DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

Co-Optimization of Fuels & Engines

Structure-property relationships & property predictions

Co-Optima review session

March 7, 2019

Anthe George
Sandia National Laboratory

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

Co-Optima is focused on outcomes which improve the blendstock value proposition

SPR-PP: Structure-property relationships and property prediction underpin Co-Optima blendstock candidate selection and evaluation

Goal

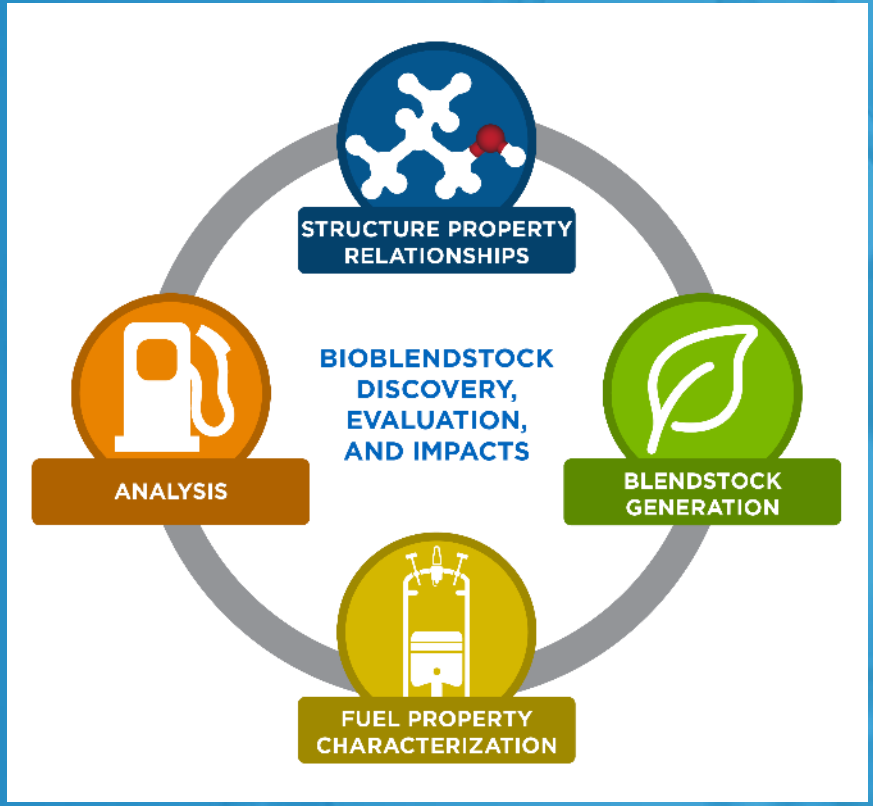
- Develop accurate chemical structure-fuel property relationships, and fuel property predictions from these, across a full set of chemical classes and structures

Outcome

- Enables Co-Optima and other researchers to identify and evaluate candidate blendstocks

Relevance

- Provides underlying science to understand and predict fuel properties of blendstock targets



SPR-PP Quad Chart Overview

Timeline

- Phase I 10/1/15 to 9/30/18
- Phase II 10/1/19 to 9/30/21
- % complete 12% of review cycle

	Total budget pre FY17	FY 17 budget	FY 18 budget	Total planned funding (FY 19-project end)
DOE funded	$4,993	$4,290	$3,515	$11,025

DOE Labs part of SPR-PP:
LANL, LBNL, NREL, ORNL, PNNL, SNL

Barriers addressed

- ADO-E. co-development of fuels & engines
- At-D. identifying new market opportunities for bioenergy and bioproduct

Objective

Tie fuel properties to chemical structure by:

- developing tools to predict SPRs
- predicting fuel properties and supplying to generation, characterization efforts

End of project goal

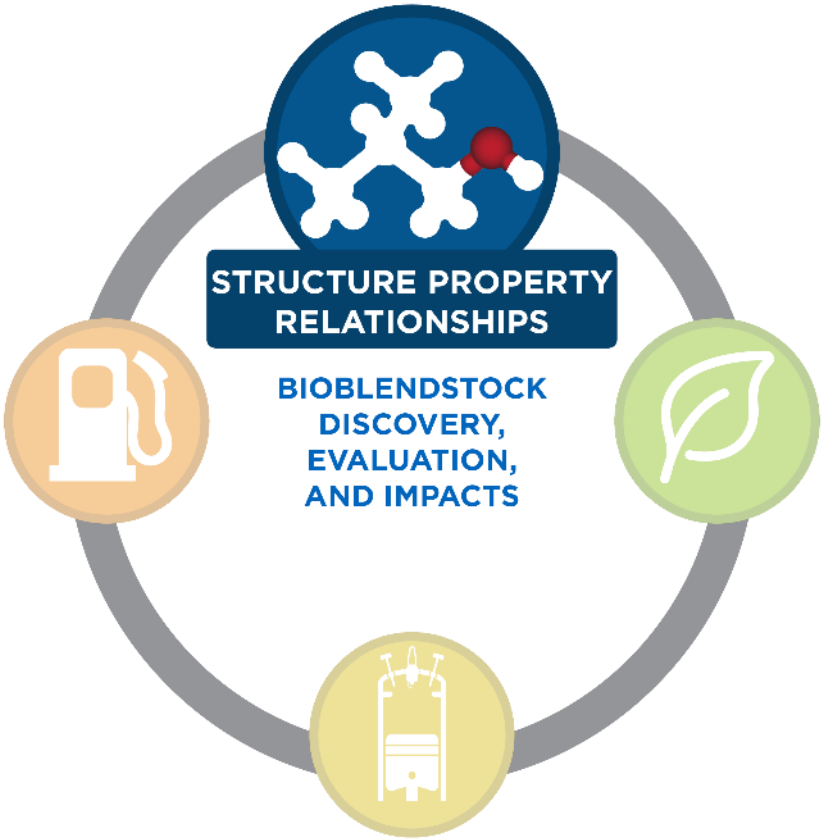
- Develop accurate chemical structure-fuel property relationships, and fuel property predictions from these, across a full set of chemical classes and structures

1 Project Overview

SPR-PP Structure-property relationships & property predictions

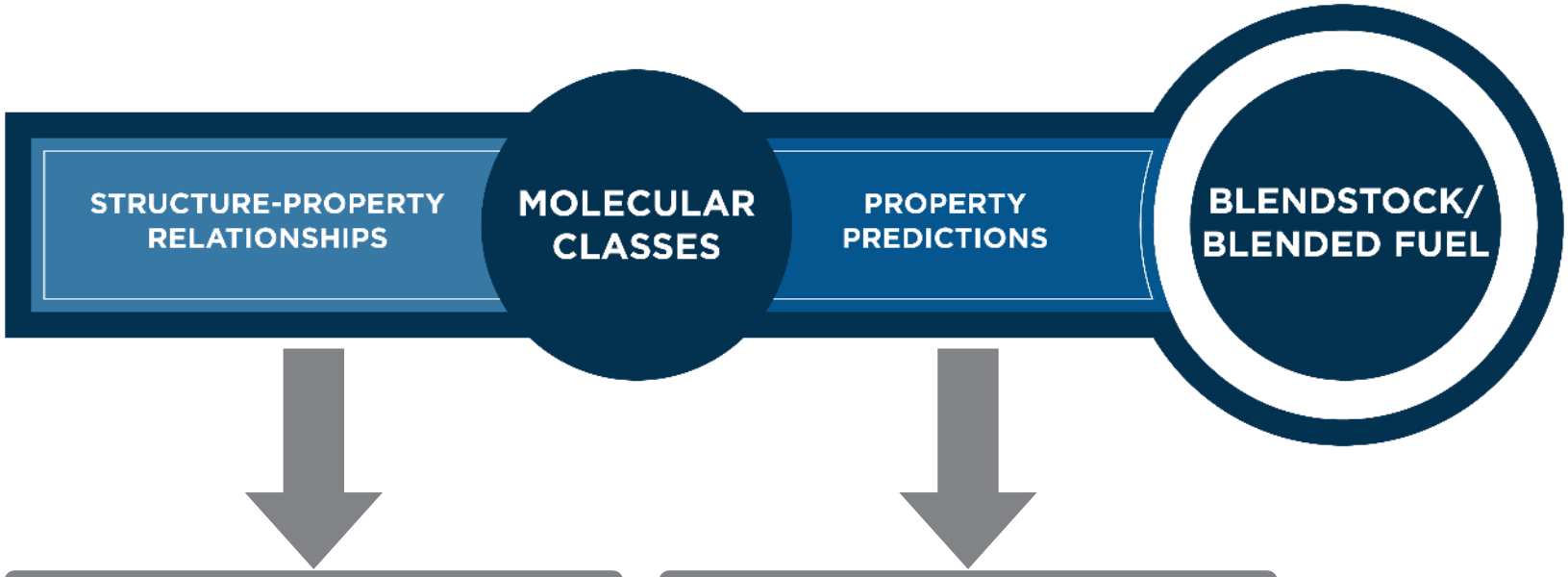
SPR-PP objectives:

- Tie fuel properties to chemical structure to enable bioblendstock selection for the generation, characterization analysis cycle



1 Project Overview

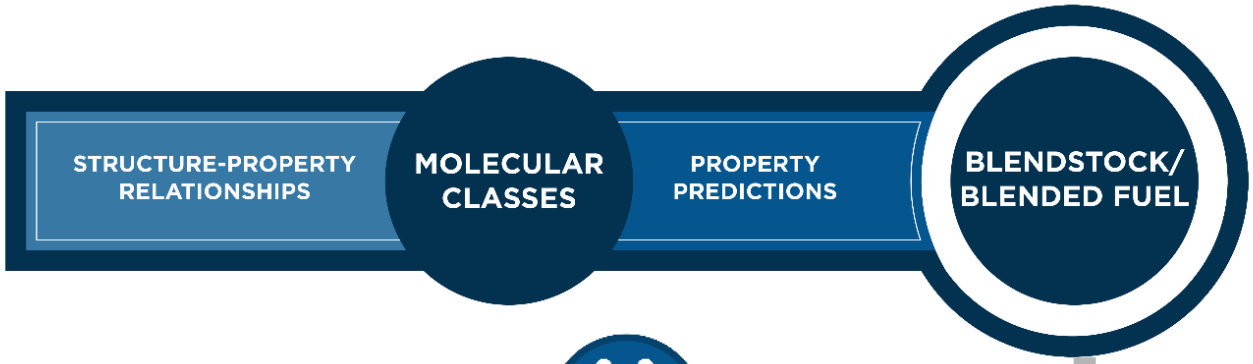
Structure-property relationships & property predictions



1. Define important properties
2. Define suite of chemistries and functional groups
3. Establish influence of these chemistries on properties

1. Develop methods to predict properties for blendstocks and blended fuels
2. Conduct predictions within qualifying molecular classes

2 Approach (Management)
All teams technically integrated



Enables decision-making on which blendstocks undergo feasibility analysis

Provides blendstock targets to be generated, where data are unavailable

Provides information on targets to be further characterized and predicted properties for unavailable fuels

2 Approach (Management)

Comprehensive inter-lab integration for all projects

National labs and principal investigators

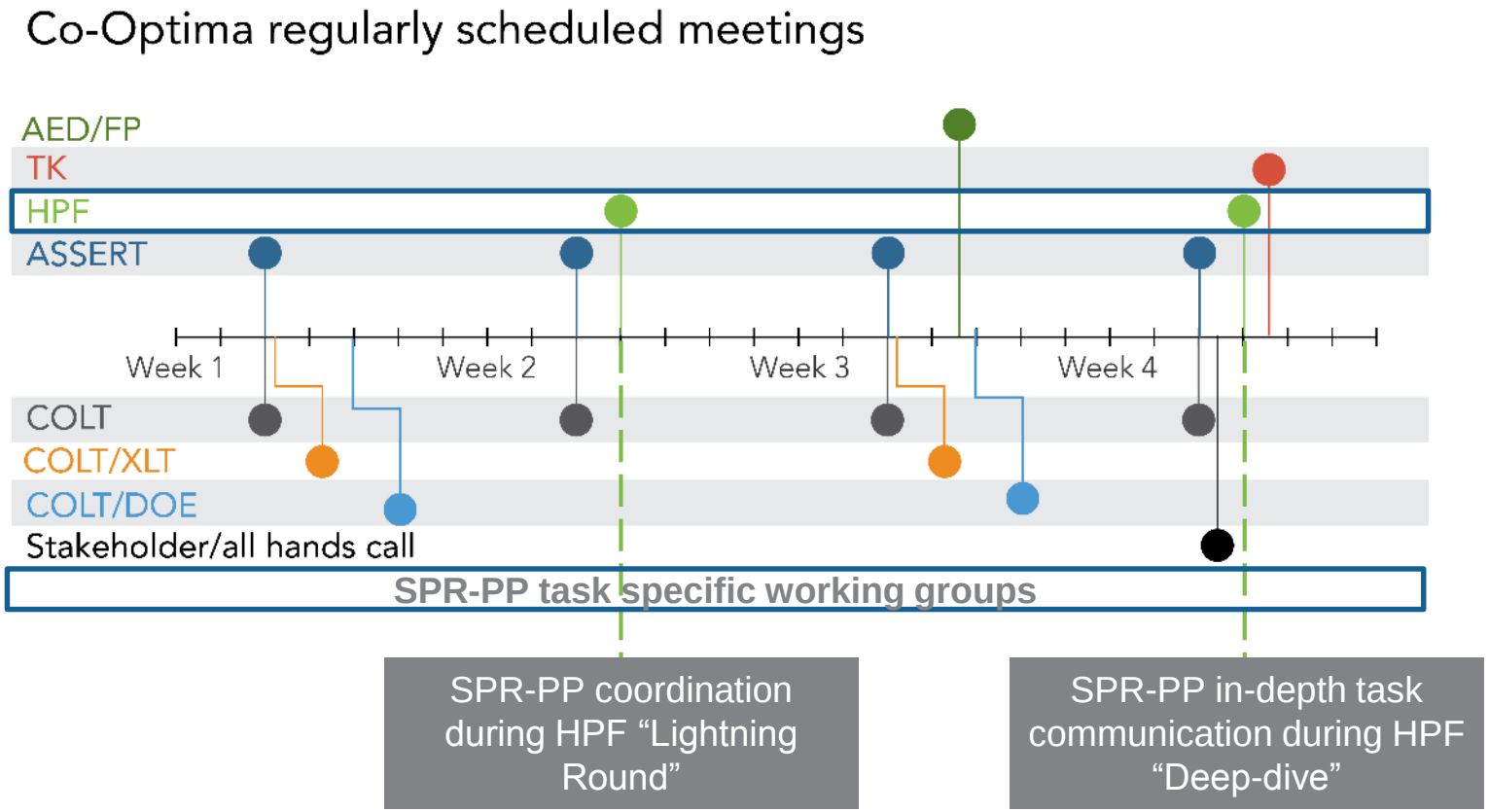
HPF Team Lead: Anthe George (SNL) **HPF Deputy: Derek Vardon (NREL)**

Los Alamos NATIONAL LABORATORY EST. 1943	**Andrew Sutton**, Kubic, Cameron Moore, Troy Semelsberger
BERKELEY LAB	**Todd Pray**, Jay Keasling, Eric Sundstrom
NREL NATIONAL RENEWABLE ENERGY LABORATORY	**Tom Foust**, Dan Ruddy, Nabila Huq, Gregg Beckham, Derek Vardon, Seonah Kim
OAK RIDGE National Laboratory	**Brian West,** Mike Kass
Pacific Northwest NATIONAL LABORATORY	**Evgueni Polikarpov,** Tim Bays, Lelia Cosimbescu, Vanessa Dagle, Dan Gaspar, Karthi Ramasamy
Sandia National Laboratories	**Anthe George,** Joey Carlson, Ryan Davis,, Corey Hudson**,** Eric Monroe

Experienced team with cross-cutting expertise in fuels and their properties

2 Approach (Management)

Communication and coordination essential for SPR-PP activities

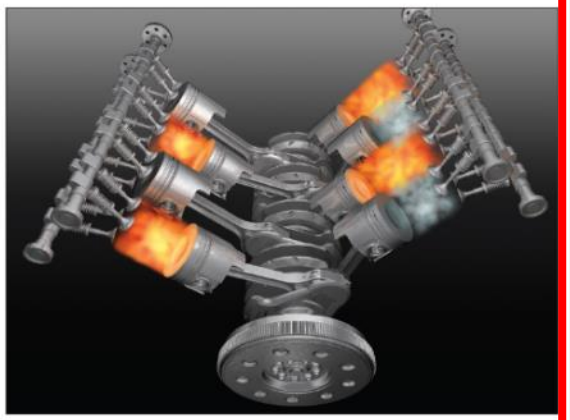


SPR – PP efforts are closely integrated in HPF & broader Co-Optima

2 Approach (Technical)

Foundational technical questions frame approach

What fuels do engines *really* want?

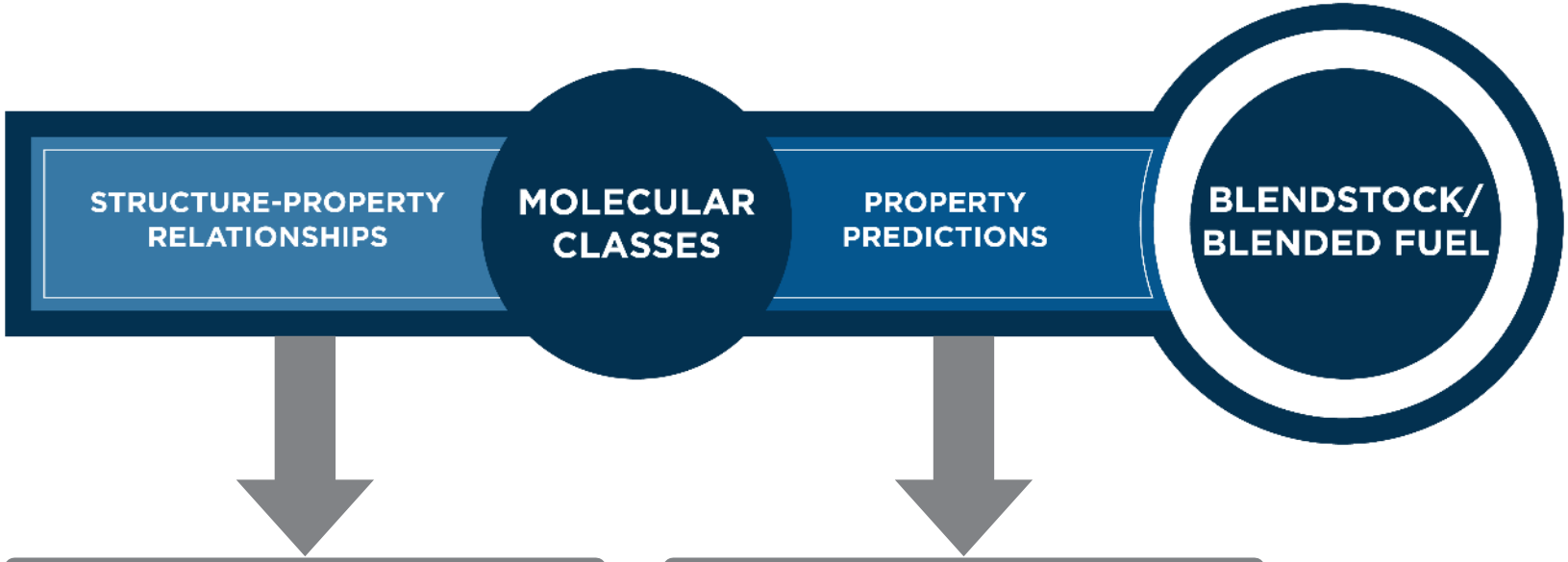


What fuel options work best?

What will work in the real world?

2 Approach (Technical)

SPR-PP workflow leads to blendstock determination

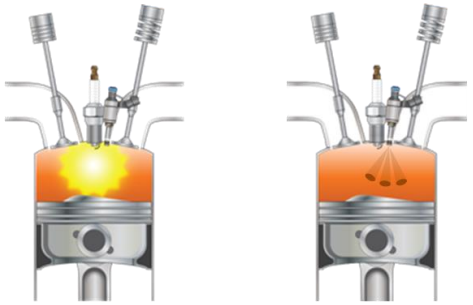


- Devise comprehensive suite of functional groups
- Mine literature, use available tools
- Devise SPRs
- Select qualifying functional groups for combustion type

- High throughput tools (computational / experimental)
- Theoretical/quantum chemistry calculations
- Machine learning
- Select experimental data for validation

2 Approach (Technical)
Defining properties by combustion mode

Light-Duty

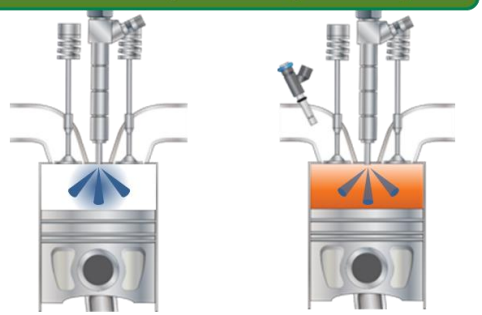


Boosted SI | Multi-mode SI/ACI

Properties

- ethers
- polyethers
- n-alkanes
- iso-alkanes
- mono-alkenes
- esters
- alcohols
- ketones
- polyketides
- cycloalkanes
- dienes
- carboxylic acids
- aldehydes
- aromatics

Medium/Heavy-Duty



Mixing Controlled | Kinetically Controlled

Properties

- ethers
- polyethers
- n-alkanes
- iso-alkanes
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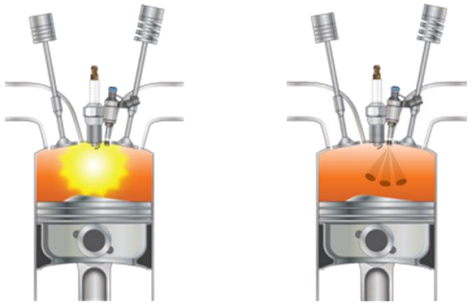
2 Approach (Technical)
Defining properties by combustion mode

Light-Duty



Boosted SI | Multi-mode SI/ACI

Performance:
RON, MON, S, HoV, Sooting

Operability:
P_{vap}, B_p, M_p, η, σ, stability

- ethers
- polyethers
- n-alkanes
- iso-alkanes
- mono-alkenes
- esters
- alcohols
- ketones
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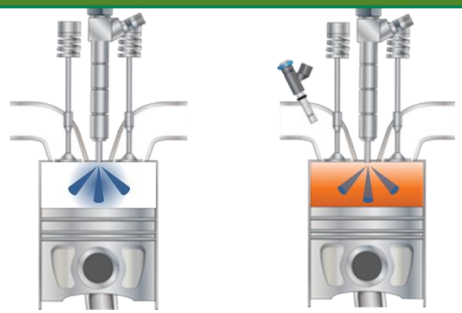
- cycloalkanes
- dienes
- carboxylic acids
- aldehydes
- aromatics

Medium/Heavy-Duty



Mixing Controlled | Kinetically Controlled

Performance:
CN, LHV, Sooting. Flash point

Operability:
M_p, η, solubility, stability

- ethers
- polyethers
- n-alkanes
- iso-alkanes
- mono-alkenes
- esters
- alcohols
- ketones
- polyketides
- cycloalkanes
- dienes
- carboxylic acids
- aldehydes
- aromatics

2 – Approach (Technical)

Critical success factors and barriers to overcome

SPR-PP Success Factors	SPR-PP Barriers to Overcome
Discover underlying science that links properties to chemical structure	Timing for devising structure-property relationships complicate work staging
Define combustion-appropriate blendstock candidates for further evaluation by Co-optima	Relevant properties for advanced combustion approaches not fully defined
Provide on-going property prediction support to broader Co-optima team	Lack of training data for novel structures can reduce reliability of models

Project activities designed to address barriers to success

2 Approach (Technical)

Well-defined milestones and strategies to address risk

SPR-PP Potential Risks

- ✓ Paucity of experimental data prevents development of models and SPR
- ✓ Time line for determining important multi-mode properties incompatible with SPR workflow

SPR-PP Risk Mitigation Strategy

- ✓ Determine essential data points and work with generation/characterization teams to produce values
- ✓ Work with fuel property and engines team to triage most critical fuel properties for evaluation

HPF Demonstrated Ability

- ✓ HPF outputs link “Structure Property” and “Bioblendstock Generation” for a given chemistry
- ✓ HPF completed >20 milestones in FY18 related to Light Duty and Heavy Duty bioblendstocks

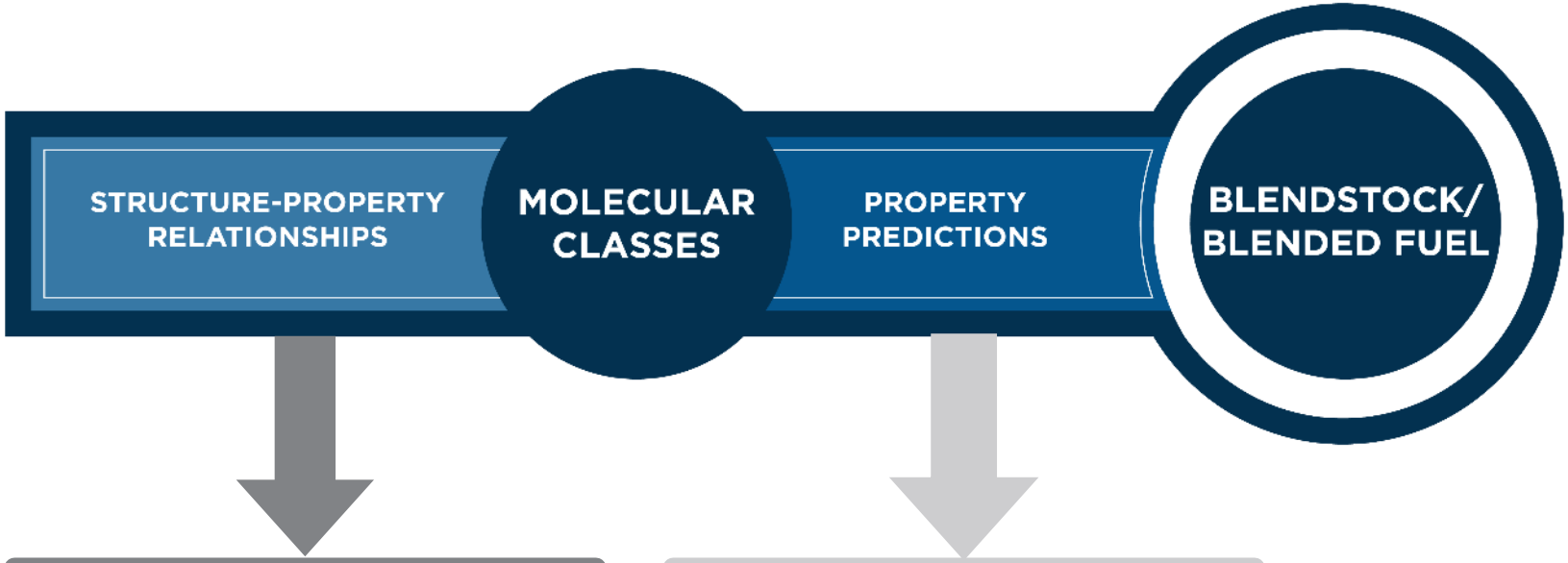
Selected SPR-PP FY18 Milestones

Submit a review article for publication detailing the newly developed thermodynamic understanding of the chemical basis for Reid vapor pressure in non-ideal fuel mixtures	Q1
Expand surrogate blend model to full composition fuels and oxygenate blends	Q3

Progress measurable with risk mitigation strategies and milestones in place

3 Progress SPR

Structure property relationships to determine blendstock targets



- Devise comprehensive suite of functional groups
- Mine literature, use available tools
- Devise SPRs
- Select qualifying functional groups for combustion type

- High throughput tools (computational / experimental)
- Theoretical/quantum chemistry calculations
- Machine learning
- Select experimental data for validation

3 Progress SPR

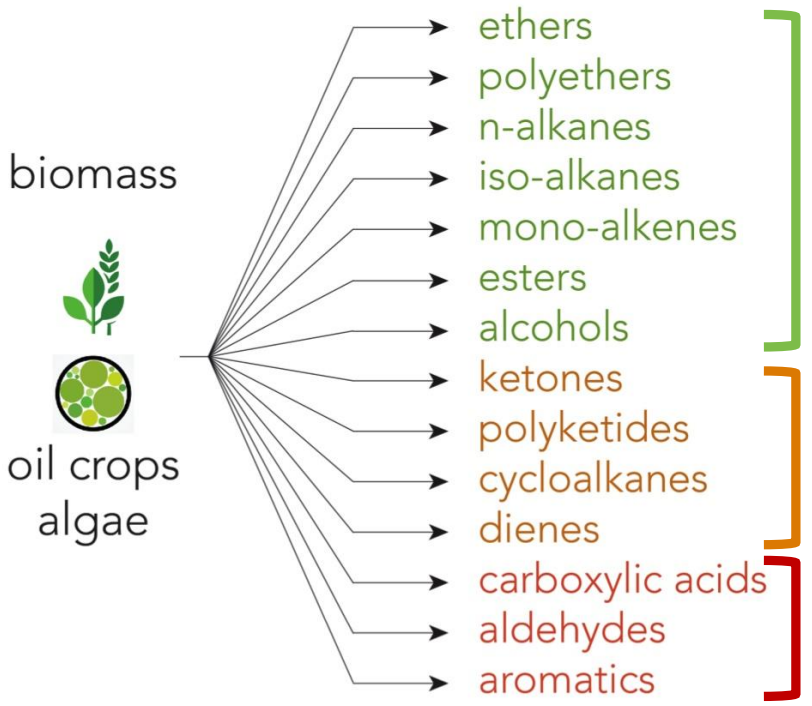
Determined chemistries with potential as diesel-like bioblend stocks

Screened functional groups based on fuel properties

- Autoignition (cetane number)
- Boiling point
- Flashpoint
- Kinematic viscosity
- Freezing point
- Biodegradability and toxicity

Evaluated 14 structural groups for MCCI bioblendstock potential

- Determined several hydrocarbon and oxygenate functional groups are (green) or may be (orange) suitable for use as diesel-like bio-blendstocks



PI: Gaspar, PNNL & McCormick NREL

Outcome: first systematic application of the fuel property-based approach to diesel-like bio-blendstocks

3 Progress SPR

Software to explain structural contributions relevant to RON, MON, CN

Software visualizes how structural differences impact fuel properties

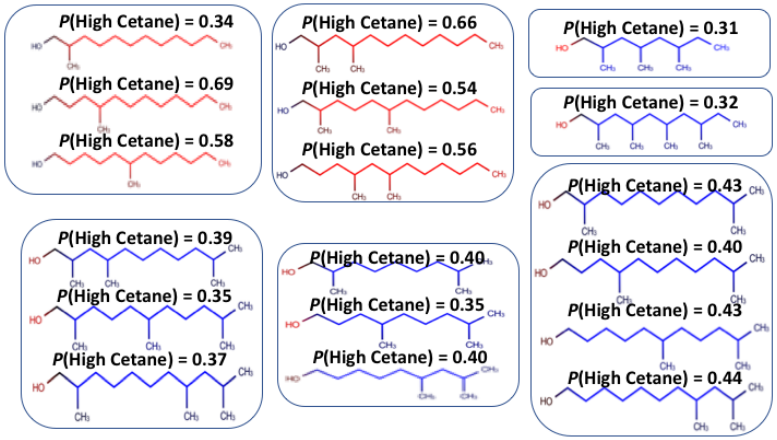
- Provided a basis for visually evaluating model performance relative to known functional groups
- Focused on properties RON, MON, CN

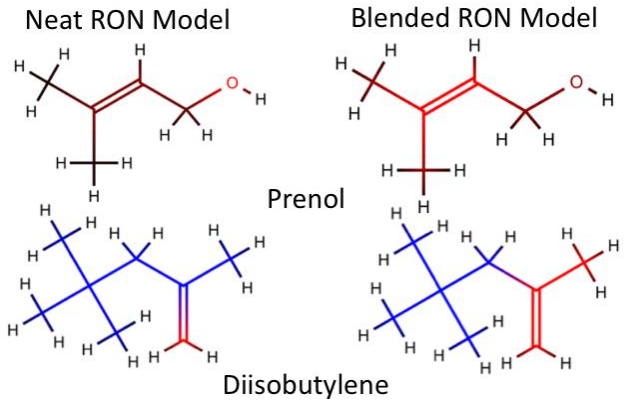
Nearly all blendstocks being considered by Co-Optima have been evaluated

- 1000s of molecules evaluated to understand impact of structure on RON MON CN

Specific outcomes include

- Determined the effect of methylation position on sparsely methylated alcohols
- Provided bases for modeling neat vs. blended effects in prenol and diisobutylene
- Software has been distributed Open Source at https://www.github.com/sandialabs/FeatureCreature





PI: Hudson, SNL

Outcome: evaluated the impact of structure on fuel properties of potential fuel chemicals that lead to MCCI and SI blendstock targets for further evaluation

3 Progress SPR

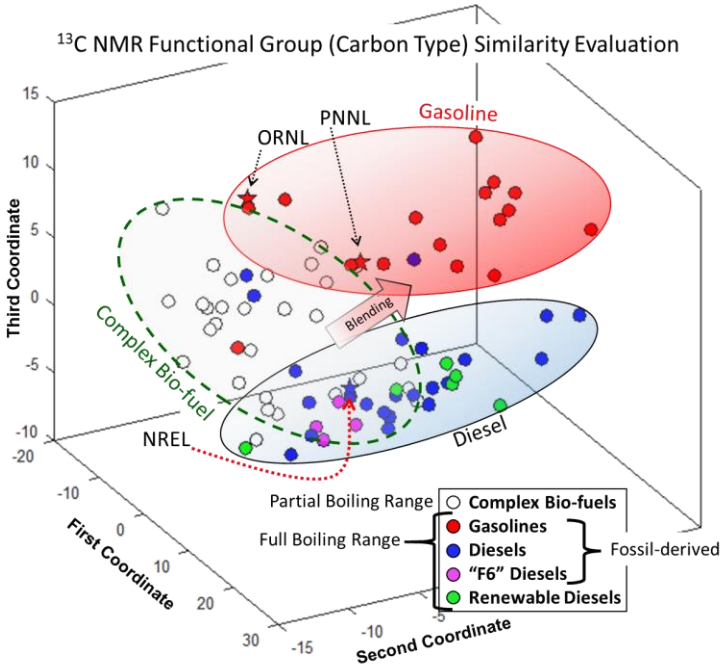
Blending/NMR models use carbon position for fuel property prediction

Fuel complexity and carbon position drive property predictions

- 250 µL NMR samples characterize blendstock properties
- Completed comparison of carbon types for 72 complex fuels (shown) and ~100 (not shown)
- Fuels generally grouped according to complexity and distillation range
- Property predictions within partial or full distillation range fuels were robust, but not extensible from less complex to more complex

Co-Optima samples characterized validate expected results

- PNNL iso-olefin sample comparable to gasoline
- NREL 20% blend of 5-ethyl-4-propylnonane in diesel comparable to diesel
- ORNL natural gasoline sample comparable to gasoline



PI: Bays, PNNL

Outcome: can successfully predict or classify fuel properties based on carbon types and aid in structure-property model development for complex mixtures

3 Progress SPR

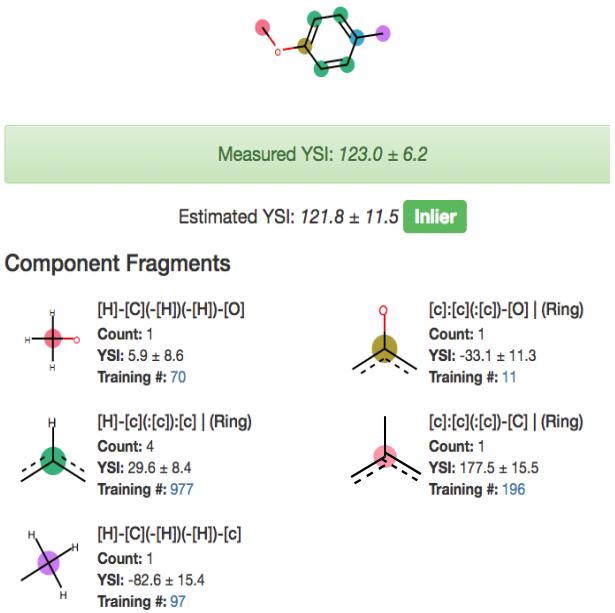
Fast screening property mapping molecular structure to sooting

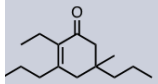
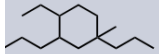
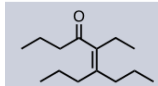
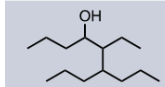
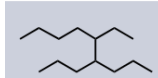
Sooting tool maps relationship between molecular structure and sooting properties

- Machine learning using molecular structure and experimentally YSI (Yield Sooting Index) values for ~500 species
- Allows screening of a wide range of chemical functionality for blendstocks that resist soot formation

Fuel design explores chemical space where we lack existing measurements

- Provides detailed information per each carbon type to design low sooting fuel candidates



Structure	CN	YSI
	16	**165**
	39	**105**
	36	**95**
	40	**90**
	49	**91**

PI: Kim & St. John, NREL

Outcome: provides user friendly web app for Co-Optima teams. This tool help to design low sooting fuel candidates based on carbon types

https://ysipred.herokuapp.com

3 Progress SPR

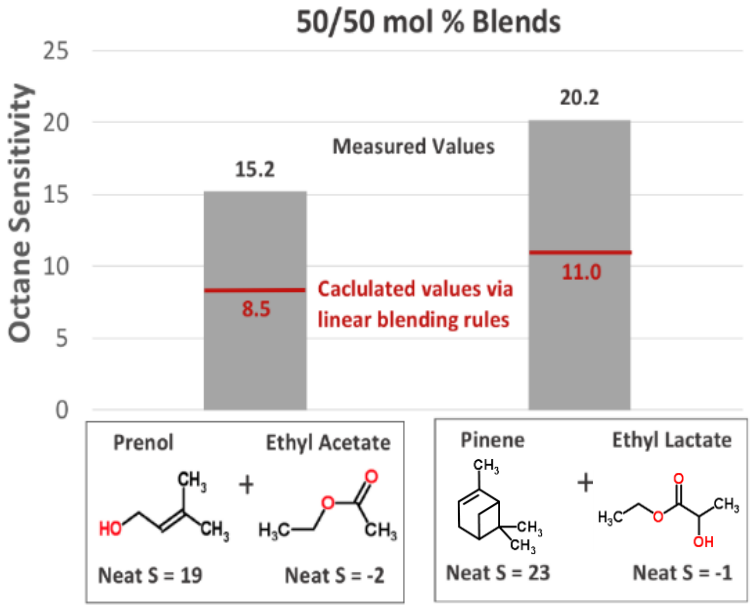
Using SPR learnings toward optimizing bioblendstock properties

From SPR learnings evaluated blends of bioblendstocks to optimize beneficial properties

- Evaluated blends of high RON low S with low S high RON

High S bioblendstocks containing double bonds tend to rapidly increase S when blended with low S bioblendstocks

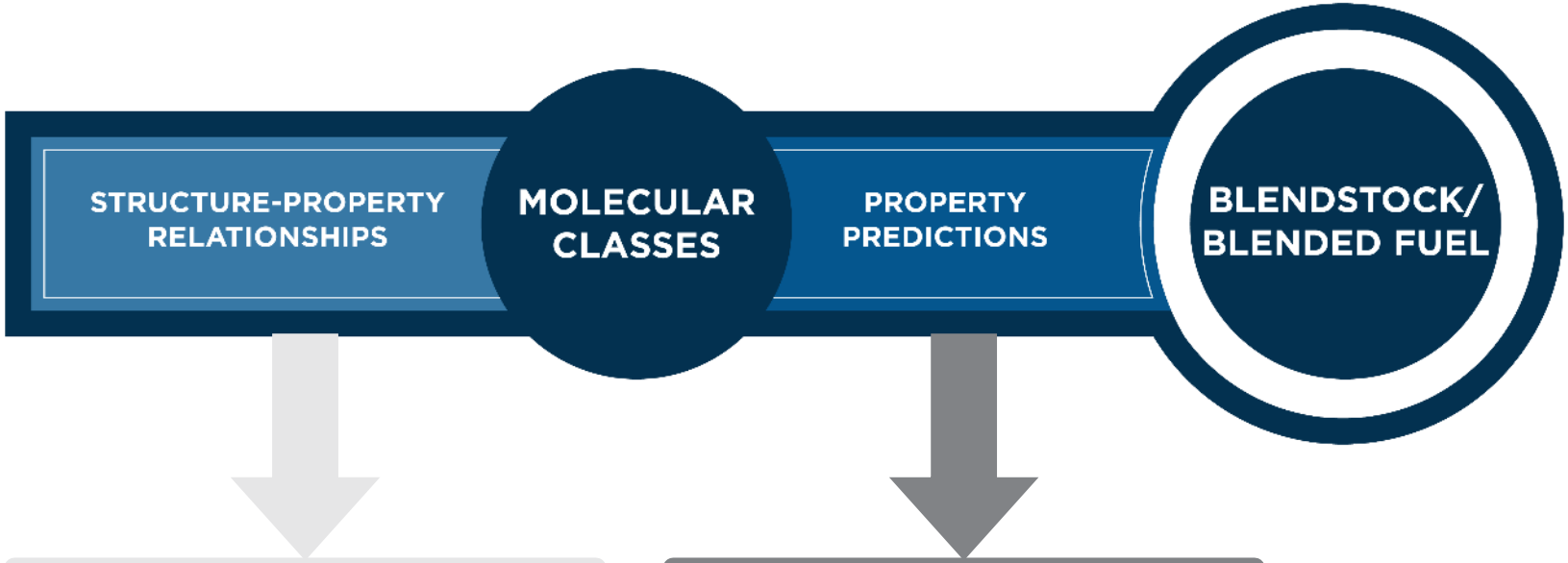
- Demonstrated clearly with ***α***-pinene and prenol
- Occurs across functional groups (esters, ketones, alcohols all interact synergistically with olefinic compounds
- Combinations of ***α***-pinene and ethyl lactate showed the strongest S synergy.
- Often occurs via extreme MON suppression and blends often overcome antagonistic RON blending



PI: Davis, SNL

Outcome: demonstrated potential for synergistic combinations of bioblendstocks for optimized octane S means compounds with strong RON performance and poor S should not be excluded

3 Progress PP
Property predictions for blendstock targets



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- High throughput tools (computational / experimental)
- Theoretical/quantum chemistry calculations
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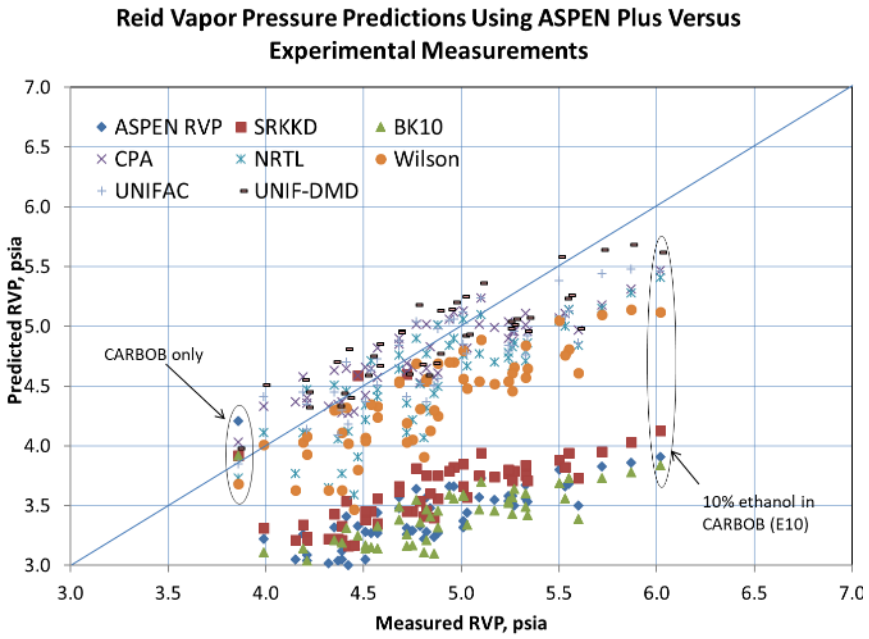
3 Progress PP

Accuracy in predicting fuel properties: vapor pressure case study

Reid Vapor Pressure (RVP) is an important fuel property which affects behavior

- Vapour pressure affects properties such as spray formation, fuel injection fuel storage and handling
- Predictions from 9 models were compared to dry vapor pressure for 19 oxygenates – alcohols, acetates, ketones, methoxy benzene, and dioxolane – in CARBOB at 10, 20, and 30 vol%
- Cubic Plus Association Equation of State model (CPA) and the UNIFAC activity coefficient method with Dortmund activity coefficients (UNIF-DMD) predicted RVP most accurately.



PI: Gaspar, PNNL

Outcome: results allow determination of vapor pressure for new blendstocks prior to synthesis or that are available in limited quantities

3 Progress PP

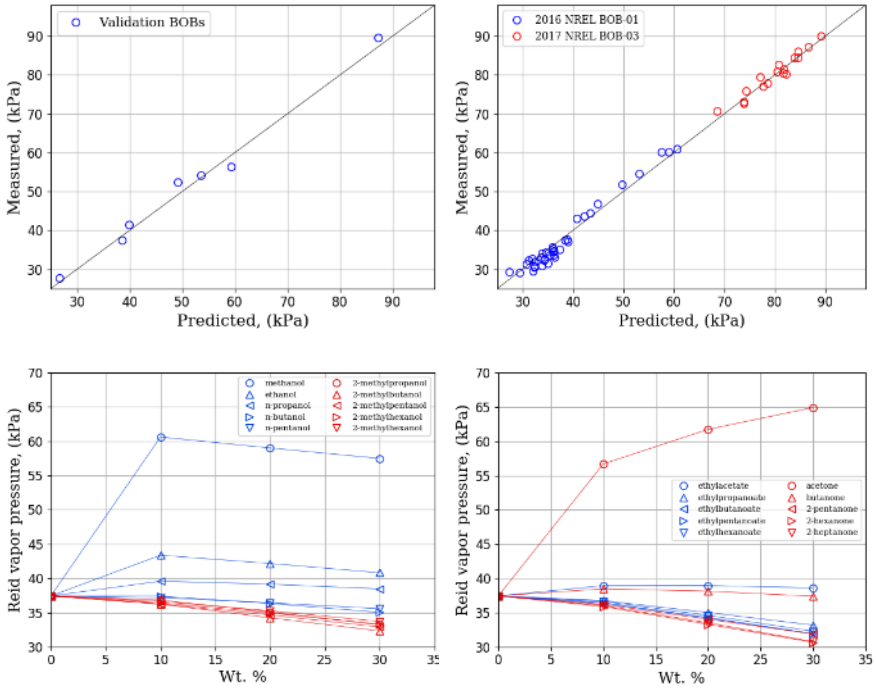
Accuracy in predicting fuel properties: vapor pressure case study

Statistically associating fluid theory produces high accuracy prediction

- Model is easily applied to SI fuels
- Benchmarked to 7 BOBs, %AAD = 3.66
- Tested against a range of oxygenates, including alcohols, esters, ketones, ethers blended into a Summer and Winter BOB
- % AAD for Summer and Winter BOB blends are 3.48 and 2.58, respectively

RVP suppression effects of oxygenates blended into a Summer BOB

- Important in refinery applications
- RVP suppression ⇒ less fuel loss due to volatility issues
- RVP suppression occurs for larger n-alcohols, branched alcohols, most esters, and some ketones – no non linear blending observed for molecules evaluated



PI: George, SNL

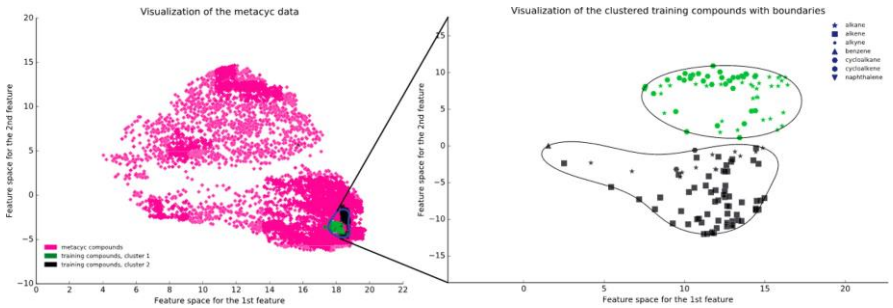
Outcome: accurate prediction model leads to better understanding of the molecular interactions controlling RVP in oxygenates and RVP suppression

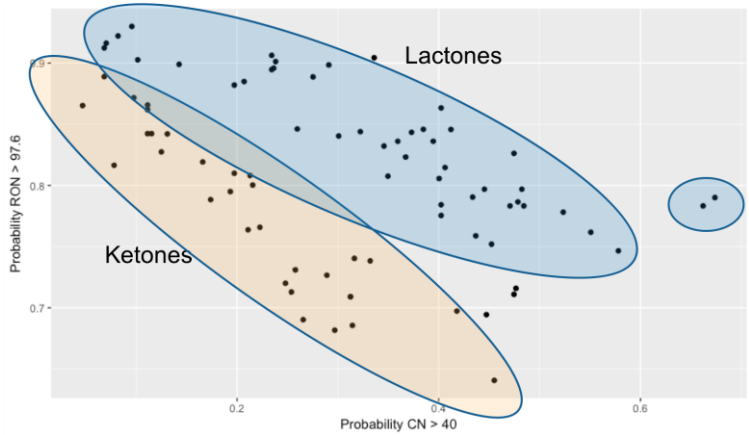
3 Progress PP

High throughput screening tool for evaluating fuel properties

Machine learning framework rapidly classifies molecules by RON, MON, Octane Sensitivity, Cetane Melting Point and Threshold Sooting Index

- Determined the positive effects of hydrogenating sesquiterpenes on cetane
- Screened thousands of molecules for light duty properties, allowing the exclusion of low quality molecules prior to costly evaluation
- Ranked potential methyl ketones by RON and Cetane, driving work in research on production of competing biological routes





Nearly every molecule under consideration by Co-Optima has been evaluated for Cetane and RON as a first order screening

PI: Hudson, SNL

Outcome: provides a tool for rapidly screening the suitability of biocompounds as potential fuels

Software has been distributed Open Source at https://www.github.com/sandialabs/BioCompoundML

3 Progress PP

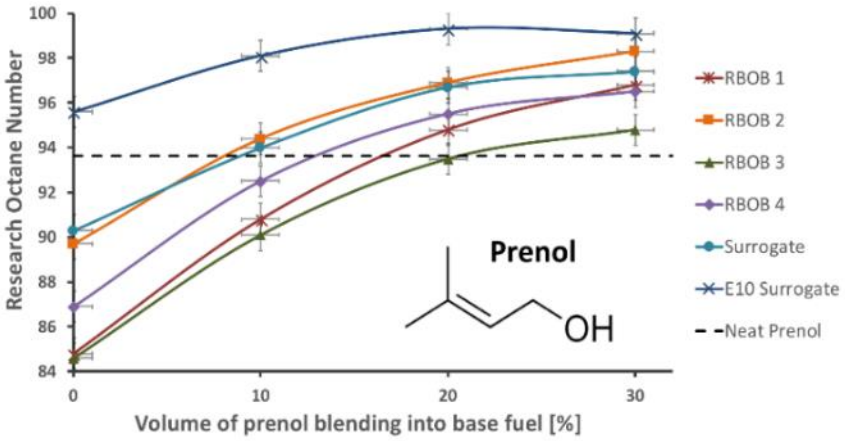
Investigation of SPRs in blends shows novel combustion behavior

Investigating structure-property relationships lead to discovery of new blending phenomenon

- Adding prenol to base fuels boosts RON beyond the neat RON of both prenol and RON
- Finding lead to prenol being included in the Top 10 Boosted SI
- Large boost in octane sensitivity

Phenomenon suggests an unexplored aspect of autoignition kinetics

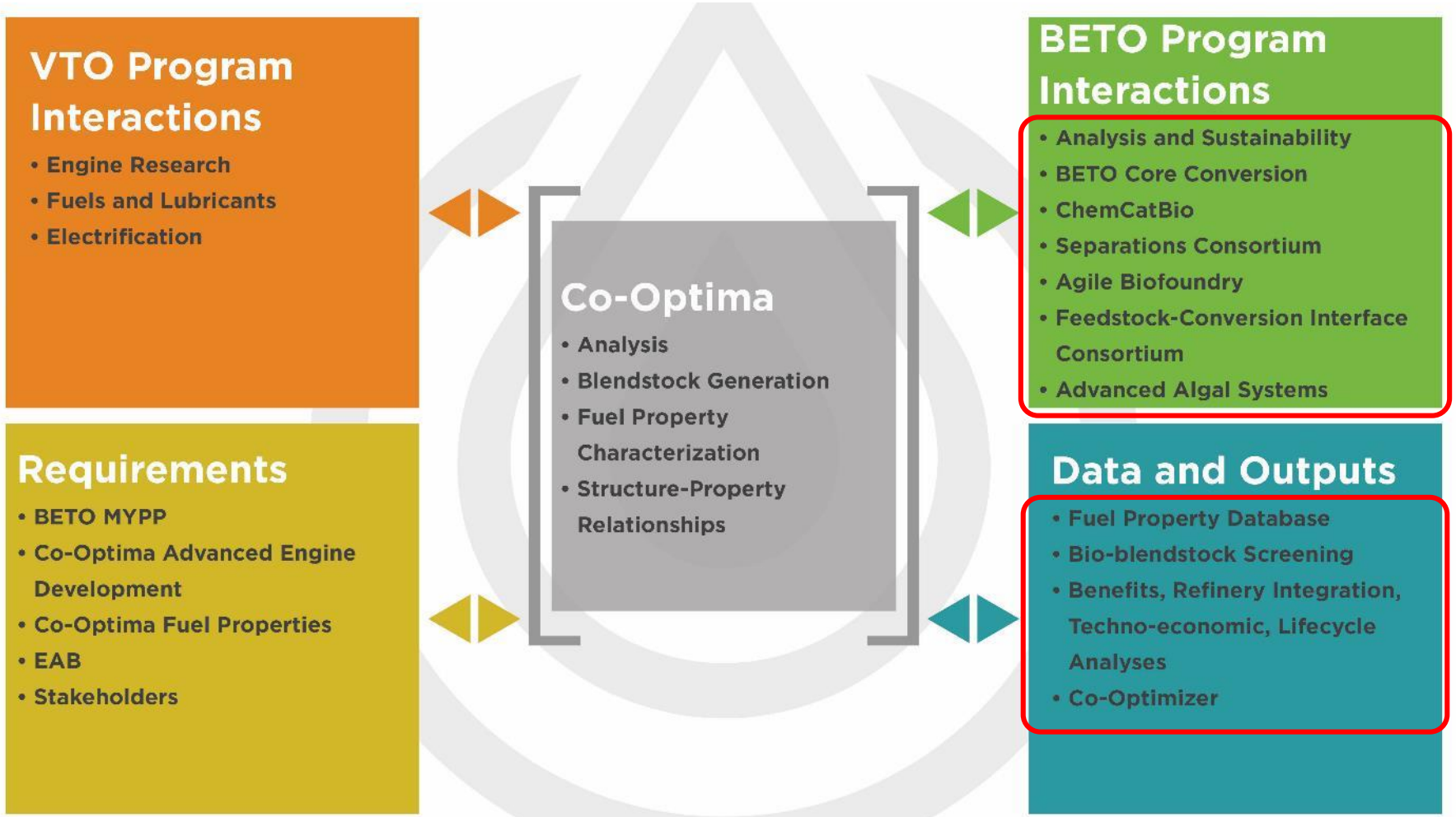
- Understanding mechanism can enable discovery of new fuels, heretofore overlooked



PI: George, SNL

Outcome: new molecule selection; prenol in base blendstock has one of the highest merit functions for boosted SI fuels. Understanding mechanism may enable discovery of new fuels.

4 Relevance
Connected to BETO and stakeholders



4 Relevance
Integral part of BETO Strategy

BETO 2016 MYPP: Conversion R&D "develops commercially viable technologies for … energy-dense, fungible, finished liquid transportation fuels …". The focus is on "**key processing components that form technology building blocks**" for "deconstruction and fractionation" and "synthesis and upgrading."

Co-Optima is identifying what fuel properties enable highly efficiency and clean engines.

- Identifies critical fuel properties (Merit Function)
- Identifies specific targets (structure-fuel property relationships)
- Provides retro-synthetic analysis that connect to BETO's pathways (and others)

This compliments BETO's focus on what "processing components" could be used to produce bio-blendstocks

Addresses what does an engine want and what should we make

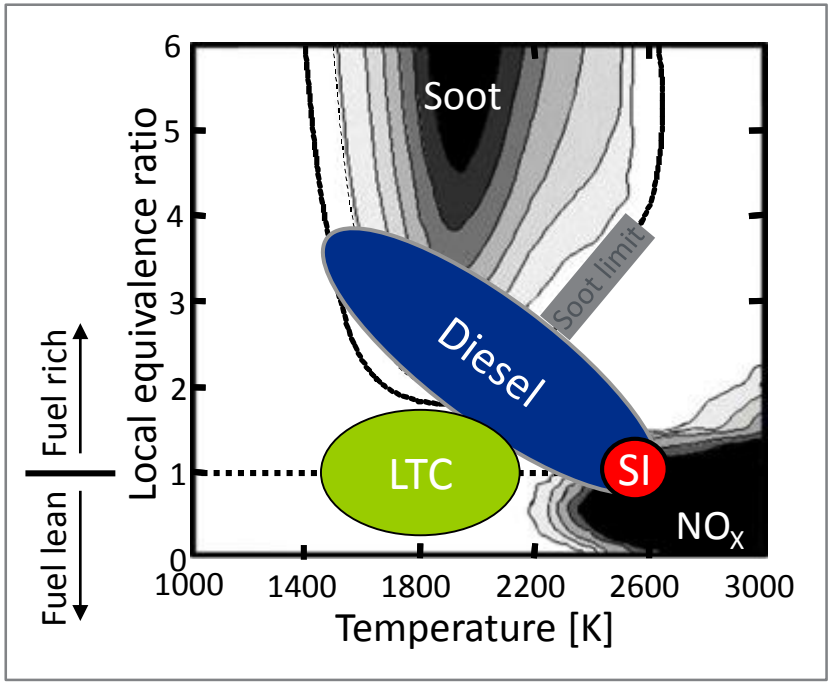
Impact: provides options for producers in a way that does not pick winners

4 Relevance
SPRs will lead to reduced emissions

BETO MYPP: "**Co-development of fuels and engines** has proved successful for **controlling** criteria **pollutants** … and **reduced** GHG **emissions**."

Co-Optima research is addressing:

- Emission profiles (on a subset of bioblendstock candidates)
- Diesel engine advancements – fuel options that burn cleaner
- Advanced compression ignition combustion modes – fuel options that approach diesel efficiency with lower emissions

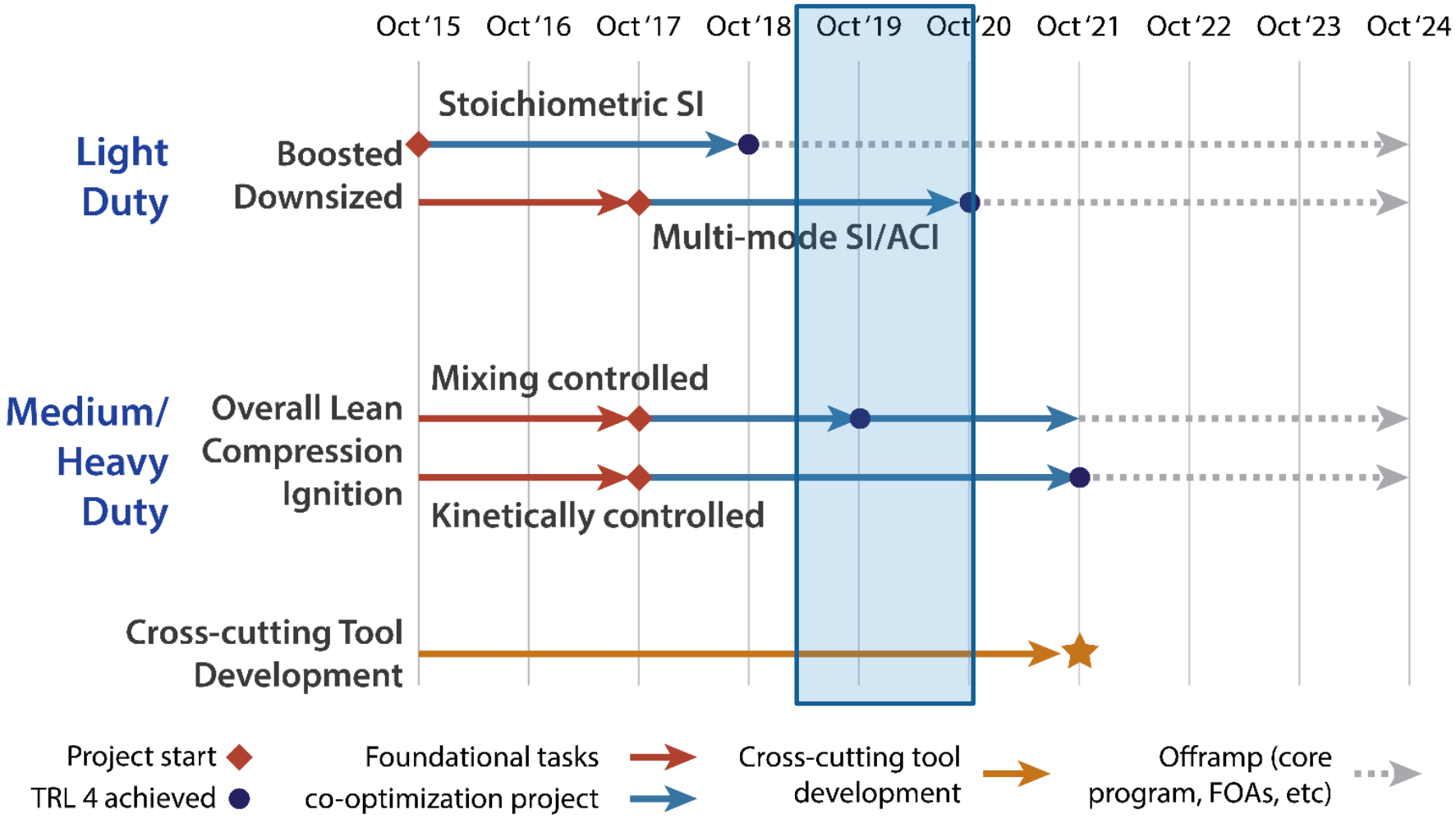


Impact: cleaner air, lower cost,* reduced greenhouse gas emissions

* Cost of emission control on heavy duty truck can approach the cost of the engine

5 Future Work

Look ahead at next 18 months



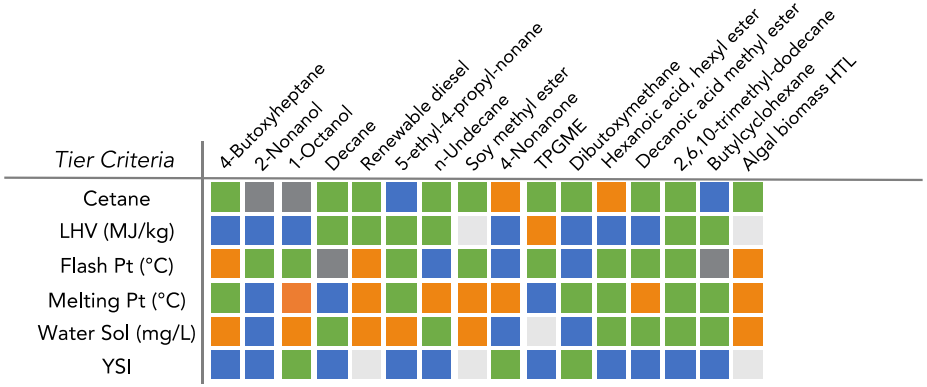
5 Future Work

Targeting other combustion modes & key challenges in next 18 months

FY19 → **FY20**

End of FY19

Complete SPR-PP work to inform MCCI merit activities

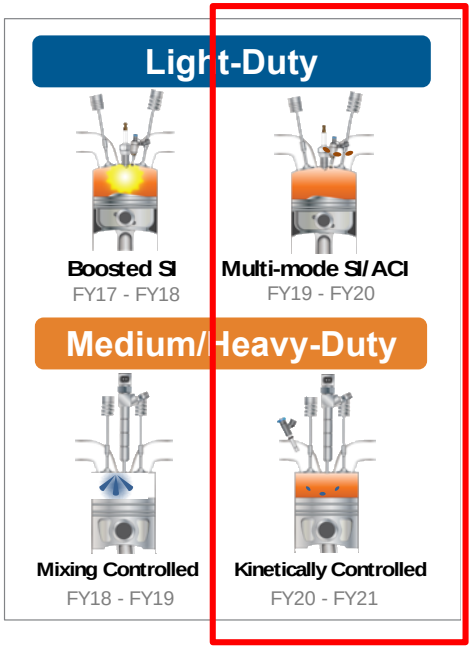


End of FY20

Establish important multi-mode properties and complete SPR-PP workflow to enable multi-mode candidate selection

FY19 to FY21

Target MM and KC



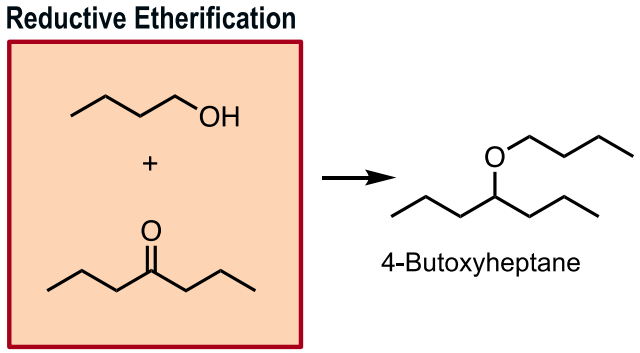
Selected FY19 Milestones		
Multi-mode	Collect octane sensitivity data for BioCompound ML tool	Q1
MCCI	MCCI + Oxygenate predictive models completed using equations of state modelling	Q3
Multi-mode combustion	Blending model able to predict fuel properties from blends of individual, Co-Optima fuel components at 10, 20, and 30% into a complex blendstock	Q4

5 Future Work

MCCI case study: Understanding ether structure on fuel properties

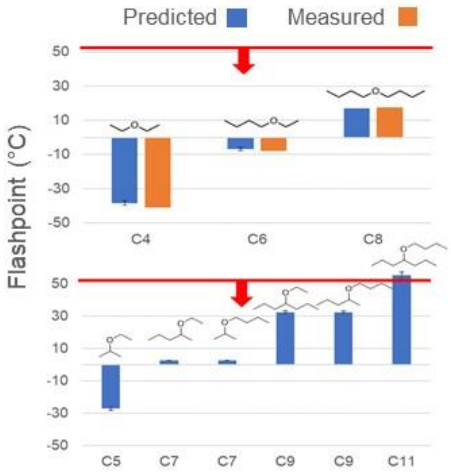
Fuel property prediction tools can be leveraged to evaluate ether structure effects on key heavy duty criteria

- Ethers have exceptionally high cetane and low sooting tendency
- However, flash point is a key ASTM and Tier 2 safety criteria for diesel fuel that can limit the application of ethers



Structure-property relationships inform targeted conversion pathways

- Carbon chain length criteria for ether flashpoint used to dictate viable C-C coupling strategies
- Approach used to evaluate both linear and branched ethers that can be accessed from short chain carboxylic acids
- Predicted vs. measured fuel properties matched well for flash point criteria, with future work to evaluate other key Tier 2 MCCI criteria



Property	Predicted
Boiling Point < 320°C	200°C
Cetane >40	76
YSI <240	63
HHV >25 MJ/kg	44.2 MJ/kg
Freezing Pt <0°C	-53°C
Flash Point >52°C	59°C

PI: Vardon, NREL

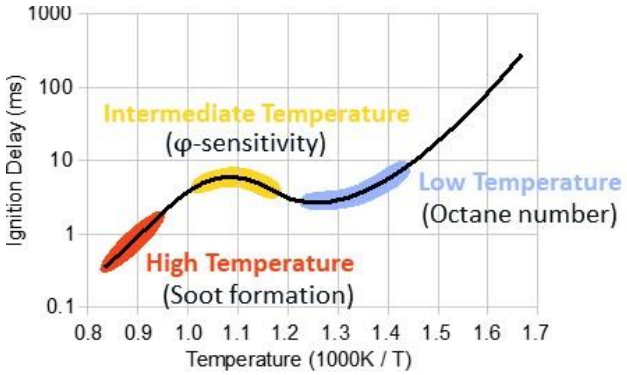
Outcome: understand impact of branching locating and chain length on ether MCCI fuel properties; enable ether candidate selection for MCCI applications

5 Future Work

Multi-mode case study: understanding mechanisms of φ -sensitivity

Theoretical chemistry can be used to understand φ-sensitivity for multi-mode applications

- φ-sensitivity is change in ignition delay with respect to air-fuel ratio, governed mainly by intermediate-temperature heat release
- Important property for multi-mode applications
- Kinetically controlled by chain branching reactions – but mechanisms poorly understood
- This task seeks to use theoretical chemistry understand the formation rates of key radicals in these reactions and how they vary by functional group



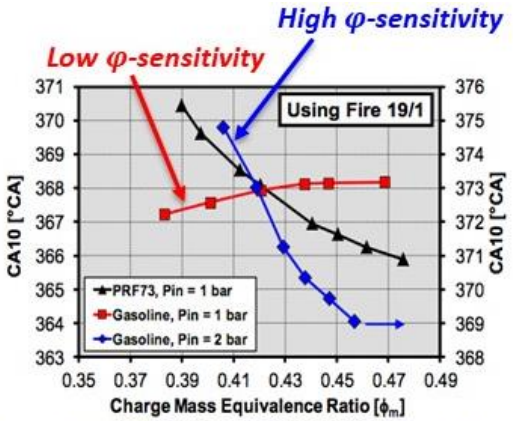


Figure from Dario Lopez-Pintor and John E. Dec

PI: Kim, St. John

Outcome: mechanistic insight into the molecular basis for phi sensitivity will enable molecule selection for multi-mode applications

Summary for SPR – PP Effort

- Determined underling science that confers particular properties to given chemical structures
- Built high-throughput property prediction tools to enable rapid evaluation of bioblendstock properties
- Generated bioblendstock candidates for the Co-Optima Bioblendstock Generation, Characterization and Analysis efforts
- Transferred data, insights and tools to other BETO programs and stakeholders
- Laid foundations to implement tools and findings to advanced combustion approaches in future efforts

Back-up slides

Summary for SPR – PP Effort

Overview	• **SPR are developed to determine which chemical families are appropriate / inappropriate for given combustion modes** • **SPR and PP are used to establish bioblendstocks within appropriate families to be evaluated in the generation-characterization-analysis cycle**
Approach	• Define key properties for given combustion mode • Define suite of chemistries and functional groups • Establish influence of theses chemical families on properties • Develop tools to predict properties of range of bioblendstocks within chemical families • Determine blendstocks to be evaluated in generation-characterization-analysis cycle
Technical Progress	• **SPR –**built new high-throughput tools to key into which structural features influence RON, MON, S, cetane and sooting. • Evaluated 1000s of samples including all bioblendstocks under consideration in Co –optima • **PP –** Developed prediction and classification tools to rapidly screen 1000s of molecules in terms of RON, MON, CN, YSI TSI • devised new methods for predicting key bioblendstock physical properties (e.g. RVP, HoV, energy density) to inform SI and MCCI bioblendstock selection. • Data fed to downstream efforts and lead to development of highest merit function BSI molecules and MCCI merit table under development.
Relevance	• **Enhance bioenergy value proposition by identifying bioblendstocks that maximize engine performance and energy efficiency, & minimize environmental impacts**
Future Work	• Complete SPR-PP work to inform MCCI merit activities • Establish important MM properties and complete SPR-PP workflow to enable MM candidate selection

Acronyms and Alphabetizations

BOB	Blendstock for oxygenated blending
Boosted SI	Boosted spark ignition for light-duty vehicles
Bp	Boiling point
bRON	Research octane number for a blend of gasoline and bioblendstock
CN	Cetane number
DCN	Derived cetane number based on ignition delay measurements
HoV	Heat of vaporization
KC	Kinetically controlled ignition for heavy-duty vehicles
LHV	Lower heating value
MCCI	Mixing controlled compression ignition for heavy-duty vehicles
Mp	Melting point
MON	Motor octane number
MM	Multi-mode ignition for light-duty vehicles
RON	Research octane number
RVP	Reid vapor pressure
S	Octane sensitivity, defined as RON minus MON
SPR-PP	Structure-property relationships and property predictions
YSI	Yield sooting index
η	Viscosity
σ	Surface tension

Publications and Presentations

FY19

- **Discovery of novel octane hyperboosting phenomenon in prenol biofuel/gasoline blends –** E. Monroe, J. Gladden, K. O Albrecht, J. T. Bays, R. McCormick, R. W. Davis, A. George, Fuel, 239, January 3, 2019
- **Measuring and Predicting the Vapor Pressure of Gasoline Containing Oxygenates –** D. Gaspar; S. .D Phillips; E. Polikarpov; K.O. Albrecht; S. B. Jones; A. George; A. Landera; D. M. Santosa; D. T. Howe; A. G Baldwin; J. T Bays, Fuel, *Accepted January 27, 2019, In Press*

FY18

- **Bio-derived Building Blocks for Various Drop in Fuels and Value Added Chemicals** – O. Staples. Presented at the 255th American Chemical Society National Meeting, New Orleans, LA, March 18 -22, 2018.
- **Biomass Market Dynamics Supporting the Large-Scale Deployment of High-Octane Fuel Production in the United States—**P. Lamers, R.T. Nguyen, D.S. Hartley, J.K. Hansen, and E.M. Searcy. Global Change Biology: Bioenergy, April 2018. https://doi.org/10.1111/gcbb.12509
- **Co-Optimization of Fuels & Engines: Efficiency Merit Function for Spark Ignition Engines: Revisions and Improvements Based on FY16–17 Research and Development –** P.C. Miles. Technical Report DOE/GO-102018-5041, 2018. https://doi.org/10.2172/1463450
- **Co-Optimization of Fuels & Engines: Fuel Blendstocks with the Potential to Optimize Future Gasoline Engine Performance; Identification of Five Chemical Families for Detailed Evaluation –** J.T. Farrell, J.E. Holladay, and R. Wagner. Technical Report, 1434413, April 2018. https://dx.doi.org/10.2172/1434413
- **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
- **Critical Fuel Property Evaluation for Potential Gasoline and Diesel Biofuel Blendstocks with Low Sample Volume Availability** – E. Polikarpov, K.O. Albrecht, J.P. Page, D. Malhotra, P. Koech, L. Cosimbescu, D.J. Gaspar. Fuel, September 24, 2018. https://doi.org/10.1016/j.fuel.2018.09.129

Publications and Presentations

FY18 continued

- **Demonstration of Fusel Alcohols as a Platform for a Tunable Suite of High Performance Biofuel Compounds for Advance Combustion Strategies –** E. Monroe, F. Liu, M. Tran-Gyamfi, A. George, and R. Davis. Oral presentation and Abstracts of Papers of The American Chemical Society, March 18, 2018
- **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
- **Explicating Feature Contribution Using Random Forest Proximity Distances;** L.S. Whitmore, A. George, and C.M. Hudson; arXiv preprint arXiv:1807.06572
- **Fuel Property Prediction and Experimental Values –** D. Vardon presented at the American Chemical Society Green Chemistry Conference in Portland, Oregon, June 18-20, 2018.
- **Discovery of a RON Hyperboosting Phenomenon in Prenol/Gasoline Blends –** A. George. ACS National Fall Conference, Boston, Massachusetts, August 2018.
- **Fuel-Film Thickness Measurements using Refractive Index Matching in a Stratified-Charge SI Engine Operated on E30 and Alkylate Fuels –** C.-P. Ding, M. Sjöberg, D. Vuilleumier, D.L. Reuss, X. He, and B. Böhm. Exp Fluids, 59:59, 2018. https://doi.org/10.1007/s00348-018-2512-5
- **Measurements and Prediction of Sooting Tendencies of Hydrocarbons and Oxygenated Hydrocarbons –** D. Das, P. St. John, C.S. McEnally, S. Kim and LD. Pfefferle. Presented at AIChE 2017, October 30, 2017.
- **Measuring and Predicting Sooting Tendencies of Oxygenates, Alkanes, Alkenes, Cycloalkanes, and Aromatics on a Unified Scale –** D.D. Das, P.C. St John, C.S. McEnally, S. Kim, and L.D. Pfefferle. Combust. Flame, 190:349-364, 2018. https://doi.org/10.1016/j.combustflame.2017.12.005
- **Sooting Tendencies of Co-Optima Test Gasolines and their Surrogates –** C.S. McEnally, Y. Xuan, P.C. St. John, D.D. Das, A. Jain, S. Kim, T.A. Kwan, L.K. Tan, J. Zhu, and L. D. Pfefferle. Proc. Comb. Inst., available online June 2018. https://doi.org/10.1016/j.proci.2018.05.071

Publications and presentations

FY17

- **A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure –** P.C. St. John, P. Kairys, D.D. Das, C.S. McEnally, L.D. Pfefferle, D.J. Robichaud, M.R. Nimols, B.T. Zigler, R.L. McCormick, T.D. Foust, Y.J. Bomble, and S. Kim. Energy & Fuels, 31(9): 9983-9990, 2017. http://pubs.acs.org/doi/pdf/10.1021/acs.energyfuels.7b00616
- **Selection Criteria and Screening of Potential Biomass-Derived Streams as Fuel Blendstocks for Advanced Spark-Ignition Engines** – R.L. McCormick, G. Fioroni, L. Fouts, E. Christensen, J. Yanowitz, E. Polikarpov, K. Albrecht, D.J. Gaspar, J. Gladden, and A. George. SAE Int. J. Fuels Lubr., 10:442-460, March 2017. https://doi. org/10.4271/2017-01-0868
- **Selection Criteria and Screening of Potential Biomass-Derived Streams as Fuel Blendstocks for Advanced Spark-Ignition Engines –** R. McCormick, G. Fioroni, L. Fouts, and E. Christensen, et al. SAE Technical Papers, Fuels Lubricants, 10(2):442-460, 2017. https://doi.org/10.4271/2017-01-0868

FY16

- **BioCompoundML: A General Biofuel Property Screening Tool for Biological Molecules using Random Forest Classifiers —** L.S. Whitmore, R.W. Davis, R.L. McCormick, J.M. Gladden, B.A. Simmons, A. George, and C.M. Hudson. Energy & Fuels, 30: 8410-8418, 2016. pubs.acs.org/doi/pdf/10.1021/acs.energyfuels.6b0195
- **The Effect of Functional Groups in Bio-Derived Fuel Candidates —** R.W. Jenkins, C.D. Moore, T.A. Semelsberger, D.J. Chuck, J.C. Gordon, and A.D. Sutton. ChemSusChem, 9: 922, 2016. onlinelibrary.wiley.com/doi/10.1002/cssc.201600552/full