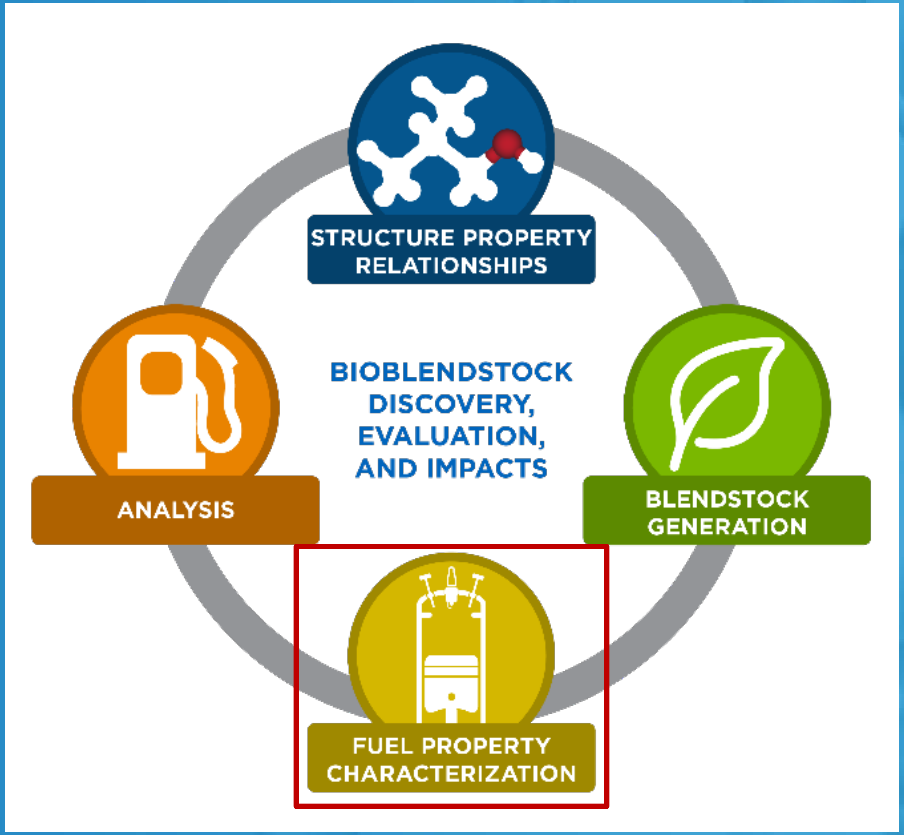
U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Co-Optima: Focused on Outcomes to Improve the Bio-Blendstock Value Proposition

Co-Optima researchers identify blendstocks derived from biomass providing critical fuel properties and assess benefits of and barriers to adoption.

Goal/Outcomes:

- Fuel properties that optimize engine performance
- Fuel-engine combinations that maximize engine efficiency while meeting all requirements, including emissions
- Bio-blendstock options for market actors to define how best to implement
- Assessment of barriers to and benefits of adoption of new blendstocks and engines



Quad Chart Overview

Fuel Property Characterization

Timeline

- **Start:** FY2016
- **Merit Review Cycle:** FY2019–2021
- **Review Cycle:** 12% complete

	Total Costs Pre FY17	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
BETO Funded	$2,252	$1,935	$1,305	$10,380

Partnering labs for work in this presentation:
- Los Alamos National Laboratory (LANL)
- National Renewable Energy Laboratory (NREL)
- Oak Ridge National Laboratory (ORNL)
- Pacific Northwest National Laboratory (PNNL)

Barriers Addressed

- ADO-E. Co-Development of Fuels & Engines
- At-D. Identifying New Market Opportunities for Bioenergy and Bioproducts

Objective

Advance underlying science needed to develop biomass-derived fuel and engine technologies that will work in tandem to achieve significant efficiency, environmental, and economic goals.

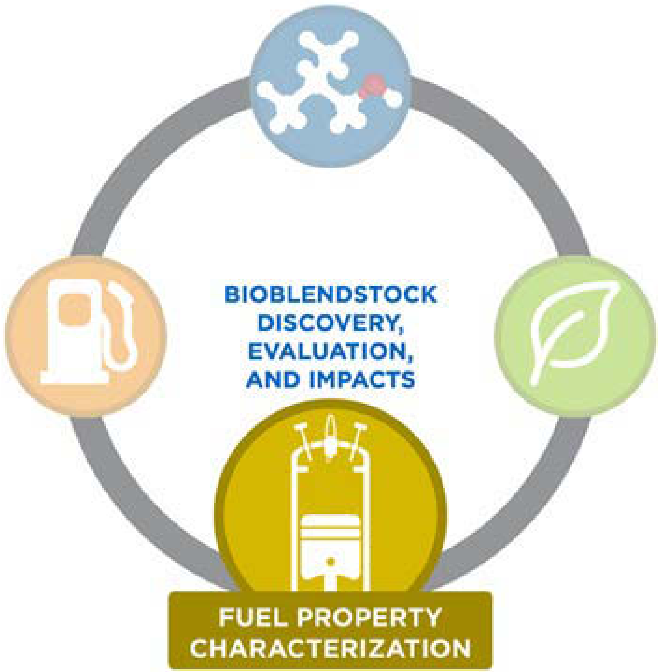
End of Project Goal

Provide critical fuel property data to inform blendstock discovery and predictive model development. Fill in data gaps for tiered screening to identify most promising candidates for multiple combustion modes.

ADO-E = At-D. =

1 – Project Overview
How Fuel Property Characterization Fits within Co-Optima

Co-Optima Presentations Today

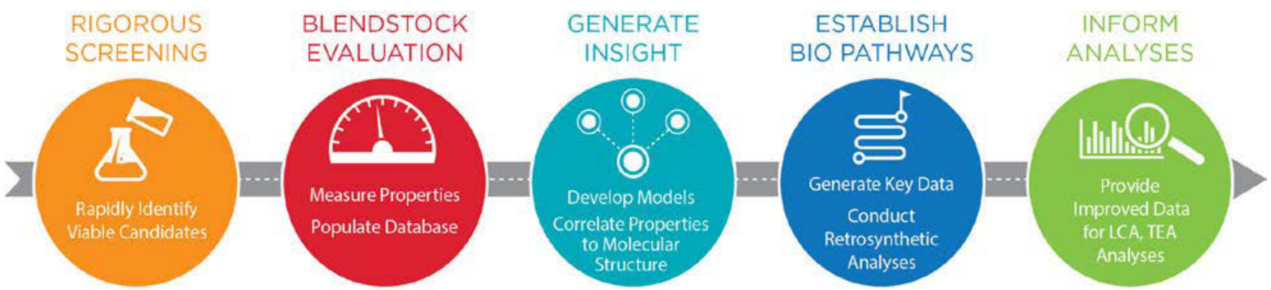


Linked Team Effort within Co-Optima

This presentation will detail efforts in:

Fuel Property Characterization

- Development and population of fuel property database
- Measurement of key fuel properties
- Tiered-screening approach to identify molecules with desirable properties
- Compatibility and toxicology assessment of blendstocks
- Reveal underlying physical chemistry for non-linear blending effects
- Mechanistic understanding of soot precursor formation

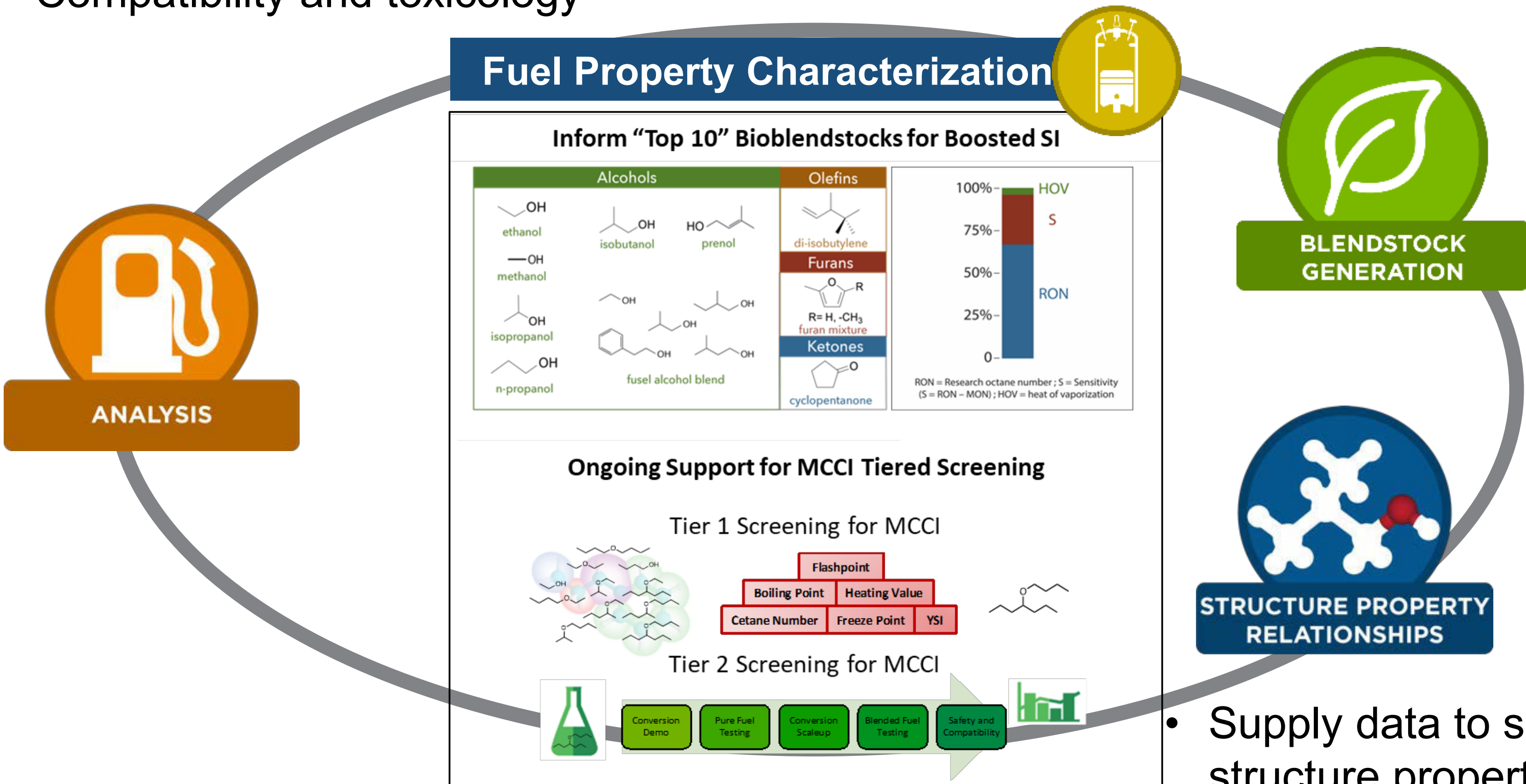


Measurement of critical fuel properties informs multiple teams within Co-Optima

2 – Approach (Management): Fuel Properties Team

Fuel Property Characterization Supports Co-Optima Mission

- Populate fuel property database
- Tiered-screening approach
- Merit function/merit table evaluation
- Compatibility and toxicology
- Reveal critical fuel properties and target ranges to guide blendstock generation
- Measure blending effects



- Supply data to support structure property analysis

MCCI = mixing-controlled compression ignition

Support blendstock discovery and predictive model development and evaluation efforts by experimental exploration and validation.

2 – Approach (Management): Fuel Properties Team

Highly Coordinated Effort Between BETO and VTO Offices

Focus of Today's Presentation

Bioenergy Technologies Office (BETO) Tasks

- NREL: Bob McCormick, Gina Fioroni, Tom Foust, Seonah Kim, Jon Burton, Teresa Alleman
- Pacific Northwest National Laboratory: Evgueni Polikarpov, Dan Gaspar
- Los Alamos National Laboratory: Andrew Sutton
- Oak Ridge National Laboratory: Mike Kass

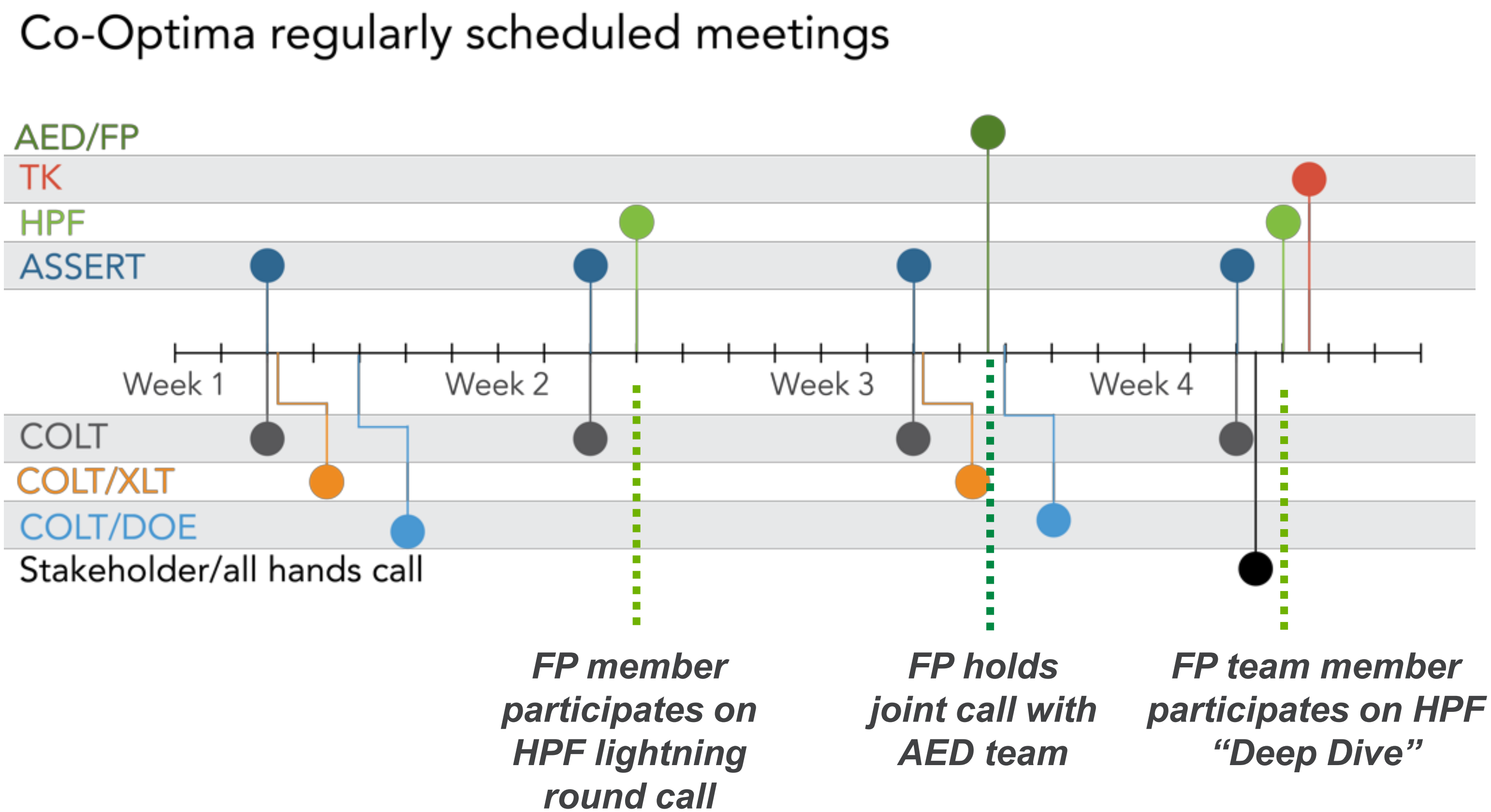
Vehicle Technologies Office (VTO) Tasks

- NREL: Bob McCormick, Gina Fioroni, Matt Ratcliff, Brad Zigler, Seonah Kim
- Pacific Northwest National Laboratory: Evgueni Polikarpov, Tim Bays
- Lawrence Livermore National Laboratory: Bill Pitz
- Sandia National Laboratories: Magnus Sjoberg, Craig Taatjes, Scott Skeen
- Argonne National Laboratory: Chris Kolodziej, Scott Goldsborough
- Oak Ridge National Laboratory: Jim Szybist, Josh Pihl, Derek Splitter

Highly experienced team knowledgeable in fuel property characterization.

2 - Approach (Management)

Communication and Coordination Essential to Success



AED = advanced engine development team
FP = fuel properties team
TK = toolkit

HPF = high performance fuels team
ASSERT = analysis of sustainability, supply, economics, risk, and trade
COLT = Co-Optima leadership team

XLT = extended leadership team
DOE = U.S. Department of Energy

Efforts integrated within fuel properties team and broader Co-Optima team.

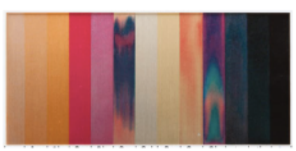
2 – Approach (Technical)

Fuel Property Evaluation: Data to Support Decision Making

Blendstock Fuel Property Characterization

Rigorous Screening

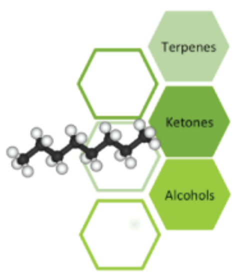
Rapidly identify viable candidates

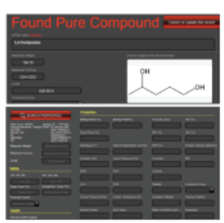


Blendstock Evaluation

Measure properties

Populate database

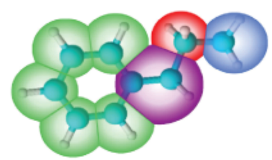


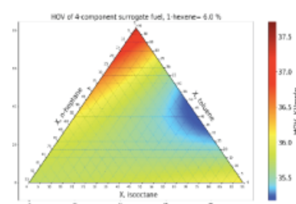


Generate Insight

Develop blending models

Correlate properties to molecular structure

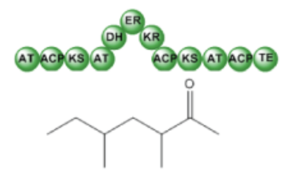




Establish Bio Pathways

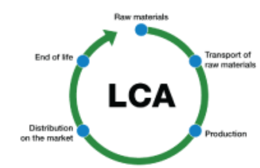
Target properties to generate key data

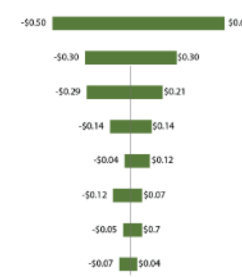
Conduct retrosynthetic analyses



Inform Analyses

Provide improved data for LCA, TEA analyses





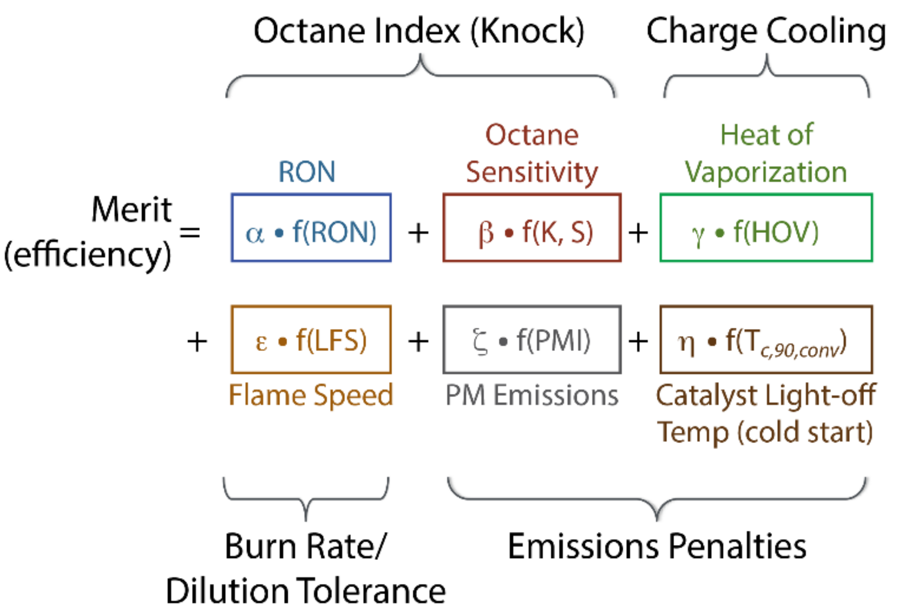
LCA = life cycle analysis, TEA = techno-economic analysis

Implemented technically sound research and development (R&D) approach to rapidly identify viable candidates.

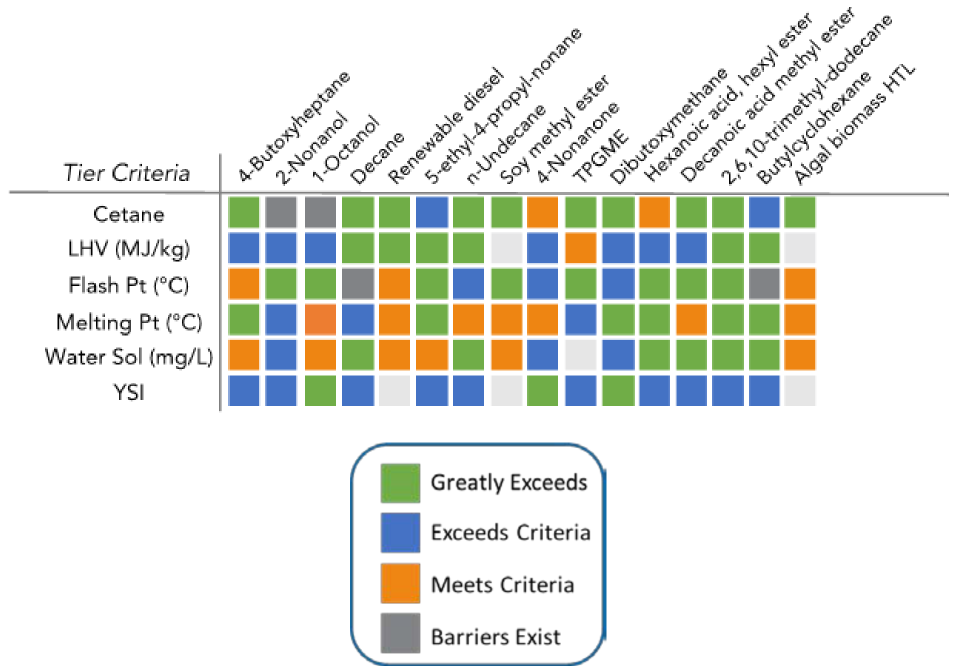
2 – Approach (Technical)

Engine R&D Determines Critical Fuel Properties

BSI Merit Function



MCCI Merit Table



Boosted spark ignition (BSI) merit function and mixing-controlled compression ignition (MCCI) merit table approach to rapidly identify most promising candidates to meet targets.

2 – Approach (Technical)

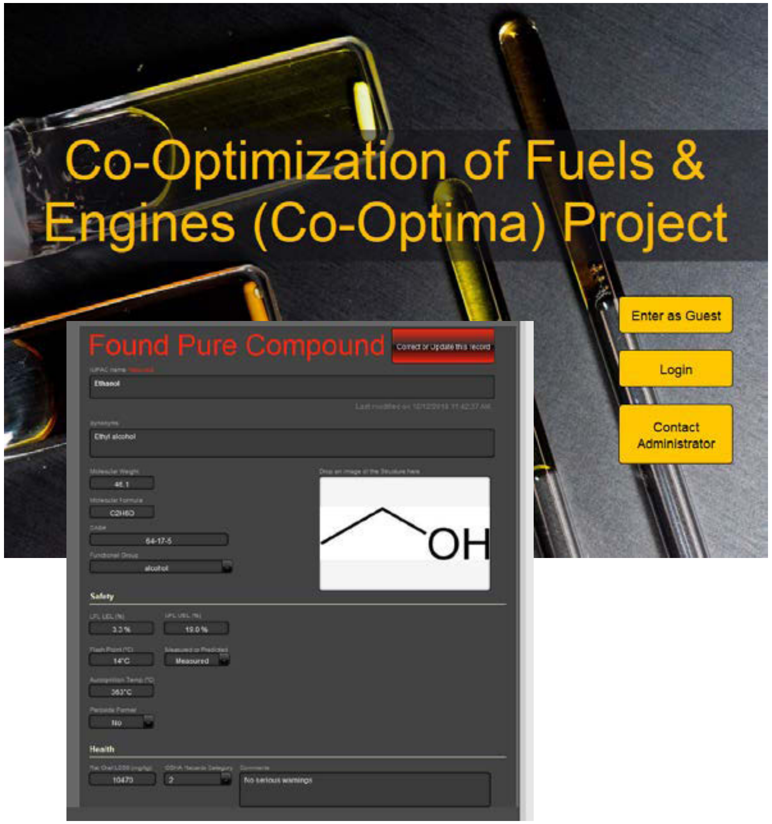
Critical Success Factors, Challenges, and Key Activities

Success Factors	Barriers to Overcome	Activities to Address
Rapidly discover promising blendstocks through tiered-screening approach for multiple combustion modes	Encompass a wide range of potential blendstocks representing several chemical families	Leverage blendstock generation efforts to expand viable candidates
Apply merit function/merit table approach to identify high-potential blendstocks	Procure and access blendstocks that are in early development stages	Continue to provide data to Co-Optima teams to fill gaps for most promising candidate identification

Project activities designed to address barriers to success.

3 – Progress
Development and Population of Fuel Property Database

- Developed a fully searchable database with fuel property candidates supplied from multiple labs and researchers
- Used extensively for BSI and MCCI candidate screening
- Database updated on a regular basis as new data is received from researchers
- Continue to utilize for future screening



https://fuelsdb.nrel.gov/fmi/webd#FuelEngineCoOptimization

Lab PIs: *Fioroni and McCormick, NREL*

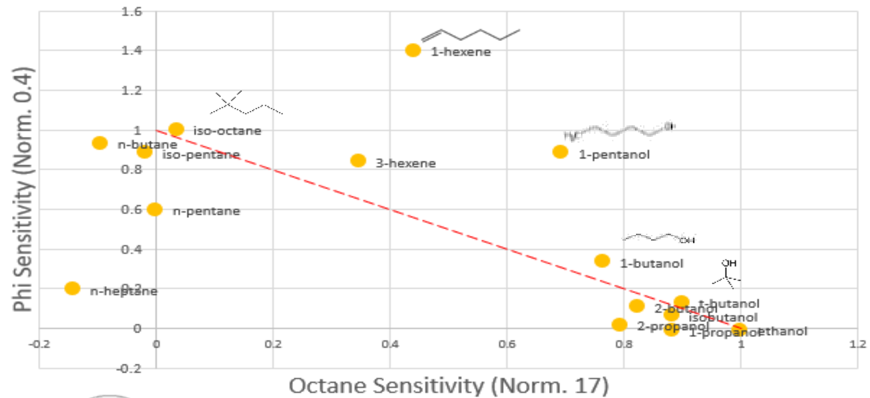
Impact: Database accessed a total of 8,165 times in the last three years. Results of BSI and MCCI screening resulted in two publications and "Most Promising Biofuels Report."

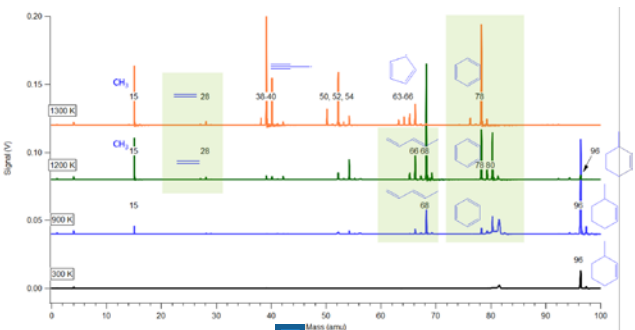
Year	Users	Guests
2016	626	385
2017	1753	1401
2018	2119	1881

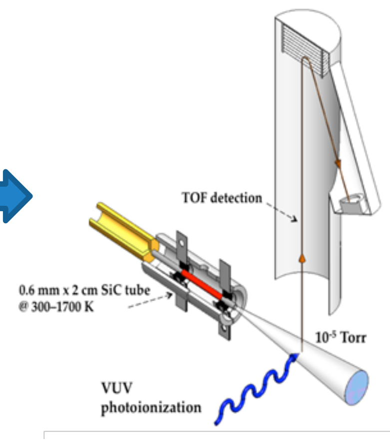
3 – Progress
Characterization of Multi-Oxygenate Fuel Blends for Multimode

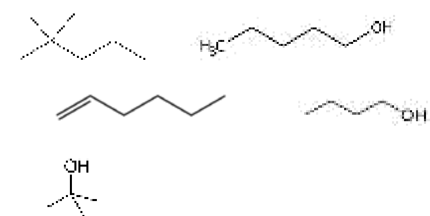
Identify multi-component bio-oxygenate blendstocks with properties well-suited for multi-mode operation targeting high:

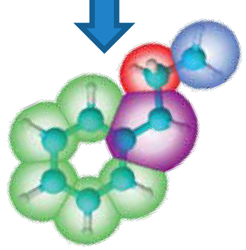
- Volatility
- Research octane number (RON)
- Octane and phi sensitivity











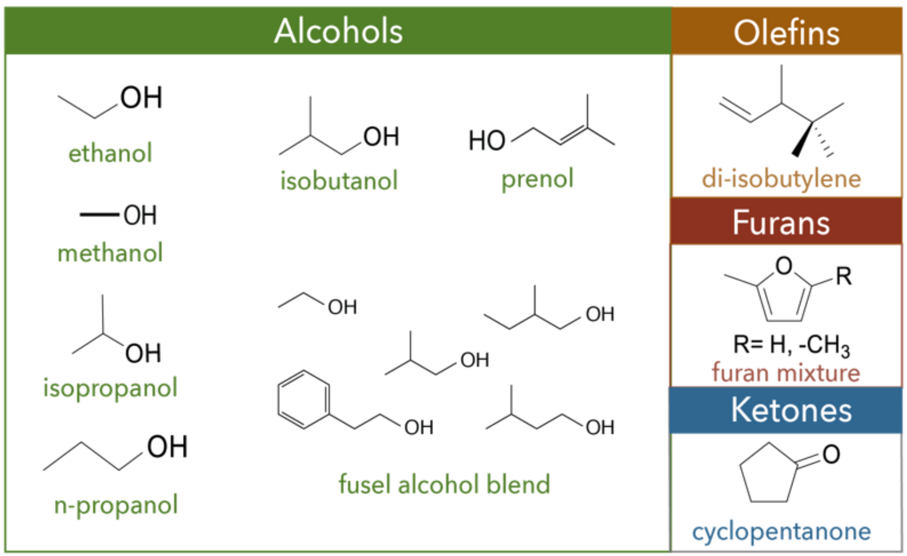
Lab PI: Foust, NREL

Impact: Leverage predictive tools in conjunction with direct experimental measurements to identify strong multi-mode fuel candidates.

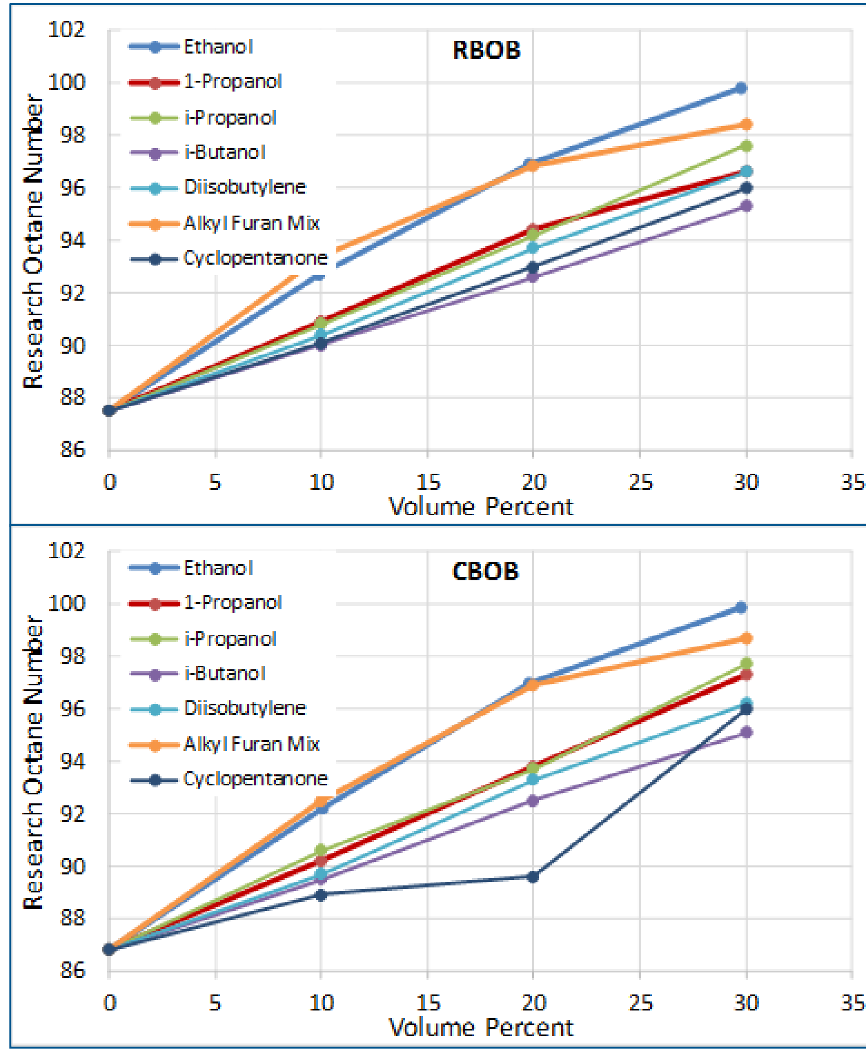
3 - Progress

Boosted SI: Measurement of Key Fuel Properties – Blends

- Applied merit function to candidate list of 40 molecules identified in FY16 and FY17
- Performed blending studies in commercial blendstock for oxygenate blending (BOB)
- Identified and reported on 10 most promising candidates



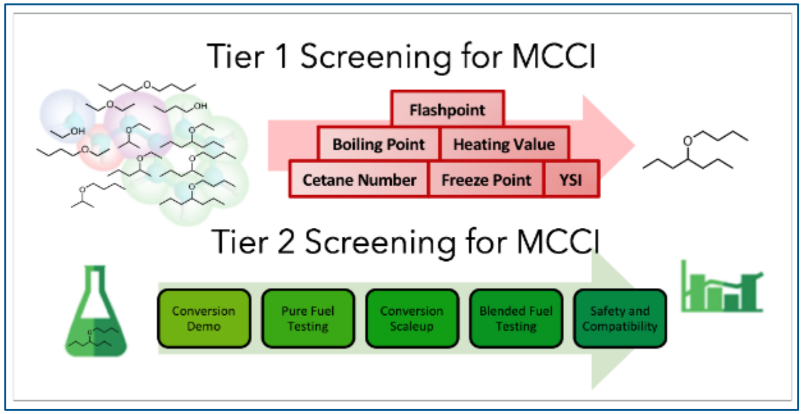
Lab PIs: Fioroni and McCormick, NREL

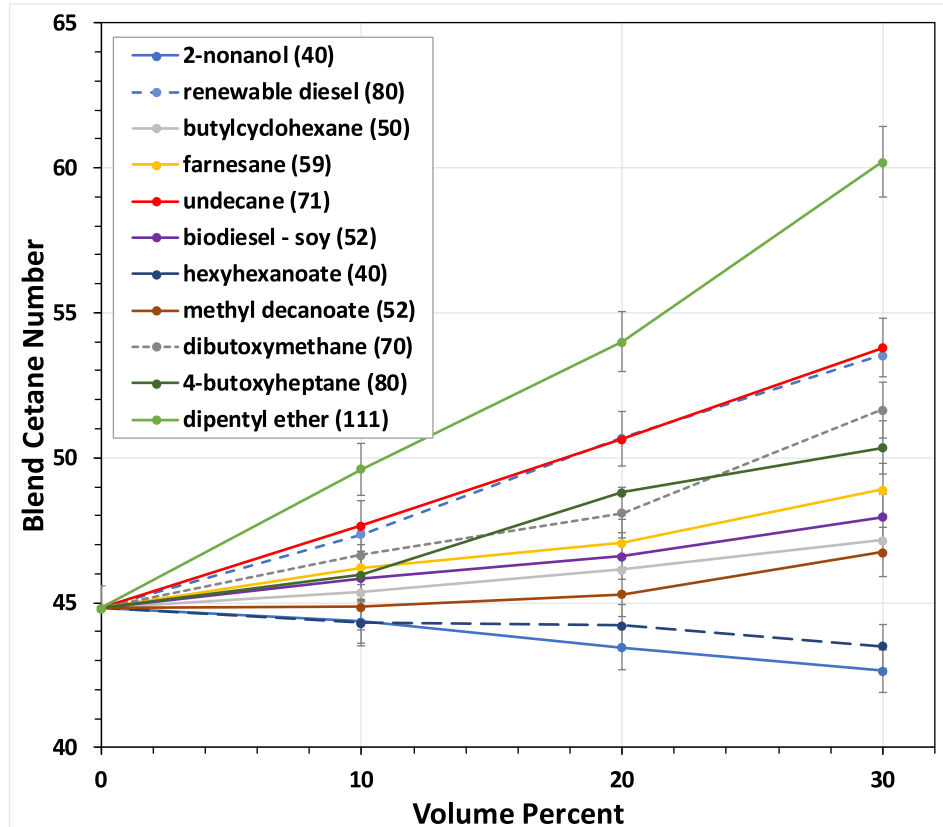


Impact: All candidates selected as promising blendstocks demonstrated synergistic blending—four functional groups represented.

3 - Progress

MCCI: Tiered Screening/Measurement of Key Fuel Properties





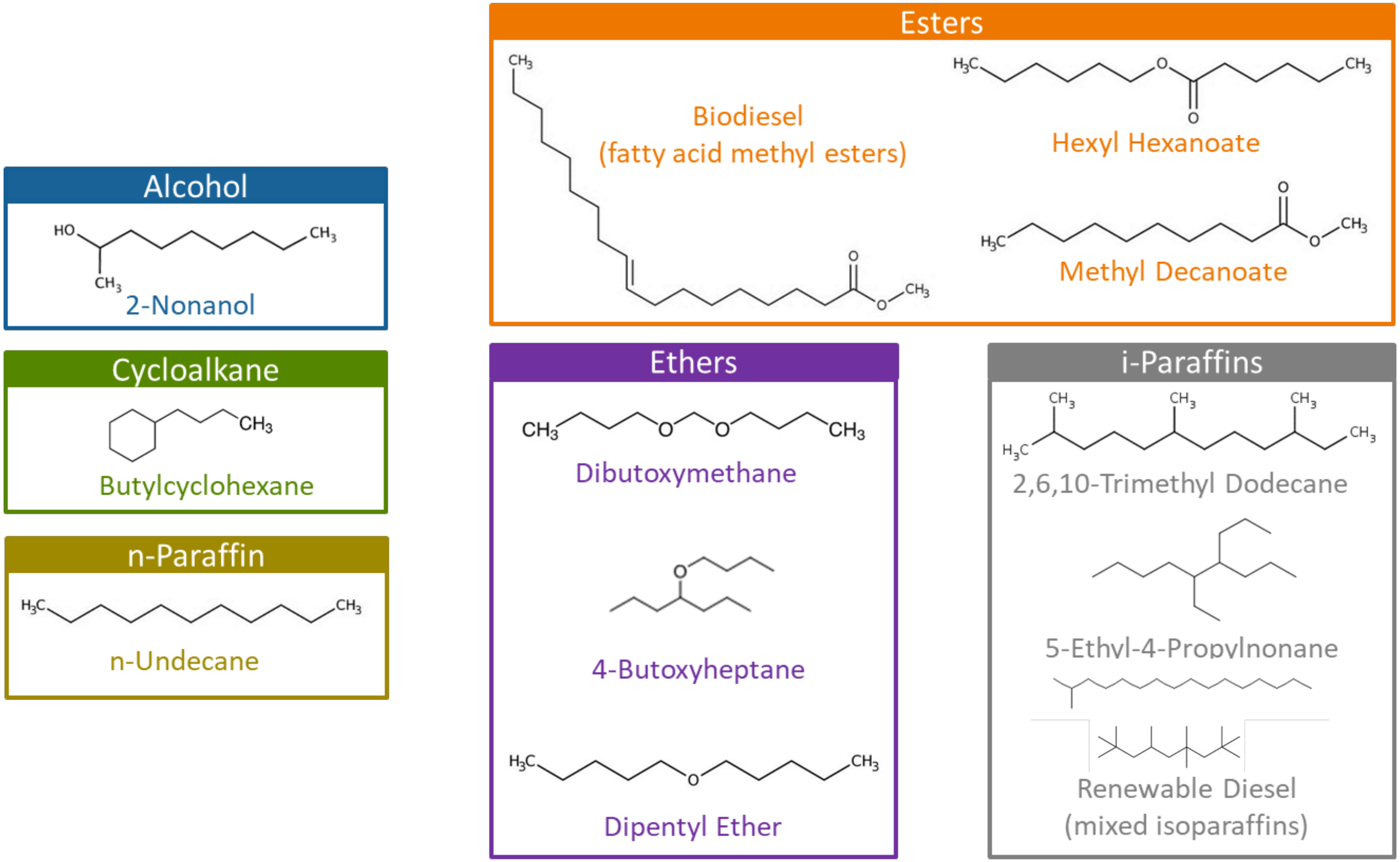
- Finalized fuel properties with input from HPF and AED teams
- Preliminary Tier I and II screening applied to database
- Identified 12 promising candidates:
  - Pure component and blend properties: oxidation stability, cetane number, lubricity, viscosity, conductivity,…
  - Solubility parameter theory assessment of materials compatibility

Lab PIs: Fioroni and McCormick, NREL

Impact: Identification and assessment of several promising candidates well Underway. Publication of screening results at SAE World Congress in 2019.

3 – Progress

MCCI: Tiered-Screening Approach



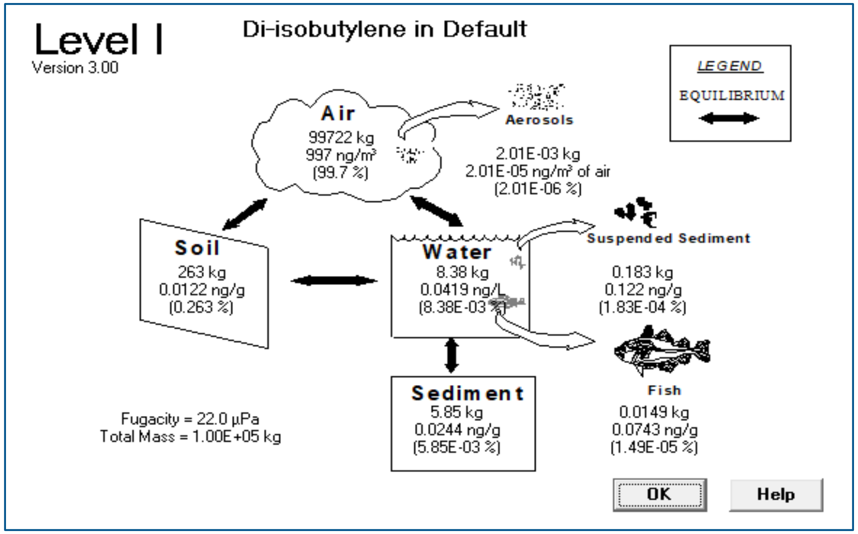
Impact: Preliminary list of 12 promising MCCI candidates spanning multiple functional groups identified

3 - Progress
Boosted SI/MCCI: Toxicology Assessment

Goal: Assess blendstocks for toxicity and environmental fate.

- Toxicity, environmental partitioning, biodegradability, fate, and transport indicators
- Literature review summarizing critical indicators for promising BSI blendstocks
- Quantitative structure-activity relationship prediction for MCCI blendstocks
- Scenario is environmental release between plant gate and consumer consumption

Compound	Air %	Soil %	Water %	Sediment %	Suspended Sediment %
Ethanol	33.2	0.0290	66.8	Trace	Trace
n-Propanol	2.36	0.154	97.5	Trace	Trace
Isopropanol	6.83	0.0925	93.1	0.00206	Trace
Isobutanol	19.5	0.408	80.1	0.00907	Trace
Cyclopentanone	73.7	0.0404	26.2	Trace	Trace
Diisobutylene	99.7	0.263	0.00838	0.00585	Trace
2-Methylfuran	97.6	0.141	2.25	0.00313	Trace
2,5-Dimethylfuran	66.5	4.46	29.0	0.0991	0.00310



Lab PI: Alleman, NREL

Impact: Boosted SI molecules do not have significant concerns, but have differing levels of partitioning and biodegradability that decision makers need to be aware of.

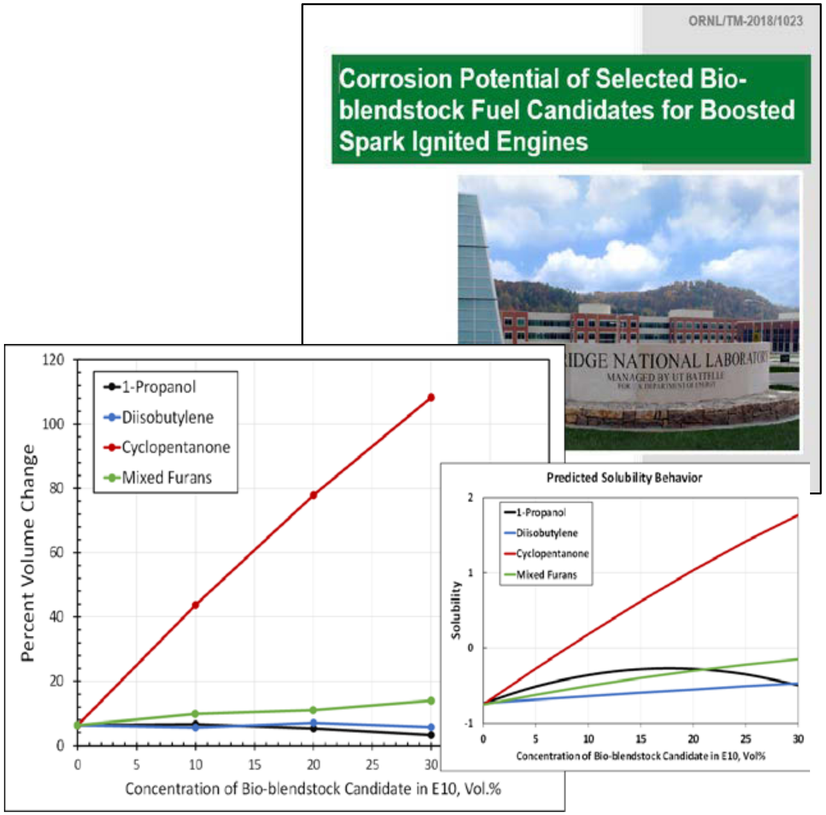
3 – Progress
Boosted SI: Compatibility Assessment

Goal: Assess materials compatibility for most promising BSI candidates.

- Completed solubility parameter-based theoretical prediction of compatibility on 39 BSI fuel candidates with six infrastructure elastomers and 14 plastics common to fueling infrastructure
- Completed exposure study on selected BSI blendstocks and elastomers
- Completed literature review of corrosion potential for metallic fueling materials

Key Findings:

- Solubility analyses showed good correlation with observed swell (elastomers)
- Blending with E10 produces more swell in polymers than blending with a BOB
- Cyclopentanone produces significant swelling in fluoroelastomers, but other Tier 3 blendstocks demonstrated good compatibility



Percent volume change of fluorocarbon elastomer vs. concentration of blendstock candidates in E10 (main figure), and Hansen solubility prediction (inset). *Figure by Michael Kass, ORNL*

Lab PI: Kass, ORNL

Impact: BSI blendstocks investigated were not likely to be corrosive—and except cyclopentanone—exhibited good compatibility with elastomers and plastics.

3 – Progress

Fuel Properties: ASTM Specification

Goal: Develop ASTM International standards for optimal fuels for boosted spark ignition (BSI), multi-mode ignition (MM), and advanced compression ignition (ACI) combustion using an understanding of the interaction between fuel effects and combustion modes.

High research octane number (RON) BSI test fuel specification is the first outcome of this task:

- Development of specification brought together a wide breadth of stakeholders
- Specification first published in 2017 and updated again in 2018
- Next iteration expected in 2019 to update with specific grades of 100 RON fuel based on Co-Optima BSI blendstocks

ASTM INTERNATIONAL

Designation: D8076 – 18

Standard Specification for
100 Research Octane Number Test Fuel for Automotive Spark-Ignition Engines[1]

Lab PI: Alleman, NREL

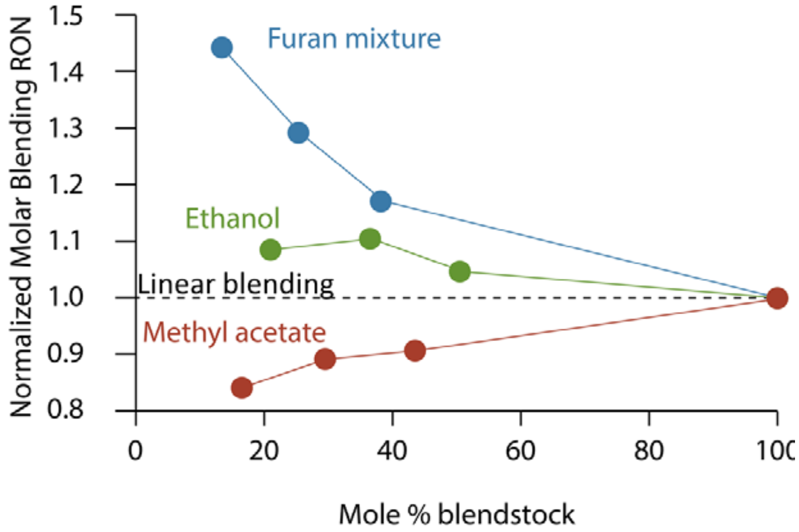
Impact: Development of 100 RON test fuel specification provides common baseline fuel for future development efforts. First ever ASTM standard to include a limit on octane number and use RON and octane sensitivity (S).

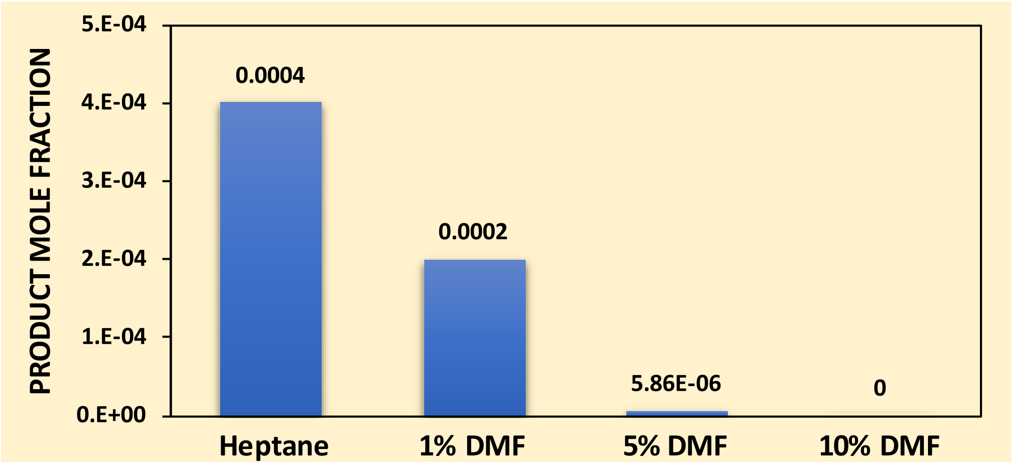
3 – Progress

BSI: Reveal Chemistry for Non-Linear Blending Effects

Goal: Understand chemical basis for synergistic and antagonistic blending for RON.

- Blended various synergistic and antagonistic compounds with a radical generator (heptane)
- Autoignition at 600 Kelvin (K)
- Synergistic compounds shut down low-temperature autoignition at low blend levels
- Identified potential common fragment in synergistic compounds that may be responsible for synergistic blending effects



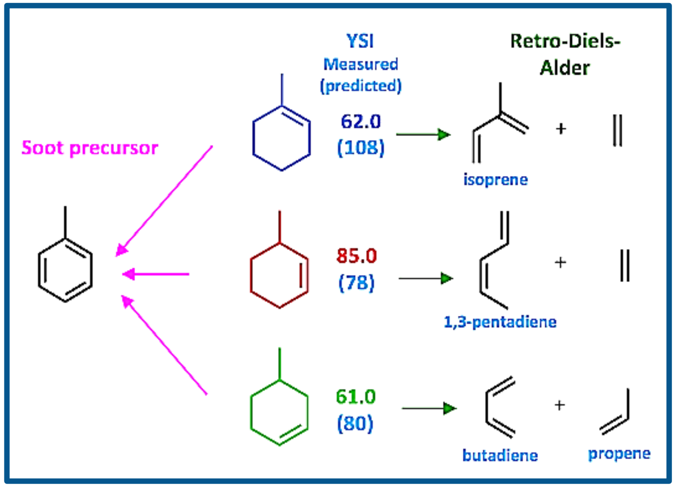


DMF =

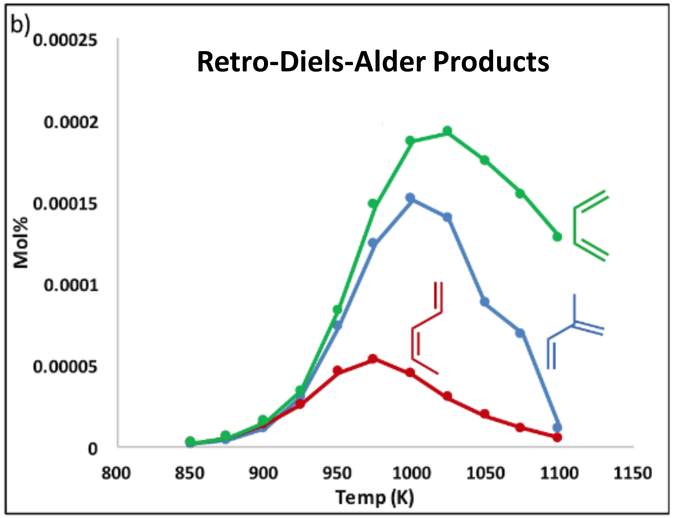
Lab PI: Fioroni, NREL

Impact: Revealing the mechanism of non-linear blending for octane number will allow design of molecules with desired blending octane behavior.

3-Progress
Mechanistic Understanding of Soot Precursor Formation

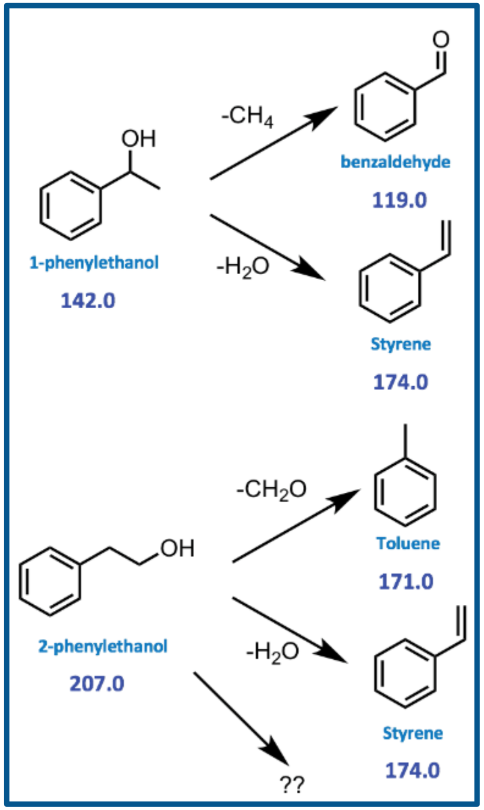


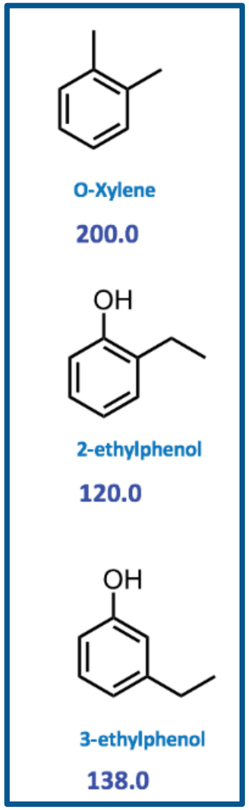
YSI = yield sooting index



Lab PIs: Kim, Fioroni, and St. John, NREL

- Flow reactor used to validate QM simulations and inform kinetic mechanism development
- Developed soot precursor mechanisms to understand effects of substituents, oxygen atom position, and isomers on soot precursor formation





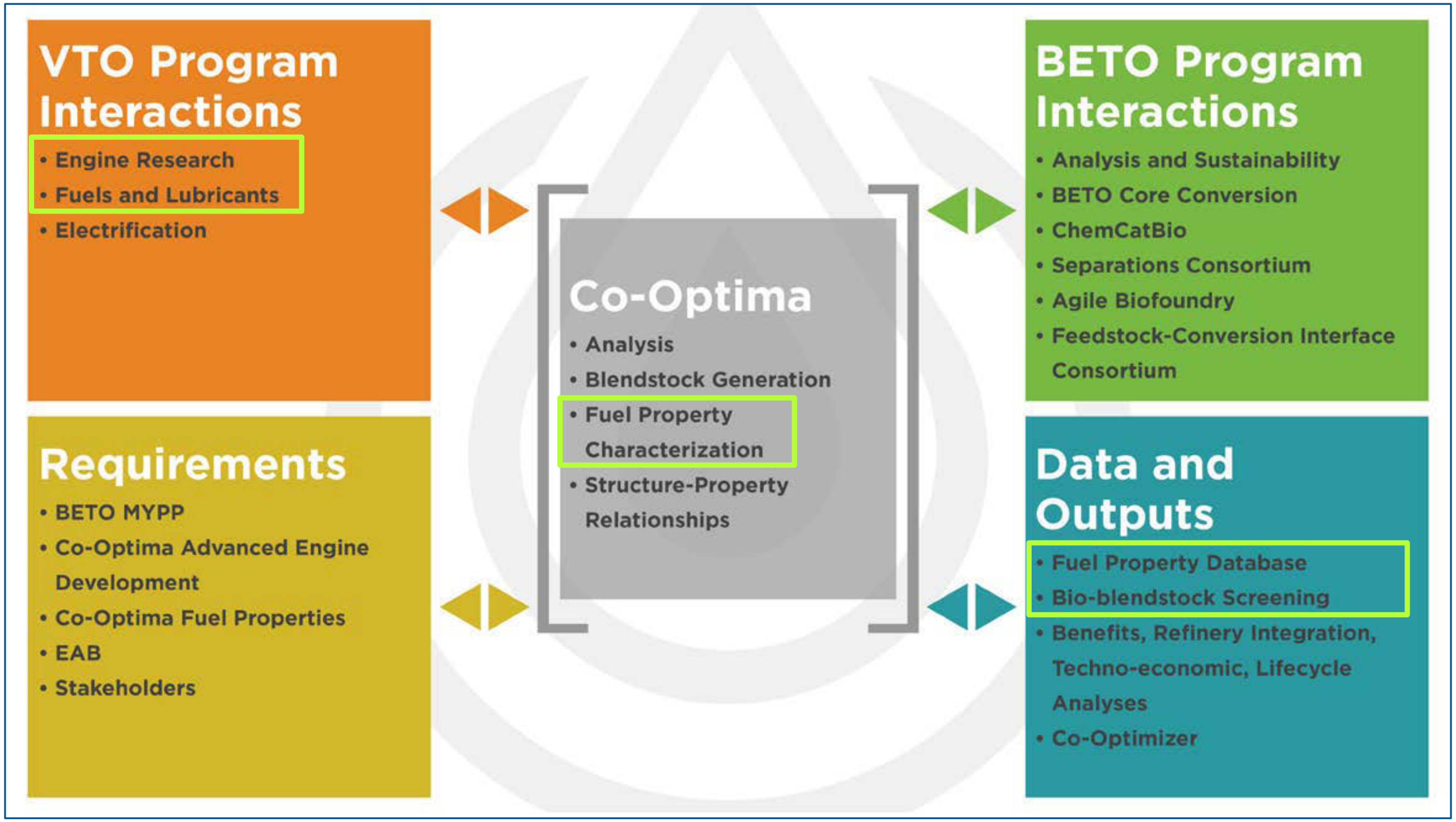
Impact: Revealing chemical structure effect on soot formation leads to cleaner fuels.

4 – Relevance

How Fuel Property Characterization Impacts BETO Goals

Specific MYP barriers addressed by fuel properties

- ADO-E. Co-Development of Fuels & Engines
- At-D. Identifying New Market Opportunities for Bioenergy and Bioproducts



MYP = MYPP = EAB =

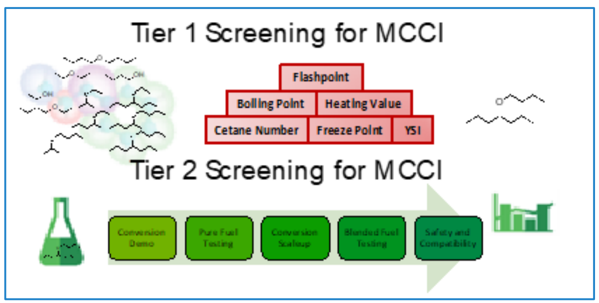
Fuel property research identifies critical properties for design of more efficient engines and relates properties to molecular structure and production pathways.

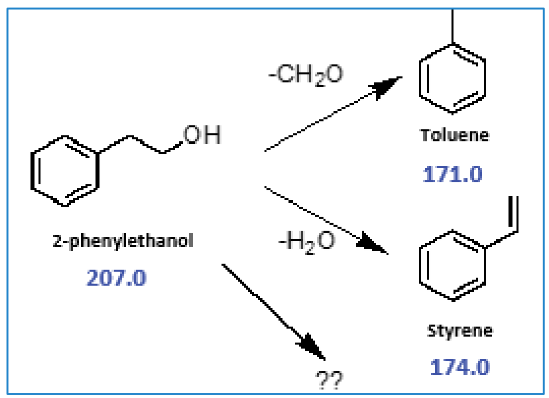
4 – Relevance

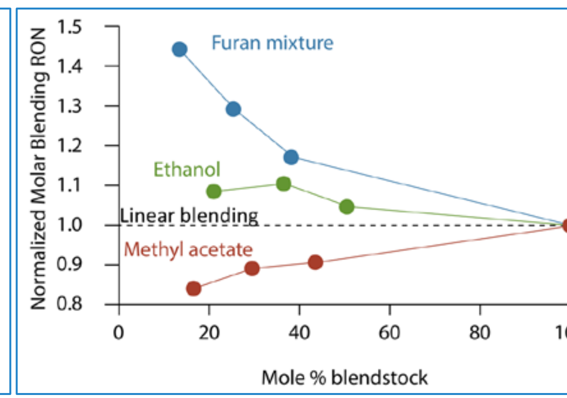
How Fuel Property Characterization Supports Co-Optima

Fuel property database available to all teams to support screening efforts for all combustion modes.

Compatibility and toxicology assessment to reduce barriers to market adoption.







Measurement of key fuel properties for tiered screening to rapidly identify blendstocks with the highest potential.

Mechanistic understanding of soot precursor formation and underlying chemical basis for non-linear blending effects.

Impact: Fuel property research informs multiple teams within Co-Optima.

5 – Future Work

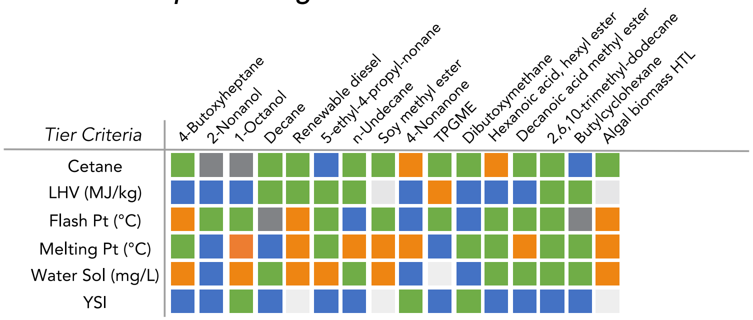
Select Planned Milestones and Upcoming Decision Points

Combustion Mode	Select Fiscal Year (FY) 2019 Milestones	Quarter
Boosted SI	A.5.5 Complete exposure study on infrastructure plastics with selected SI blendstocks (ORNL).	Q3 FY19
Boosted SI	F.1.4.1 Draft journal article explaining the chemical basis for synergistic and antagonistic blending for RON and S (NREL).	Q2 FY19
Boosted SI	A.5.6 Identify 5 new compounds or mixtures that improve octane sensitivity when blended into BOB or E10. Measure RON, MON, and S for each in an E10 and BOB blend (PNNL).	Q3 FY19
MCCI	A.4.10 Complete polymer exposure studies on selected MCCI blendstocks (ORNL).	Q4 FY19
MCCI	A.4.9 Complete Hansen solubility analysis on up to 40 MCCI candidates (ORNL).	Q2 FY19
MCCI	A. 5. 1. Identify the blendstock molecular structures or individual BOB component that leads to the highest antagonistic blending effect to raise RON and S for MMCI (LANL).	Q4 FY19
Multi-Mode	A.5.9 Quantify the upper limit of moisture tolerance of BOB/ester blends towards hydrolysis of esters by LCA of carboxylic acids in the aged-fuel sample with and without residual acids (PNNL).	Q3 FY19

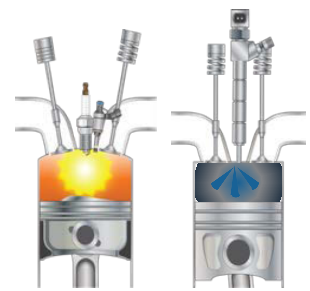
FY19 plan will finalize MCCI work and continue MM effort.

5 – Future Work
Upcoming Decision Points and Remaining Issues

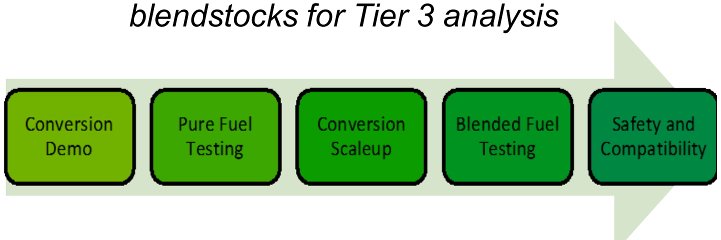
DECISION POINT
End of FY19 – *Determine most promising candidates for MCCI*



FUTURE FOCUS
FY19 to FY21 – *Target MM and KC*



DECISION POINT
End of FY20 – *Select blendstocks for Tier 3 analysis*



REMAINING ISSUES
FY19 to FY21 – *Determine target values of key fuel properties and ranges for MM and KC combustion modes*

KC = kinetically-controlled ignition

Decision Points: *Select MCCI blendstocks for Tier 3 screening; identify future targets for MM and KC.*
Remaining Issues: *How are key fuel properties and target ranges for MM and KC combustion modes defined?*

Summary for Fuel Property Characterization

Overview	**Measure key fuel property data to:** • Fill data gaps and support tiered screening and merit evaluation approaches to advance development of new fuel and combustion options
Approach	• Identify promising blendstocks through tiered-screening approach • Measure key fuel properties to fill data gaps and supply information for merit evaluation • Perform compatibility and toxicology assessment of promising candidates • Reveal underlying chemistry for non-linear blending effects, validate quantum mechanical simulations, and inform kinetic mechanism development
Technical Progress	• Developed publicly accessible fuel property database • Utilized tiered-screening approach to rapidly identify promising blendstocks • Measured blending behavior of chemically diverse blendstocks • Completed initial material compatibility and toxicology assessment on promising candidates • Examined the chemical basis for non-linear blending effects through flow reactor auto-ignition experiments • Provided experimental results to validate quantum mechanical simulations for soot pre-cursor formation
Relevance	• Implemented technically sound approach for evaluating blendstocks • Identified key blendstocks that enable engines to operate efficiently
Future Work	• Complete measurement of key fuel properties for MCCI candidates and facilitate selection of most promising candidates • Identify key fuel properties for light duty (multi-mode) and heavy duty (kinetically-controlled) blendstock options • Apply tiered-screening approach to select promising candidates for multi-mode and kinetically-controlled combustion modes

List of Acronyms

CO-OPTIMA TEAMS & THRUSTS

- **AED** – advanced engine development team
- **FP** – fuel properties team
- **HPF** – high performance fuels team
- **SAE** – Society of Automotive Engineers
- **VTO** – Vehicle Technologies Office

ENGINE COMBUSTION MODES

- **ACI** – advanced compression ignition, heavy duty
- **BSI** – boosted spark ignition, light duty
- **KC** – kinetically-controlled ignition, heavy duty
- **MCCI** – mixing-controlled compression ignition, heavy duty
- **MM** – multi-mode ignition, light duty

FUEL PROPERTY MEASUREMENTS

- **BOB** – blendstock for oxygenate blending
- **cBOB** – conventional blendstock for oxygenate blending
- **RBOB** – reformulated blendstock for oxygenate blending
- **HoV** – heat of vaporization
- **LCA** – life cycle analysis
- **MON** – motor octane number
- **RON** – research octane number
- **QM** – Quantum mechanics
- **S** – Octane sensitivity, defined as RON - MON
- **YSI** – yield sooting index

GENERAL ACRONOYMS (not listed to the left but were in the slide deck)

- **ADO-E –** ????
- **ASSERT –** analysis of sustainability, supply, economics, risk, and trade
- **At-D.** – ???
- **BETO** – Bioenergy Technologies Office
- **COLT** – Co-Optima leadership team
- **DMF – ????**
- **DOE** – U.S. Department of Energy
- **EAB** – ???
- **MYP** – ??
- **MYPP** – ???
- **R&D** – research and development
- **TEA** – techno-economic analysis
- **XLT** – extended leadership team

Disclaimer

Thank you

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Additional Slides

Responses to Previous Reviewers' Comments

Reviewer comments:

- No guarantee that industry will use information to provide better fuels
- No plan of attack for impetus for industry change
- Lots of calls and meetings

Response:

- These risks are real. To mitigate these risks, Co-Optima has focused on extensive outreach to communicate the technical foundation we have developed, so that market actors can act. Our outreach plan includes direct engagement with biofuel companies at all scales, as well as with automakers and all parts of the fuel supply chain, including Octane Workshops in 2018 (next slide), and a concerted effort to solicit feedback from biofuel companies in 2018 (report is being drafted).
- We have made an effort to manage the work more efficiently, reducing the number of meetings across Co-Optima by 1/3, and reduced travel for the leadership team by another 1/3.

List of Publications and Presentations (1)

FY19 Publications and Presentations

1. **Screening of Potential Biomass-Derived Streams as Fuel Blendstocks for Mixing Controlled Compression Ignition Combustion -** Fioroni, G.M., Fouts, L., McCormick, R.L. et al., to be published, *SAE Technical Paper No. 2019-01-0730*.
2. **Heat of Vaporization and Species Evolution During Gasoline Evaporation Measured by DSC/TGA/MS for Blends of C1 to C4 Alcohols in Commercial Gasoline Blendstocks -** Fioroni, G.M., Fouts, L., Christensen, E.D., McCormick, R.L. *SAE Technical Paper 2019-01-0014*, doi:10.4271/2019-01-0014.
3. **Discovery of Novel Octane Hyperboosting Phenomenon in Prenol/gasoline Blends -** Monroe, E., Gladden, J., Albrecht, K., Bays, J.T., McCormick, R.L., Davis, R.W., George, A. *Fuel* 239 1143-1148.
4. **Dual-Alcohol Blending Effects on Gasoline Properties -** Saeid Aghahossein Shirazi , Bahareh Abdollahipoor, Jake Martinson, Bret Windom, Kenneth F. Reardon, Thomas Foust, Submitted to *Fuel* January 2019.
5. **Development and Application of a Fuel Property Database for Mono-Alcohols as Fuel Blend Components for Spark Ignition Engines -** Saeid A Shirazi, Thomas D Foust, Kenneth F. Reardon, Accepted by *Fuel* January 2019, publication forthcoming shortly.
6. **Autoignition and Select Properties of Low Sample Volume Thermochemical Mixtures from Renewable Sources -** Olarte, Mariefel V., Karl O. Albrecht, J. Timothy Bays, Evgueni Polikarpov, Balakrishna Maddi, John C. Linehan, Molly J. O'Hagan, and Daniel J. Gaspar, *Fuel* 238 (2019): pp 493-506.
7. **Critical Fuel Property Evaluation for Potential Gasoline and Diesel Biofuel Blendstocks with Low Sample Volume Availability-** Polikarpov, Evgueni, Karl O. Albrecht, Jordan P. Page, Deepika Malhotra, Phillip K. Koech, Lelia Cosimbescu, and Daniel J. Gaspar, *Fuel* 238 (2019): pp 26-33.
8. **Measuring and Predicting the Vapor Pressure of Gasoline Containing Oxygenates -** Daniel J. Gaspar; Steven D. Phillips; Evgueni Polikarpov; Karl O. Albrecht; Susanne B. Jones; Anthe George; Alexander Landera; Daniel M. Santosa; Daniel T. Howe; Anna G. Baldwin; J. T. Bays, *Fuel* (2019, accepted; in press).

List of Publications and Presentations (2)

FY18 Publications and Presentations

1. **Measurement of Heat of Vaporization for Research Gasolines and Ethanol Blends by DSC/TGA -** Fioroni, G.M., Fouts, L., Christensen, E.D., Anderson, J.E., McCormick, R.L. *Energy Fuels* DOI: 10.1021/acs.energyfuels.8b03369.
2. **Screening Fuels for Autoignition With Small Volume Experiments and Gaussian Process Classification -** Lunderman, S., Fioroni, G.M., McCormick, R.L., Nimlos, M., Rahimi, M.J., Grout, R.W. *Energy Fuels* 32 9581−9591.
3. **Experimental and Theoretical Insight into the Soot Tendencies of the Methylcyclohexene Isomers –** S Kim, G. M. Fioroni, J. Park, D. J. Robichaud, D.D. Das, P.C. St. John, T. Lu, C.S. McEnally, L.D. Pfefferle, R.S. Paton, T.D. Foust, and R.L. McCormick. *Proc. Comb. Inst.*, available online, July 2018. https://doi.org/10.1016/j.proci.2018.06.095.
4. **Investigation of the Impact of Fuel Properties on Particulate Number Emissions of a Modern Gasoline Direct Injection Engine -** Fatouraie, M., Frommherz, M., Mosburger, M., Chapman, E., Li, S., Fioroni, G.M., McCormick, R.L. *SAE Technical Paper 2018-01-0358*.
5. **Measured and Predicted Vapor Liquid Equilibrium of Ethanol-Gasoline Fuels with Insight on the Influence of Azeotrope Interactions on Aromatic Species Enrichment and Particulate Matter Formation in Spark Ignition Engines -** Burke, S., Rhoads, R., Ratcliff, M., McCormick, R.L., Windom, B., *SAE Technical Paper 2018-01-0361*, doi:10.4271/2018-01-0361.
6. **The Use of Biomass Oxygenates to Reduce Particulate Matter Formation in Direct Injected Spark-ignited Engines -** T. Foust, P. C. St John, R. L. McCormick, C. A. Farberow, S. Kim, "*Renew Sus. Energy* Reviews submitted January 2018 – under review.
7. **Measuring and Predicting Sooting Tendencies of Oxygenates, Alkanes, Alkenes, Cycloalkanes, and Aromatics on a Unified Scale -** Dhruhajyoti D. Das, Peter St. John, Charles S. McEnally, Seonah Kim, Lisa D. Pfefferle, *Combustion and Flame*, 190, 349-364 (2018).
8. **Experimental and Theoretical Study of Oxidative Stability of Alkylated Furans Used as Gasoline Blend Components –** E. Christensen, G.M. Fioroni, S. Kim, L. Fouts, E. Gjersing, R.S. Paton, and R.L. McCormick. *Fuel*, 212:576-585, January 2018. https://doi.org/10.1016/j.fuel.2017.10.066.
9. **Annual Merit Review and Peer Review Evaluation Presentations –** 12 presentations: A. Agrawal, S. Curran, J. Farrell, G. Fioroni, C. Kolodziej, G. Lavoie, C. McEnally, M. McNenly, C. Mueller, J. Pihl, I. Schoegl, and S. Sluder. https://www.energy.gov/eere/vehicles/annual-merit-review-presentations.

List of Publications and Presentations (3)

FY18 Publications and Presentations

10. **Sooting Tendencies of Co-optima Test Gasolines and Their Surrogates -** Charles S. McEnally, Yuan Xuan, Peter C. St. John, Dhrubajyoti D. Das, Abhishek Jain, Seonah Kim, Thomas A. Kwan, Lance K. Tan, Junqing Zhu, Lisa D. Pfefferle, Proceedings of the Combustion Institute (2018), https://doi.org/10.1016/j.proci.2018.05.071.
11. **Small Ester Combustion Chemistry: Computational Kinetics and Experimental Study of Methyl Acetate and Ethyl Acetate -** Ahfaz Ahmed, William J.Pitz, Carlo Cavallotti, Marco Mehl, Nitin Lokachari, Eln, J.K. Nilsson, Jui-Yang Wang, Alexander A. Konnov, Scott W. Wagnon, Bingjie Chen, Zhandong Wang, Seonah Kim, Henry J. Curran, Stephen J. Klippenstein, William L. Roberts, S. Mani Sarathy, Proceedings of the Combustion Institute (2018), https://doi.org/10.1016/j.proci.2018.06.178.
12. **Sooting Tendencies of Aromatic Hydrocarbons with Oxygen- Containing Side-Chains -** Brian P. Beekley, Charles S. McEnally, Peter C. St. John, Seonah Kim, Abhishek Jain, Hyunguk Kwon, Yuan Xuan, Lisa D. Pfefferle, ESSCI (Eastern States Section of the Combustion Institute) Spring 2018, Proceedings of the Combustion Institute.
13. **Co-Optimization of Fuels & Engines: Properties of Co-Optima Core Research Gasolines –** R. McCormick, L.A. Fouts, G.M Fioroni, E.D. Christensen, M.A. Ratcliff, B.T. Zigler, S. Sluder, J.P. Szybist, S. Ciatti, J.T. Bays, W. Pitz, M. Mehl, J.E. Dec, and P.C. Miles. Technical Report 1467176, August 2018. https://dx.doi.org/10.2172/1467176.
14. **Compatibility Assessment of Fuel System Thermoplastics with Bio-Blendstock Fuel Candidates Using Hansen Solubility Analysis –** M. Kass, B. West. *SAE Int. J. Fuels Lubr.* 11(1):43-104, 2018 https://doi.org/10.4271/04-11-01-0004.
15. **Experimental and Surrogate Modeling Study of Diesel Fuel –** G. Kukkadapu, R. Whitesides, M. Wang, SS Wagnon, K. Zhang, M. Mehl, W.J. Pitz, C.-J. Sung and C. Westbrook. 37th International Combustion Symposium, Dublin, Ireland, July 29-August 3, 2018.
16. **Fueling Infrastructure Materials and Isobutanol Compatibility** – M. Kass and K. Moriarty. Webinar Presentation to the Steel Tank Institute, May 31, 2018.
17. **National Labs Examine Effects of New Fuels on Current Equipment –** M. Kass and K. Moriarty. PEI Journal, Second Quarter, 2018.

List of Publications and Presentations (4)

FY18 Publications and Presentations

18. **Near-azeotropic Volatility Behavior of Hydrous and Anhydrous Ethanol Gasoline Mixtures and Impact on Droplet Evaporation Dynamics –** B. Abdollahipoor, S.A. Shirazi, K.F. Reardon, and B.C. Windom. *Fuel Processing Technology*, 181:166-174, December 2018. https://doi.org/10.1016/j.fuproc.2018.09.019.

19. **Physiochemical Property Characterization of Hydrous and Anhydrous Ethanol Blended Gasoline –** S.A. Shirazi, B. Abdollahipoor, J. Martinson, K.F. Reardon, and B.C. Windom. *Industrial and Engineering Chemistry Research*, 57(32):11239-11245, August 2018. https://pubs.acs.org/doi/10.1021/acs.iecr.8b01711.

20. **Selection Criteria for Sustainable Fuels for High-Efficiency Spark-Ignition Engines with Examination of their Storage Stability, Impact on Engine Knock, and Fine Particle Emissions –** R.L. McCormick. Presented at Colorado State University, May 2018. https://www.nrel.gov/docs/fy18osti/71627.pdf.

List of Publications and Presentations (5)

FY17 Publications and Presentations

1. **A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure -** St. John, P., Kairys, P., Das, D., McEnally, C.S., Pfefferle, L.D., Robichaud, D.J., Nimlos, M.R., Zigler, B.T., McCormick, R.L., Foust, T.D. Bomble, Y., Kim, S. *Energy Fuels* 31 9983−9990.
2. **Understanding Trends in Autoignition of Biofuels: Homologous Series of Oxygenated C5 Molecules -** Bu, L., Ciesielski, P.N., Robichaud, D.J., Kim, S., McCormick, R.L., Foust, T.D., Nimlos, M.R. *J. Phys. Chem. A* 121 5475–5486.
3. **Distillation-based Droplet Modeling of Non-Ideal Oxygenated Gasoline Blends: Investigating the Role of Droplet Evaporation on PM Emissions -** Burke, S., Ratcliff, M., McCormick, R.L., Rhoads, R., Windom, B. *SAE Int. J. Fuels Lubr.* 10(1):69-81, doi:10.4271/2017-01-0581.
4. **Selection Criteria and Screening of Potential Biomass-Derived Streams as Fuel Blendstocks for Advanced Spark-Ignition Engines -** McCormick, R.L., Fioroni, G.M., Fouts, L., Christensen, E., Yanowitz, J., Polikarpov, E., Albrecht, K., Gaspar, D.J., Gladden, J., George, A. *SAE Int. J. Fuels Lubr.* 10(2):2017, doi:10.4271/2017-01-0868.
5. **Co-Optimization of Fuels & Engines –** A. Lindauer. Transportation Research Board 96th Annual Meeting, Washington, DC, January 8-12, 2017.
6. **Co-Optimization of Fuels & Engines: FY16 Year in Review –** January 2017. https://www.nrel.gov/docs/fy17osti/67595.pdf.
7. **Co-Optimization of Fuels & Engines (Co-Optima) Initiative –** J. Farrell. SAE 13th International Conference on Engines and Vehicles, Capri, Italy, September 13, 2017. https://www.nrel.gov/docs/fy18osti/70200.pdf.
8. **Annual Merit Review and Peer Evaluation Presentations –** 8 presentations: J. Dec, J. Farrell, C. Kolodziej, R.L. McCormick, M. McNenly, M. Sjöberg, J.P. Szybist, and T. Toops. Vehicle Technologies Office Annual Merit Review and Peer Evaluation, Washington, DC, June 5-9, 2017. https://energy.gov/eere/vehicles/annual-merit-review-presentations.
9. **Bioblendstocks that Enable High Efficiency Engine Designs –** R.L. McCormick, G.M. Fioroni, M.A. Ratcliff, B.T. Zigler, and J. Farrell. 2nd CRC Advanced Fuel and Engine Efficiency Workshop, Livermore, California, November 3, 2016. https://www.nrel.gov/docs/fy17osti/67629.pdf.

List of Publications and Presentations (6)

FY17 Publications and Presentations

10. **Compatibility of Fuel System Elastomers with Bio-Blendstock Fuel Candidates Using Hansen Solubility Analysis – ** M. Kass and B. West. *SAE Int. J. Fuels Lubr.* 10(1):138-162, 2017. http://papers.sae.org/2017-01-0802.
11. **Understanding Trends in Autoignition of Biofuels: Homologous Series of Oxygenated C5 Molecules –** L. Bu, P.N. Ciesielski, D.J. Robichaud, S. Kim, R.L. McCormick, T.D. Foust, and M.R. Nimlos. *Journal of Physical Chemistry A*, 121:5475-5486, 2017. https://doi.org/10.1021/acs.jpca.7b04000.

List of Publications and Presentations (7)

FY16 Publications and Presentations

1. **Effects of Iso-octane/Ethanol Blend Ratios on the Observance of Negative Temperature Coefficient Behavior within the Ignition Quality Tester —** G.E. Bogin, Jr., J. Luecke, M.A. Ratcliff, E. Osecky, and B.T. Zigler. *Fuel* 186:82-90, 2016 www.sciencedirect.com/science/article/pii/S0016236116307578.
2. **Exploring the Relationship Between Octane Sensitivity and Heat-of-Vaporization —** R. McCormick, M. Ratcliff, and B.T. Zigler. *SAE Int. J. Fuel Lubr.*, 9:80-90, 2016. papers.sae.org/2016-01-0836/.
3. **Fuel Properties and Chemical Kinetics —** R.L. McCormick, G. Fioroni, J. Szybist, T. Bays, P. Miles, M. McNenly, B. Pitz, J. Luecke, M. Ratcliff, B. Zigler, S. Goldsborough. DOE 2016 Annual Merit Review and Peer Evaluation Meeting for the Vehicles Technologies Office, Washington, DC, June 5-9, 2016. www.energy.gov/sites/prod/files/2016/07/f33/ft038_mccormick_szybist_fuel_properties_2016.pdf.
4. **Investigation of Iso-octane Ignition and Validation of a Multizone Modeling Method in an Ignition Quality Tester —** E.M. Osecky, G.E. Bogin, Jr., S.M. Villano, M.A. Ratcliff, J. Luecke, B.T. Zigler, and A.M. Dean. *Energy & Fuels*, 30 (11): 9761– 9771, 2016. pubs.acs.org/doi/abs/10.1021/acs.energyfuels.6b01406.
5. **Knock Resistance and Fine Particle Emissions for Several Biomass-Derived Oxygenates in a Direct-Injection Spark-Ignition Engine —** M.A. Ratcliff, J. Burton, P. Sindler, E. Christensen, G.M. Chupka, L. Fouts, and R.L. McCormick. *SAE Int. J. Fuel Lubr.*, 9:59-70, 2016. papers.sae.org/2016-01-0705/.