2021 DOE Vehicle Technologies Office
Annual Merit Review

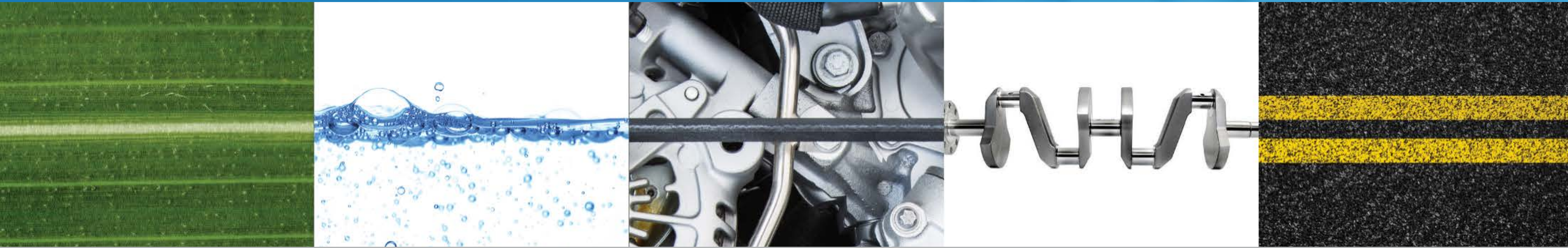
Fuel Properties and Kinetics

Principal Investigator: Gina M. Fioroni
Organization: National Renewable Energy Laboratory
Project ID # FT094

CO-OPTIMIZATION OF
FUELS & ENGINES

better fuels | better vehicles | sooner

June 24, 2021



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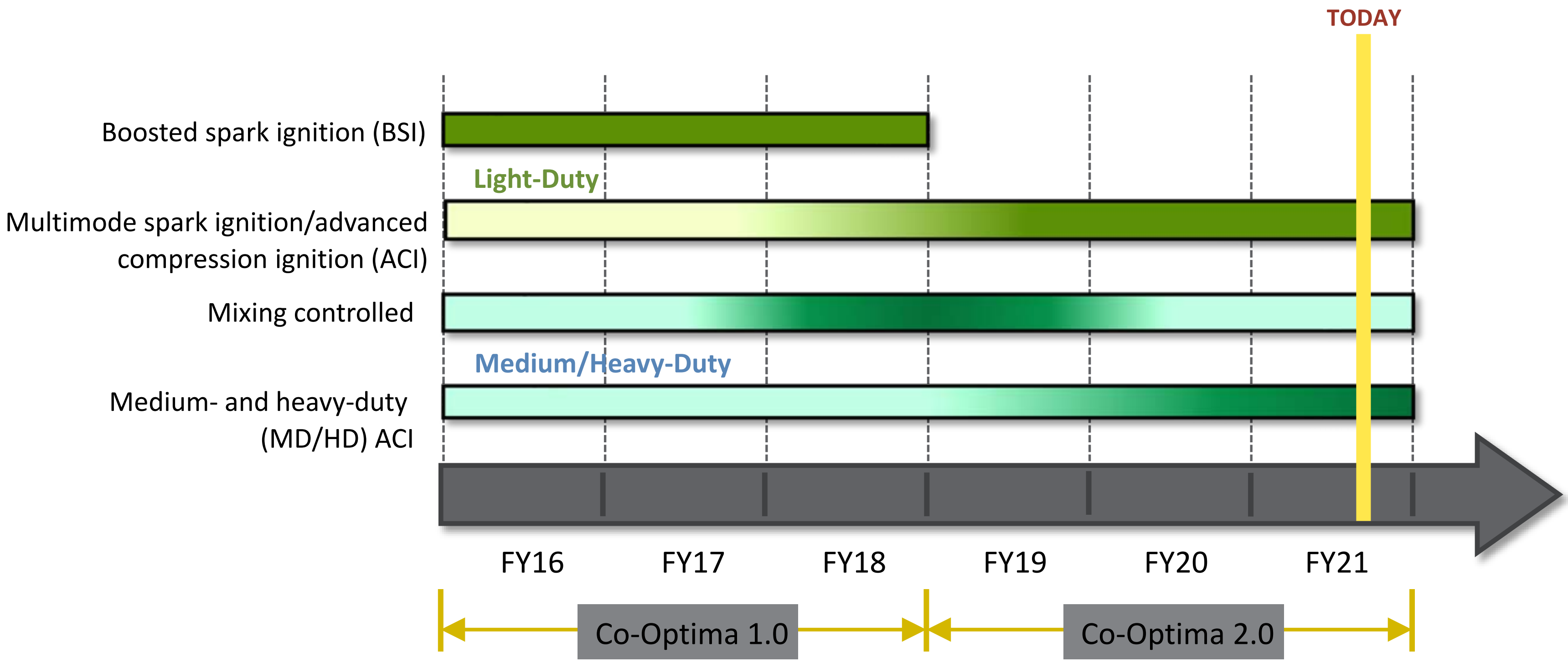
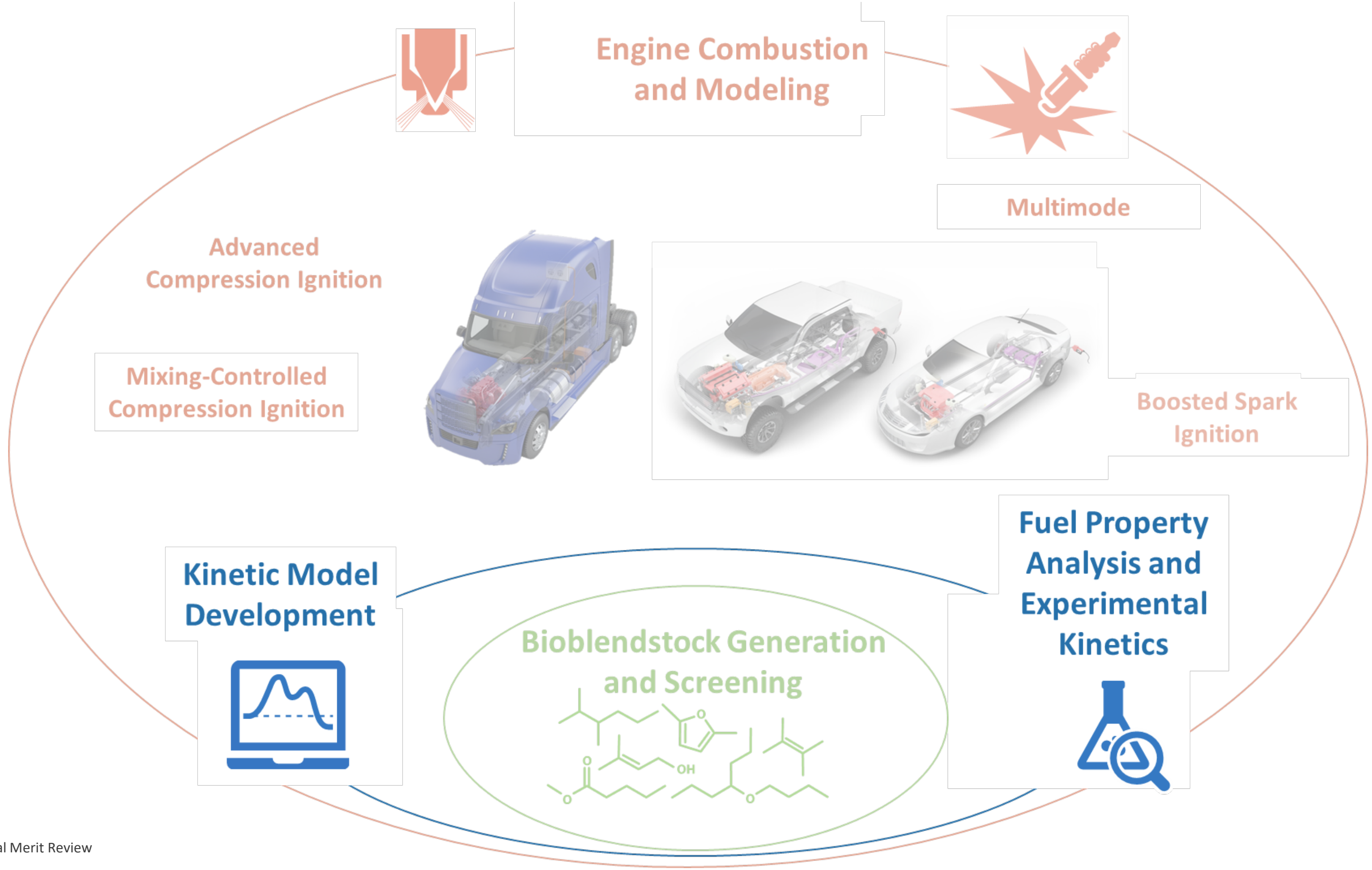
Overview | Timeline



Co-Optima Program Integrated to Deliver Better Engines Sooner



Relevance: Fuel Properties and Experimental Kinetics

Impact:

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

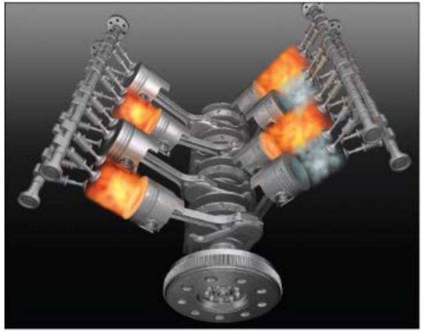
Objectives:

- **Develop list of key fuel properties in collaboration with Advanced Engine Design (AED) team that enable advanced combustion strategies**
- **Bench-scale experimental measurement of key fuel properties (small-volume autoignition)**
  - *Advanced Fuel Ignition Delay Analyzer (AFIDA) and rapid compression machine (RCM) for autoignition metrics and measurement of key fuel properties*
  - *ϕ-sensitivity, research octane number (RON), octane sensitivity (S), and heat of vaporization (HOV)*
  - *Flow reactor studies for skeletal reaction mechanisms*
- **Development of kinetic simulations**
  - *Development of kinetic models for autoignition, NO_x, flame speeds, and soot-precursor formation over a wide range of pressures, temperatures, equivalence ratios, and exhaust gas recirculation (EGR)*

Identifying Promising Blendstocks

Approach: Development of Key Fuel Properties, Screening, and Characterization

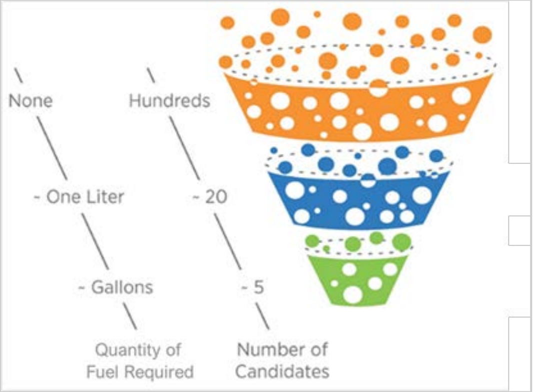
What Do Engines Want?



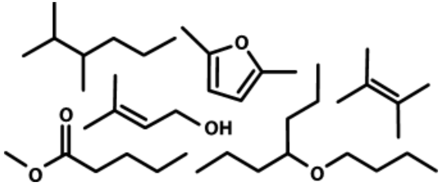
Generate List of Properties

RON and S
ϕ-sensitivity
HOV
Cetane number
Flame speed

Tiered Screening



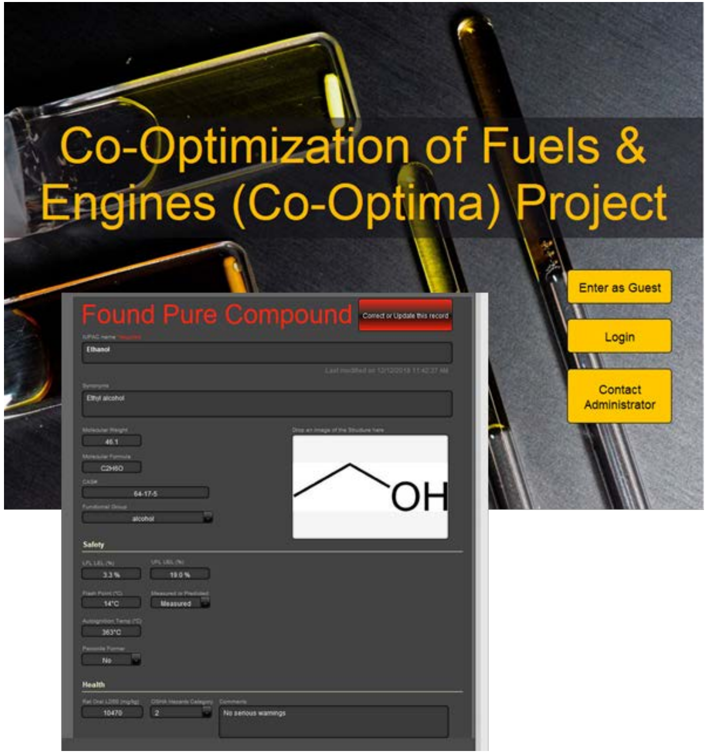
Most Promising Blendstocks



For more details on screening results, see back-up slides

Developed Fuel Property Database for Screening and Data Organization

- Fully searchable database with fuel property candidates supplied from multiple labs and researchers
- Used extensively for candidate screening
- Database updated on a regular basis as new data are received from researchers
- Thousands of pure components and mixtures included.



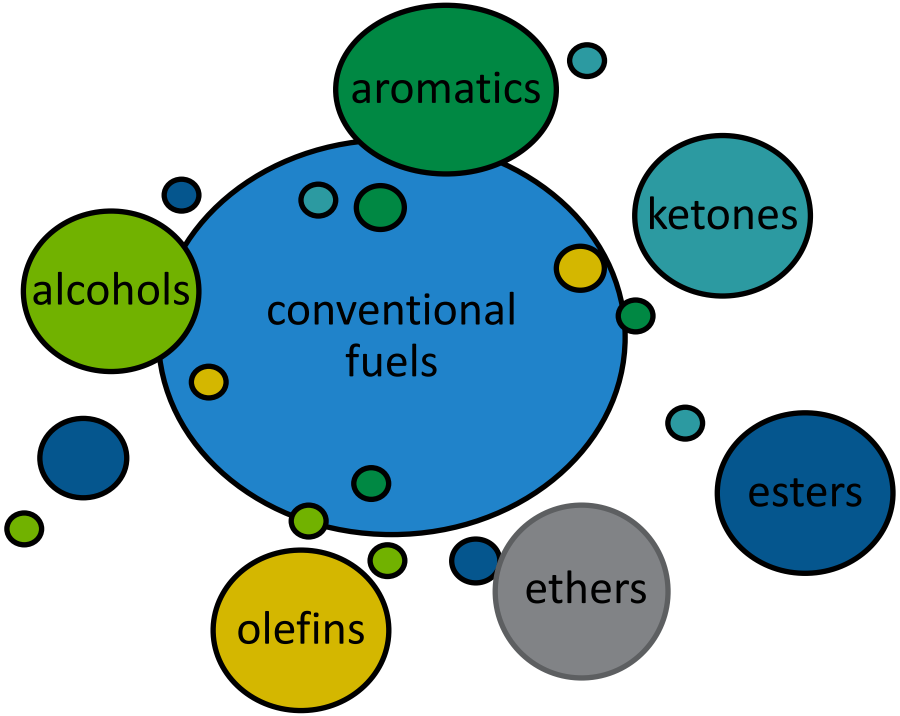
Year	Users	Guests
2016	626	385
2017	1,753	1,401
2018	2,119	1,881
2019	2,168	2,056
2020	2,174	2,003
2021*	606	595

* Through May 8, 2021

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

Highlights: Combined Experimental and Kinetic Model Development for Key Fuel Property Metrics

Kinetic Mechanism Development



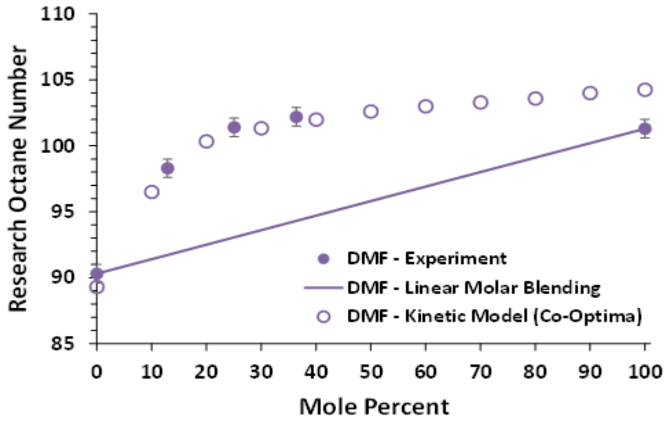
- ***Kinetic models developed for conventional fuels and oxygenates***
- ***Kinetics required to include combustion into large-scale models***

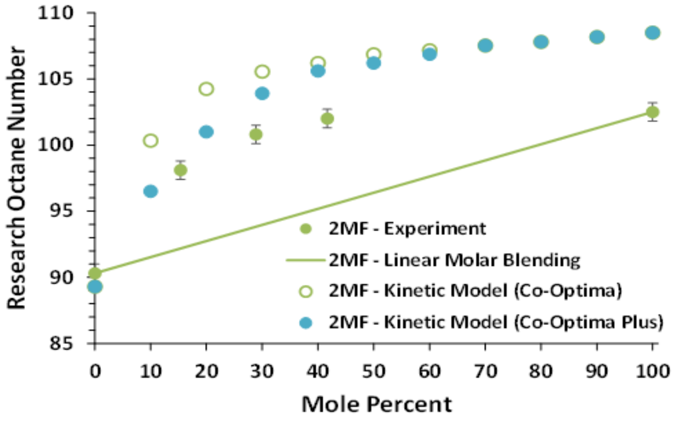
"Co-Optima" model:
~4,200 species
~19,100 reactions

Key fuel properties from kinetics:
- **RON prediction**
- **ϕ-sensitivity**

- **Autoignition and soot precursors**
- **NO_x effects (EGR)**
- **Polyaromatic hydrocarbons (PAH)/ soot**

Kinetic Simulations for RON Prediction Led to Detailed Understanding of Key Low-Temperature Reactions





- RONs for several blendstocks blended into gasoline were predicted using the Co-Optima mechanism
- Mechanism was interrogated to reveal key reactions responsible for nonlinear blending behavior
- Utilized density functional theory to calculate key reaction rates
- Updated kinetic model with new reaction rates for improved RON prediction.

Manuscript in preparation

Gasoline surrogate

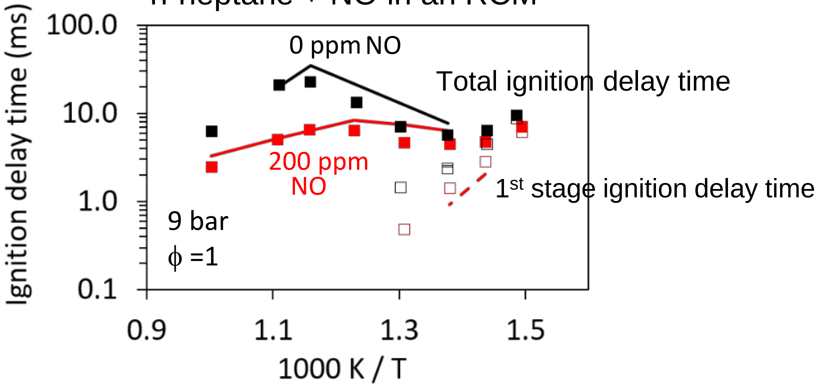
Species	Volume fraction	Mass fraction	Mole fraction
Isooctane	0.55	0.519	0.469
Toluene	0.25	0.296	0.331
n-Heptane	0.15	0.140	0.144
1-Hexene	0.05	0.046	0.056

PIs: Gina Fioroni and Mohammad Rahimi, NREL, and Seonah Kim, CSU

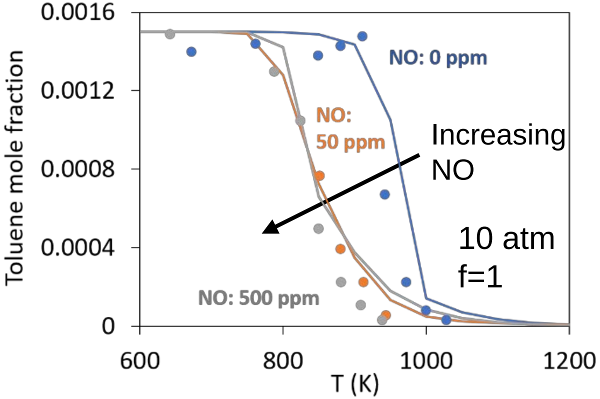
Predict NO_x Promotion/Inhibition of Autoignition of Gasoline Surrogate Components

- Nitric oxide (NO) in EGR can affect engine knock and ACI combustion phasing
- Ignition promoting: example: $NO+HO_2=NO_2+OH$
- Ignition inhibiting, R = fuel radical: example: $RO_2+NO=RO+NO_2$
- Extended NO_x kinetics to more surrogate components:
  - iso-pentane (new)
  - cyclopentane (new)
  - 1-hexene (new)
  - n-heptane, updated
  - toluene, updated

n-heptane + NO in an RCM

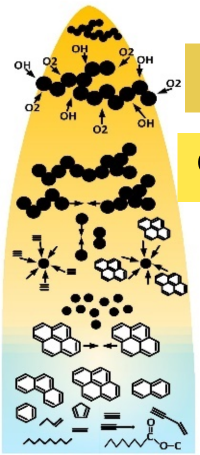


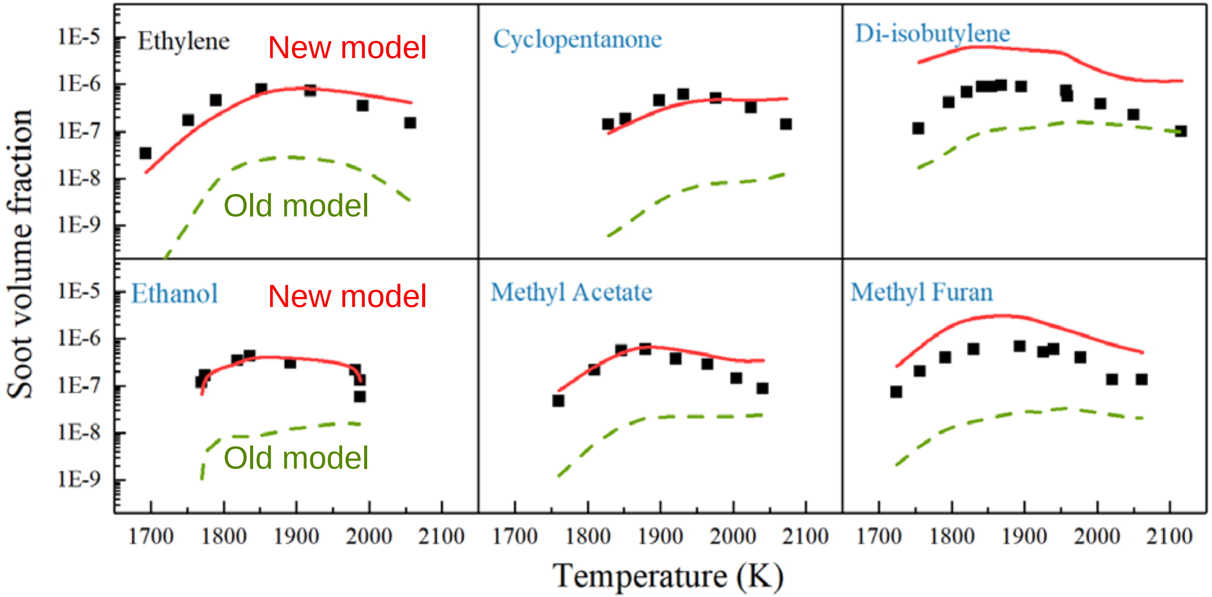
Toluene + NO in jet stirred reactor



PI: William J. Pitz, LLNL

Improved PAH Model Helps Accurately Predict Soot Formation





https://thomsonlab.mie.utoronto.ca/detailed-and-fundamental-modeling-of-soot-formation/

Used PAH kinetic model + sectional model for soot

Measurements: University of Central Florida shock tube
New model: New LLNL PAH mechanism
Old model: Literature PAH mechanism

PI: William J. Pitz, LLNL

Highlights: Fuel Property Bench-Scale Measurements

Developed Bench-Scale Experiments for Kinetic Model Validation and to Measure Key Fuel Properties

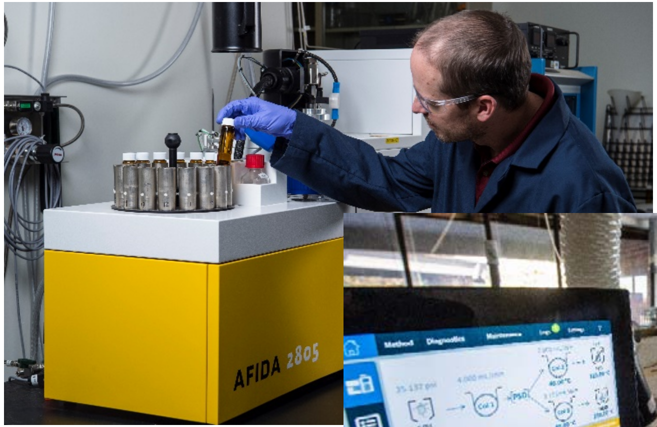
Bench-scale measurements enable research on small volumes of fuel and rapid screening of fuel candidates

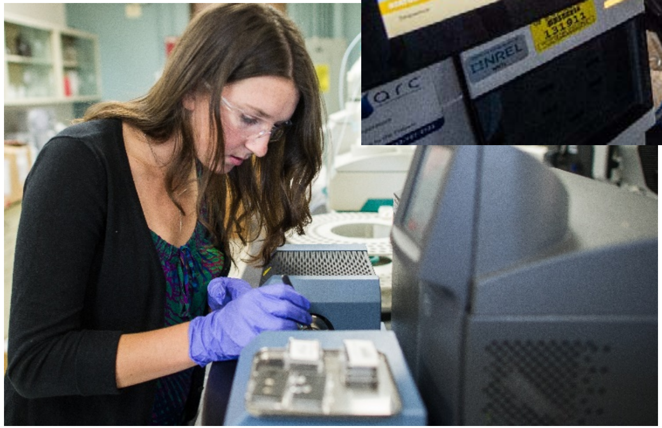
Key Fuel Properties:

- RON/S
- HOV
- ϕ-sensitivity (new property)

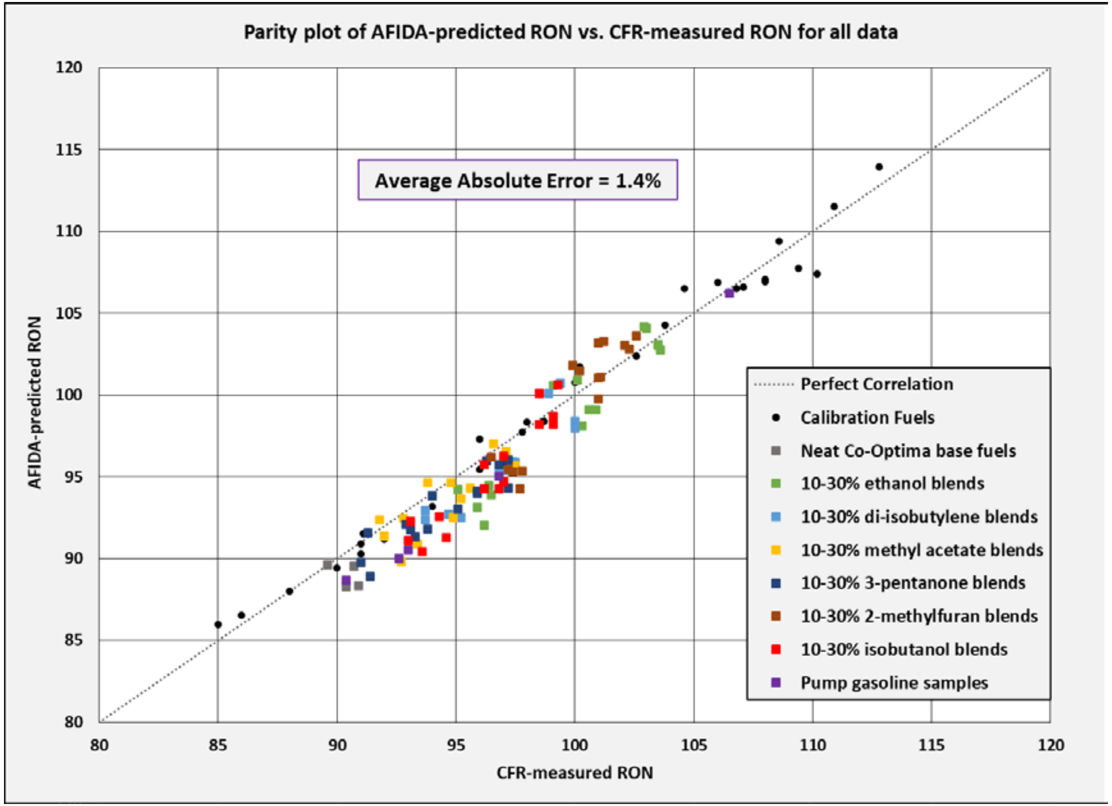
Bench-Scale Instruments:

- AFIDA
- RCM
- Differential scanning calorimeter (DSC)/ thermogravimetric analyzer (TGA)/ mass spectrometer (MS)
- Flow reactor





Bench-Scale Fuel Candidate Screening Development: RON and S

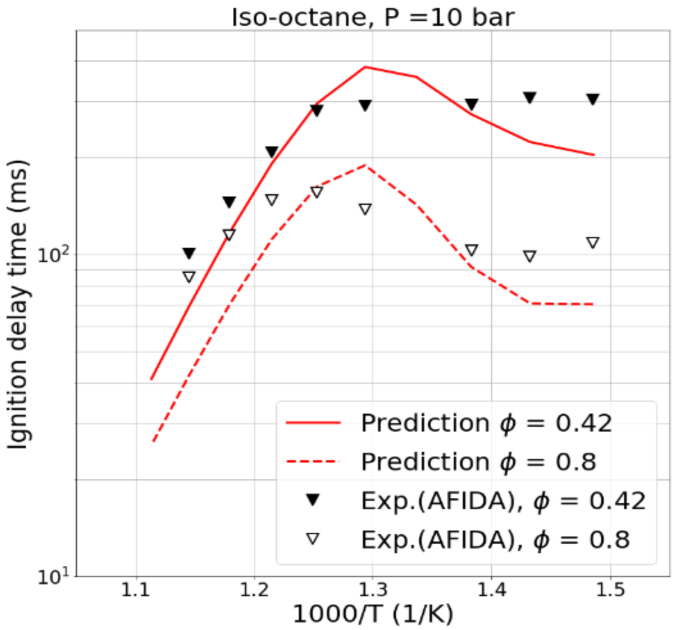


- AFIDA-based small-volume (~40-mL) rapid screening (~1-hour) methodology accurately predicts RON and S over a wide variety of chemistries
- Enabled fast screening for candidate compounds as well as determining blend behavior.

https://doi.org/10.1016/j.fuel.2021.120969

PIs: Bradley T. Zigler and Jon Luecke, NREL

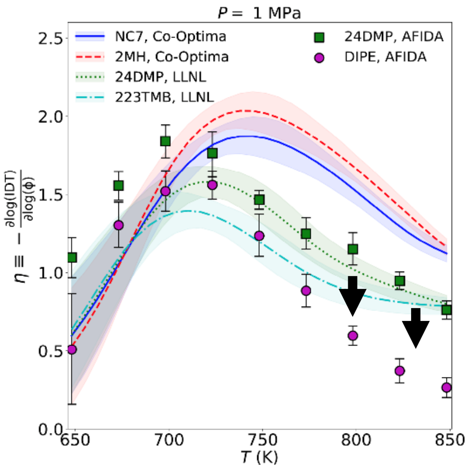
AFIDA Bench-Scale Measurement: Phi-Sensitivity

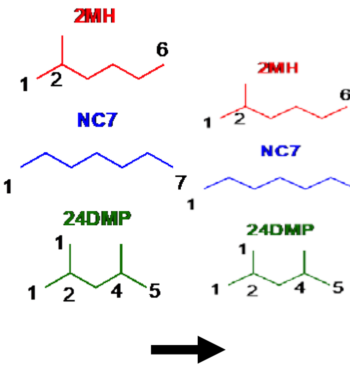


$$-\frac{d\log(\tau)}{d\log(\phi)}\Bigg|_{T,P} = \eta$$

Temperature sweeps of ignition delay across different ϕ and pressures expanded development of new ϕ-sensitivity metric

- This new definition was applied to compounds with developed kinetic mechanisms and compounds of interest (without mechanisms) to study molecular structure effects on ϕ-sensitivity, coupled with EGR species





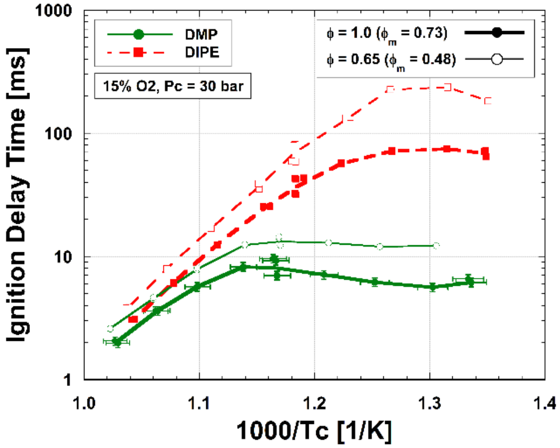
Oxygen addition

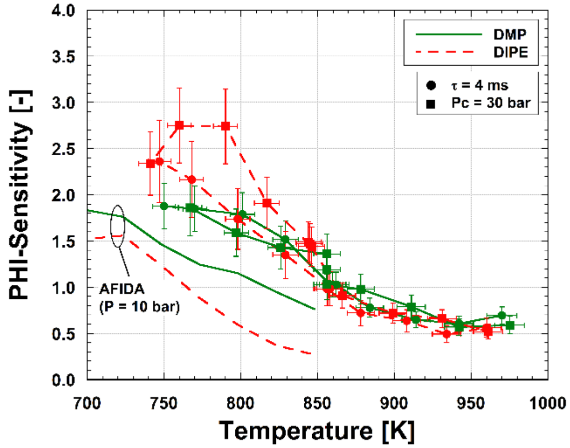
https://doi.org/10.1016/j.combustflame.2019.12.019
https://doi.org/10.1016/j.combustflame.2020.11.004

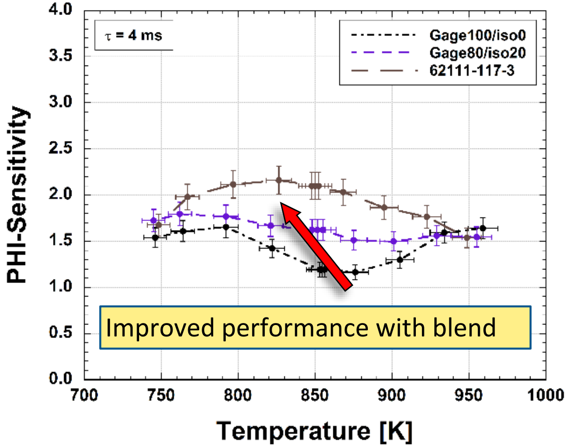
PIs: Bradley T. Zigler, Jon Luecke, NREL, and Seonah Kim, CSU

RCM: Development/Application of Multi-Mode/ACI Fuel Quality Metric

- Investigated various ways to define/measure phi-sensitivity, using the RCM and engine data to quantify blended fuel behavior
- Conducted tests with 2,4 dimethyl pentane and diisopropyl ether in collaboration with NREL to refine phi-sensitivity definition and compare against AFIDA measurements at P = 10 bar
- Conducted tests with PNNL dimethyl-hexene-rich olefin blendstock + full boiling range gasoline to verify phi-sensitivity improvement at 20% v/v blend level. Improvements are confirmed with single-cylinder engine tests.

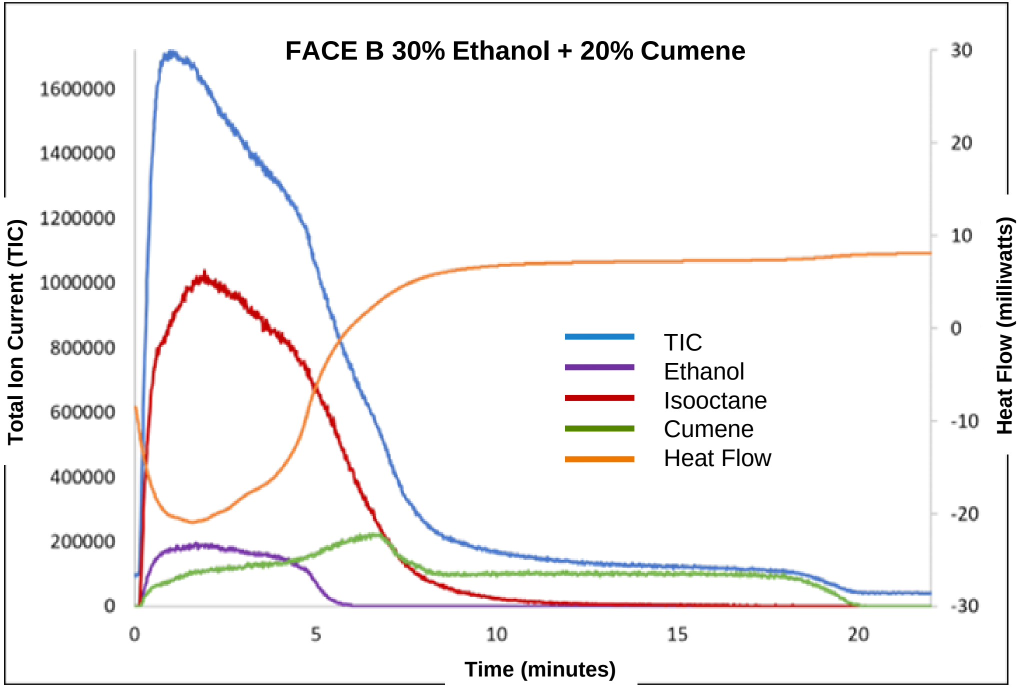






PI: S. Scott Goldsborough, ANL

Development of HOV Measurement Utilizing DSC/TGA/MS



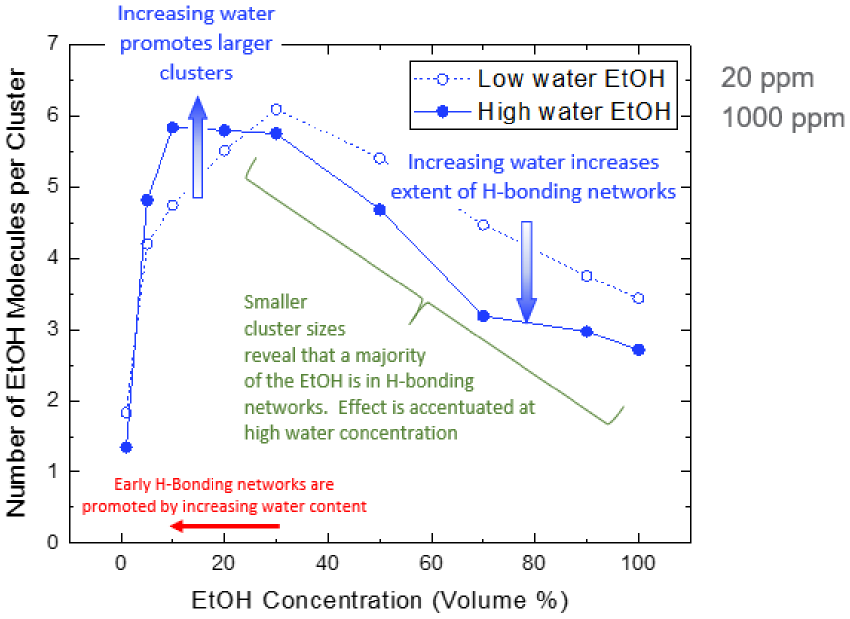
- Coupled MS to DSC/TGA to track species evolution during evaporation
- Highly accurate method for measuring HOV of gasoline and gasoline blends
- Shows heat effects during alcohol evaporation as well as suppression of evaporation of aromatic components
- Coupling with molecular dynamics and multicomponent spray droplet vaporization simulations to translate the impact of azeotropic solutions, water, and increased HOV on mixture stratification due to spray evaporation

https://doi.org/10.1021/acs.energyfuels.8b03369
https://doi.org/10.4271/2019-01-0014

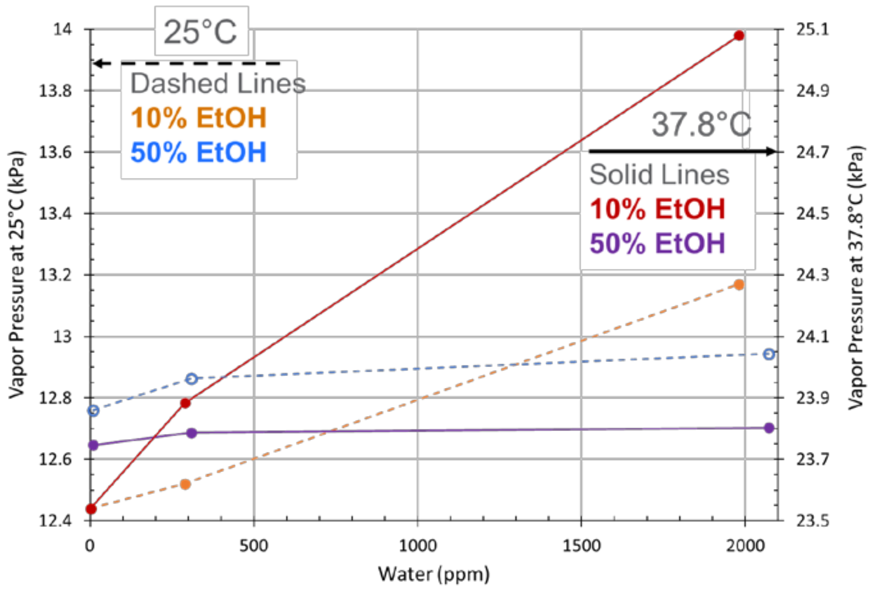
PI: Gina M. Fioroni, NREL

Impact of Water on Alcohol Clustering and Vapor Pressure

Water Effects on Cluster Size and Networks



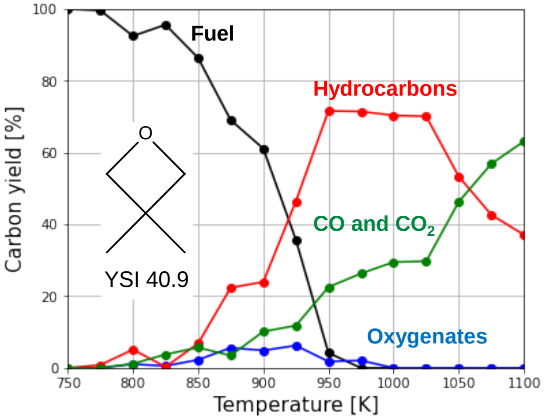
Water Effects on n-Heptane Vapor Pressure

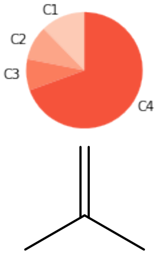


- Diffusion measurements and molecular dynamic simulations reveal effect of water on cluster size distribution and vapor pressure changes
- Utilized in combination with DSC/TGA/MS experiments and multicomponent spray droplet vaporization simulations to understand the impact of clustering on mixture stratification due to spray evaporation.

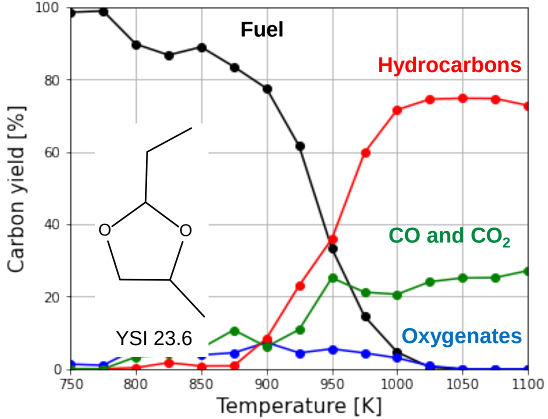
PI: J. Tim Bays, PNNL

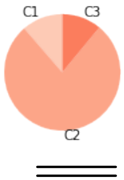
Flow Reactor Experiments Reveal Key Species Responsible for Soot Precursor Formation





Isobutene





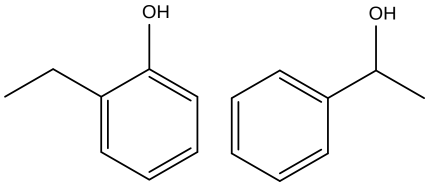
Ethylene

Carbon #	YSI
1	~0
2	~5.6
3	~12.1
4	~18.5

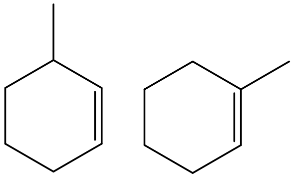
Yield sooting index (YSI) value related to the size of the product molecule from high-temperature reaction

- Combined quantum mechanical and experimental approach has led to development of multiple soot-precursor and autoignition kinetic models: ***Significant knowledge gained in structural impacts***
- Recent experiments highlight structural impacts of ethers on sooting tendency.

Multiple Structural Motifs Investigated



Oxygen position in oxygenated aromatics



Substituent position on ring

PIs: Gina M. Fioroni, NREL and Seonah Kim, CSU

https://doi.org/10.1016/j.proci.2020.06.321
https://doi.org/10.1016/j.proci.2020.06.072

Remaining Challenges and Barriers and Future Work

- **Fuel-engine experiments and high-fidelity simulations cannot generate enough data to discover hidden fuel properties using unsupervised learning (data mining)**
  - Create a framework to fairly compare the benefits of different multimode strategies and fuel combinations.
- **There is a need to develop kinetic models for new, low-carbon-intensity fuels for MD/HD**
- **Ethers represent promising blendstocks for MD/HD, but there remain barriers to their adoption in the market**

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

Summary

Relevance:

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

Approach:

- Utilize combined expertise from across national laboratories, universities, and industry to develop unique testing capabilities and modeling analysis competencies

Technical Accomplishments:

- Created tools to screen, characterize, and identify the most attractive bio-blendstocks to enable various combustion strategies
- Developed several kinetic mechanisms, including the Co-Optima mechanism and kinetics to both predict key fuel properties and describe PAH/soot formation chemistry
- Designed experiments to measure key fuel properties to inform structure property relationships and provide rapid screening of fuel candidates

Collaborations:

- Nine national laboratories, 20+ universities, two DOE offices, industry, and stakeholders

Thank you!

Contributors to this presentation:

S. Scott Goldsborough

Bradley T. Zigler

Robert L. McCormick

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Marco Arienti

Acronyms

ACI	advanced compression ignition
AED	Advanced Engine Design
AFIDA	Advanced Fuel Ignition Delay Analyzer
ANL	Argonne National Laboratory
BSI	boosted spark ignition
CFR	Cooperative Fuel Research
Co-Optima	Co-Optimization of Fuels & Engines
CSU	Colorado State University
DSC	differential scanning calorimeter
EGR	exhaust gas recirculation
FACE	fuels for advanced combustion engines
FY	Fiscal Year
HOV	heat of vaporization
LLNL	Lawrence Livermore National Laboratory
MCCI	mixing-controlled compression ignition
MD/HD	medium/heavy duty
MS	mass spectrometer
NO_x	oxides of nitrogen
NREL	National Renewable Energy Laboratory
PAH	polyaromatic hydrocarbons
ϕ	phi (equivalence ratio)
PM	particulate matter
PMI	particulate matter index
PNNL	Pacific Northwest National Laboratory
ppm	parts per million
RCM	rapid compression machine
RON	research octane number
RVP	Reid vapor pressure
S	octane sensitivity (S = RON − MON)
SI	spark ignition
SNL	Sandia National Laboratories
τ	tau, ignition delay time
TGA	thermogravimetric analyzer
YSI	yield sooting index

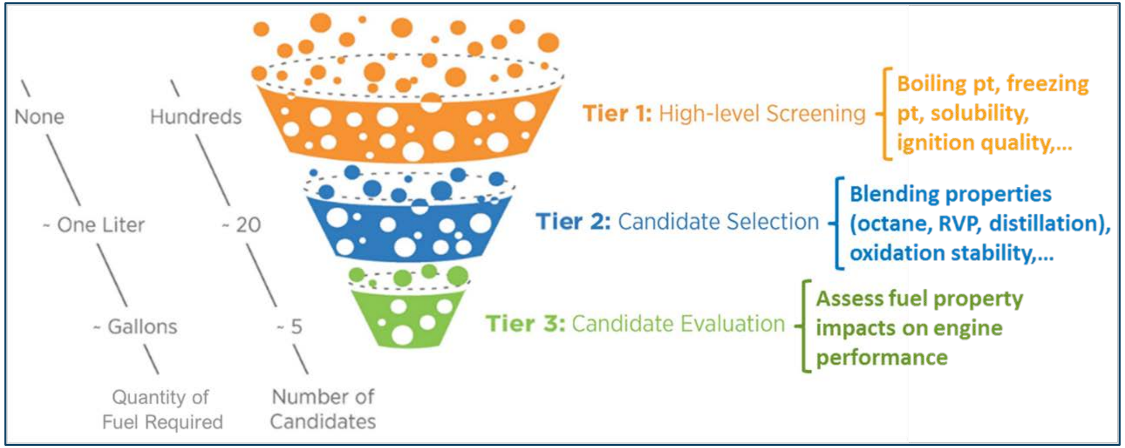
Special Note

This presentation is a part of a series that gives an overview of the 6-year **Co-Optimization of Fuels and Engines** initiative, and therefore does not adhere to the standard Annual Merit Review presentation guidance

CO-OPTIMIZATION OF
FUELS & ENGINES

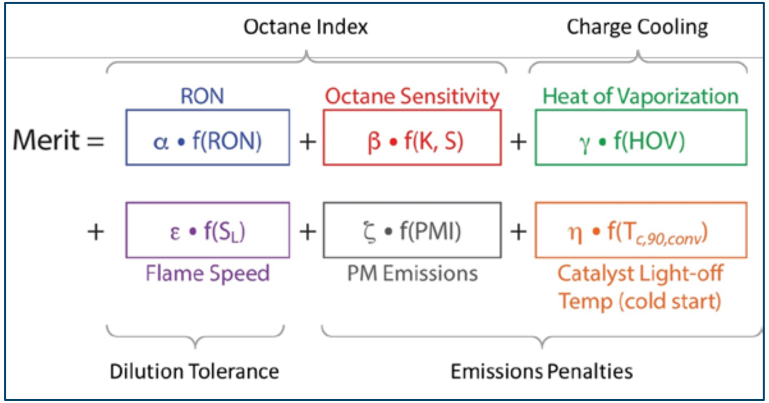
Technical Back-Up Slides

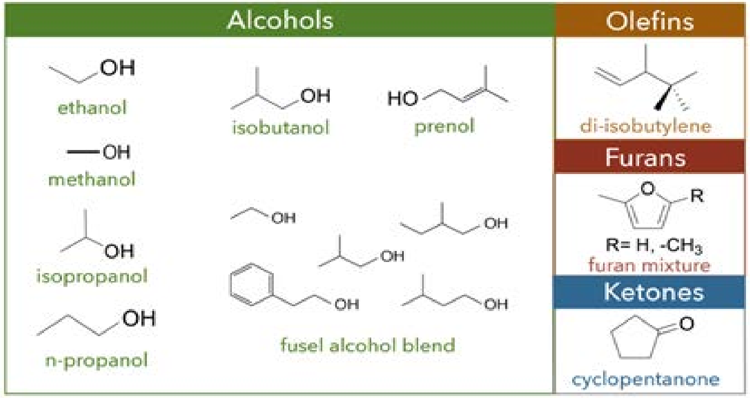
Boosted Spark-Ignition Screening Results



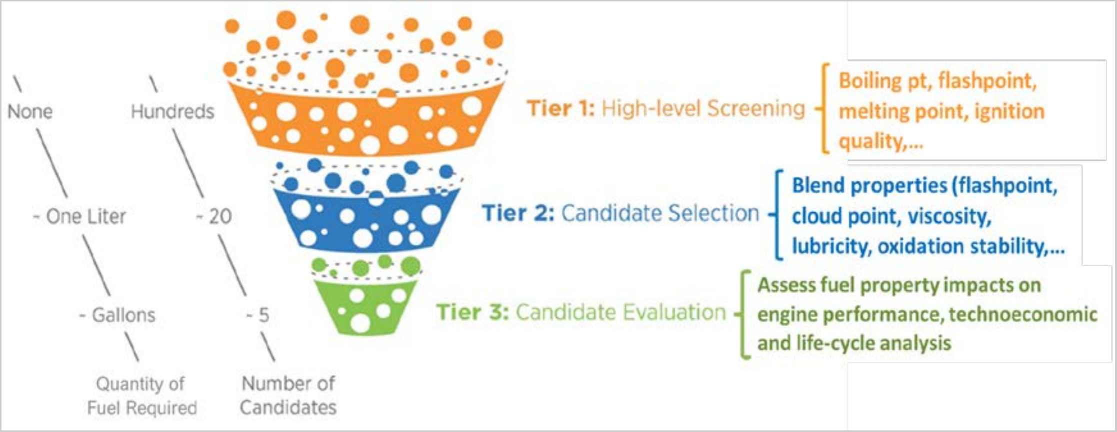
Defining what SI engines want

- Tiered screening process
- Can it be a fuel?
- Determine key fuel property metrics
- Design bench-scale measurements
- Develop kinetic models



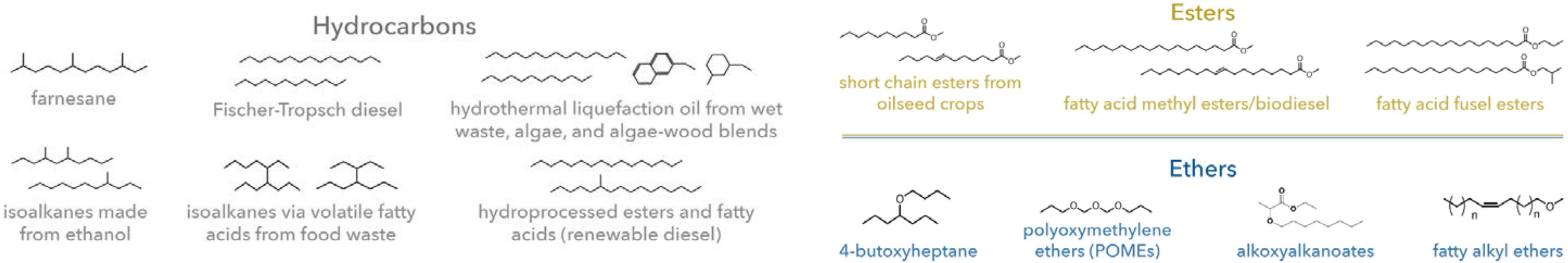


Mixing-Controlled Compression Ignition Screening Results



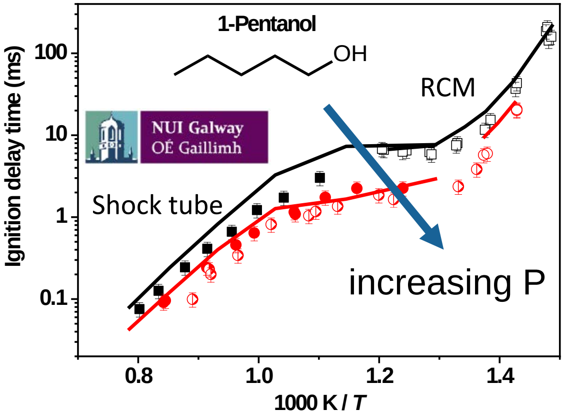
Defining what MCCI engines want

- Tiered screening process
- Can it be a fuel?
- Determine key fuel property metrics
- Design bench-scale measurements
- Develop kinetic models



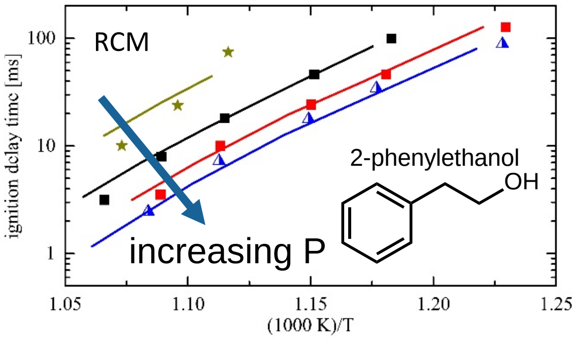
Kinetic Model Development: Co-Optima Blendstocks

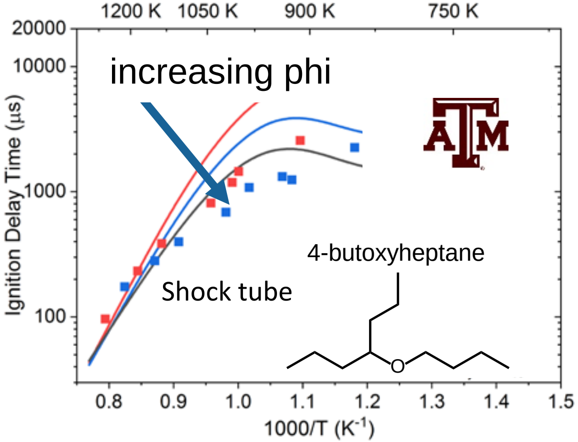
PI: William Pitz, LLNL



Coordinating with Labbe group for new alcohol ab initio rate constants

Additional 2-phenylethanol data on binary blends with n-heptane (not shown)



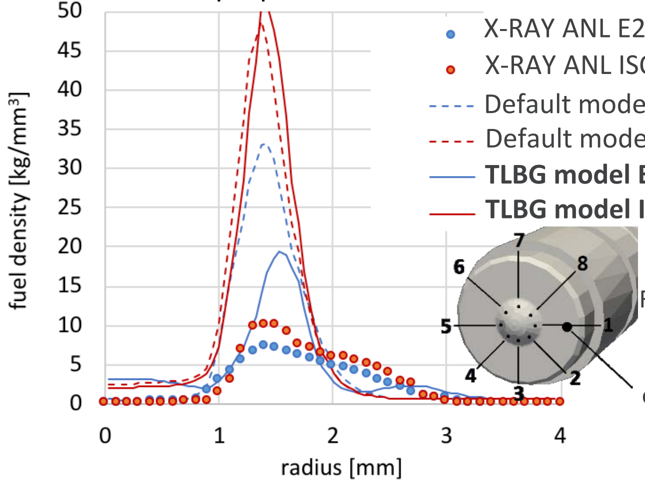


Additional 4-butoxyheptane data from a flow reactor now available (NREL).
Jet-stirred reactor planned, N. Hansen

Improving Sensitivity of Computational Fluid Dynamics Flash-Boiling Models to Fuel Thermophysical Properties

New thermally limited bubble growth (TLBG) model helps distinguish the effect of fuel composition on spray cone angle

E20 vs. iso-octane example: The change in fuel radial mass distribution is due to the different thermophysical properties of the two fuels



Radial fuel density is averaged over the 8 holes

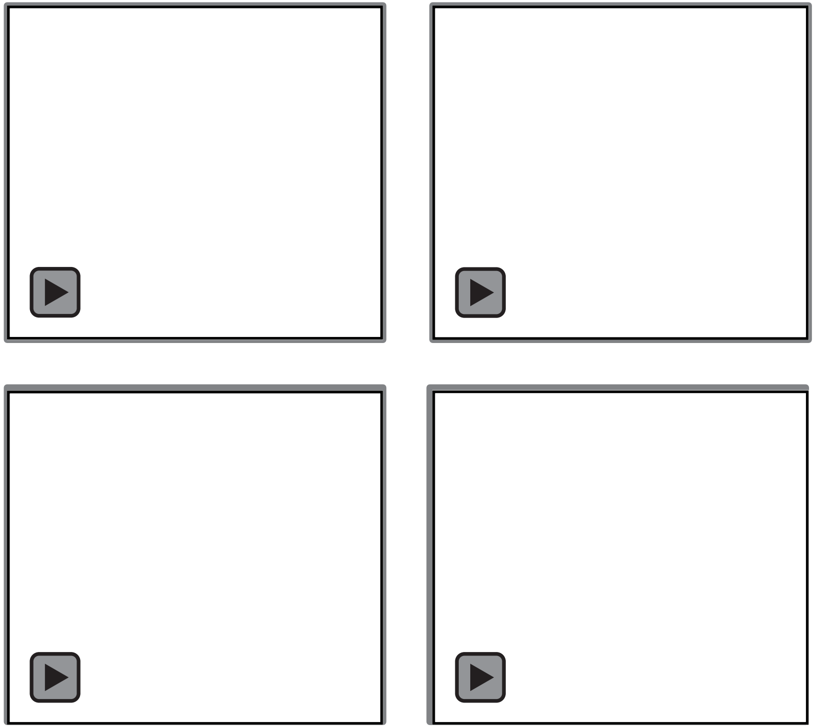
- The new TLBG model was made available in CONVERGE as a user-defined function
- In collaboration with Convergence Science Inc., work continues in modeling liquid fuel behavior at pressures lower than saturation.

Neat iso-octane

20% ethanol 80% iso-octane

Default model (empirical)

TLBG

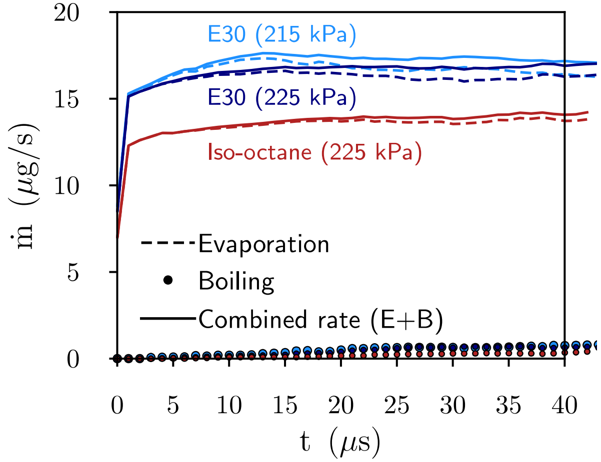


PI: Marco Arienti, SNL

Predictive Film Evaporation/Boiling at Engine Conditions

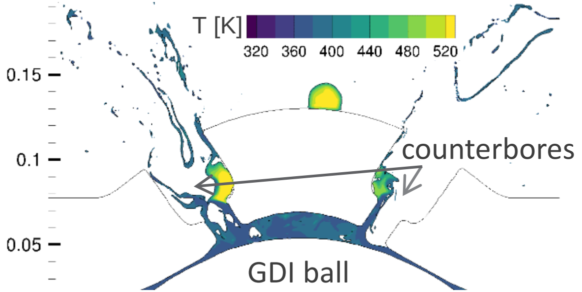
Enabled study of phase-change behavior for newly developed fuels in realistic engine environments

Demonstration calculation for droplet near hot surface (573 K): quantification of changing boiling/evaporation of E30 as a function of ambient pressure



DNS captures GDI's end-of-injection dribbling phenomenon (2019)[1]

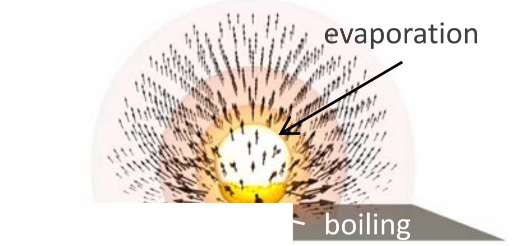
- Based on advanced interface-capturing methodology
- Differentiates evaporation from cavitation



Fuel phase change near hot surface (2020)

- Achieved accurate prediction of evaporation and boiling of real fuels (as generated by the REFPROP library) without need of empirical correlations[2,3]
- Applied to tip wetting, this type of results can be used to predict film drying
- This implementation establishes the framework to examine the behavior of surrogate components (end of 2021)

E30 vapor mass fractions: $Y = 0.55, 0.75, 0.90$, and 0.97 (outermost to innermost)



1. Arienti et al., "Effects of detailed geometry and real fluid thermodynamics on Spray G atomization," Proceedings of the Combustion Institute 2021.
2. Wenzel and Arienti, "A new approach for the modeling and simulation of liquid/vapor phase change at engine-relevant conditions," Proceedings of the 31st ILASS-Americas, May 2021.
3. Wenzel and Arienti, "A conservative framework for the modeling and simulation of evaporation in compressible flow systems," in preparation for submission to *J. Comput. Phys*.

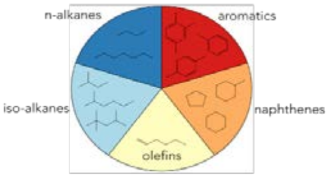
PI: Marco Arienti, SNL

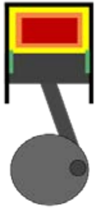
Virtual Properties, Reduced Mechanisms, Blending of Kinetics, and Modeling of Fuel

Impact: Accelerate hypothesis testing using accurate fuel chemistry models for broad blend explorations

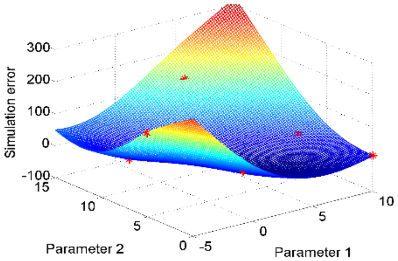
$$Q\begin{pmatrix} RPM \\ CR \\ C_2H_5OH \\ n\text{-}C_7H_{16} \\ i\text{-}C_8H_{18} \\ \cdots \end{pmatrix}$$

LLNL Task: simulations





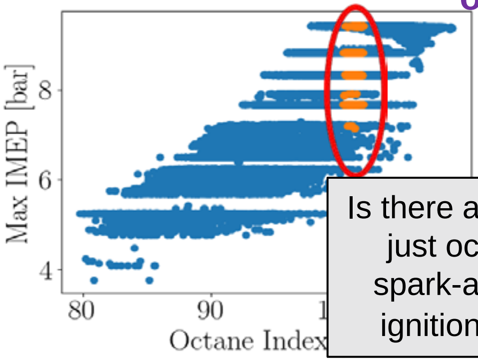
$$\max \text{Load Range}\begin{pmatrix} C_2H_5OH \\ n\text{-}C_7H_{16} \\ i\text{-}C_8H_{18} \\ \cdots \end{pmatrix}$$



e.g., Multimode fuel property exploration

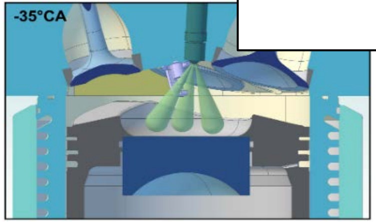
see Sjoberg's talk FT070

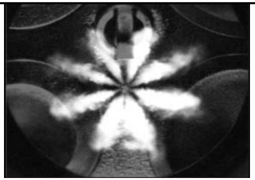
LBNL task: Efficient co-optimization



Is there another dimension than just octane index affecting spark-assisted compression ignition (SACI) load range?

SNL task: Multimode engine experiments
LLNL/SNL/ANL task: System efficiency over real-world drive cycles



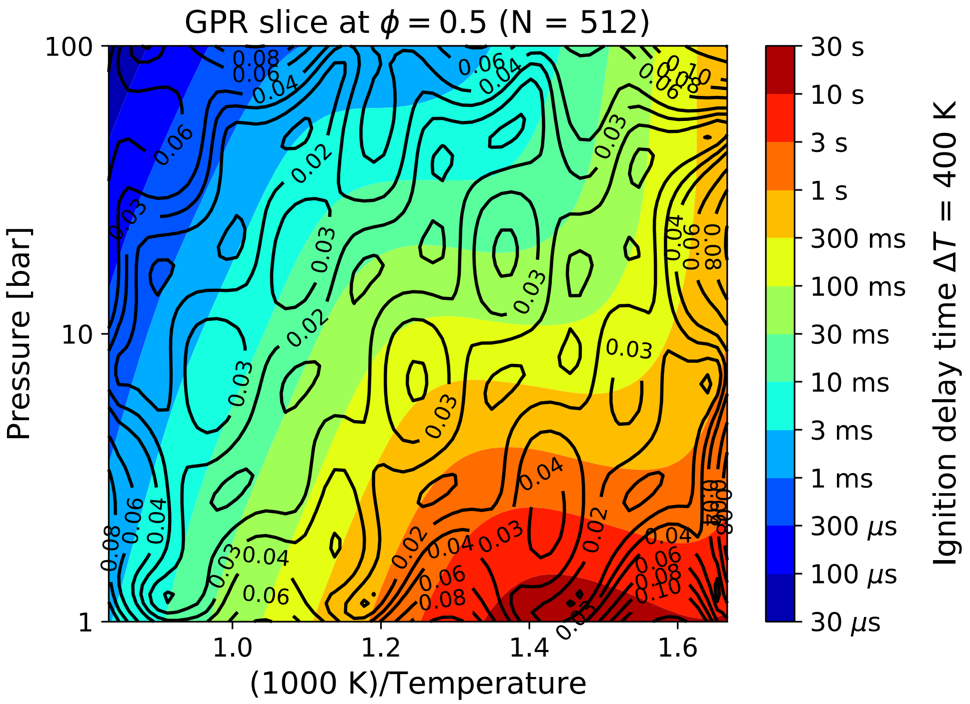


PI: Matt McNenly, LLNL

Virtual Properties, Reduced Mechanisms, Blending of Kinetics, and Modeling of Fuel

Database of 10,000 different HPF+BOB blends created to rapidly explore new engine-chemistry metrics

e.g., GPR model for E10 regular surrogate



- Six base BOBs (clustered at RON = 90.5 and MON = 85.4) using 9-hydrocarbon palette
- 17 bio-derived high-performance fuels (HPFs)
- All HPFs and HPF mixtures blended in the base BOBs at 10%, 20%, 30%, and 40% (v/v)
- Binary mixtures (25/75 and 50/50) of all 17 HPFs = ***over 10,000 blends***
- Database stores a Gaussian process regression (GPR) model for log(autoignition)

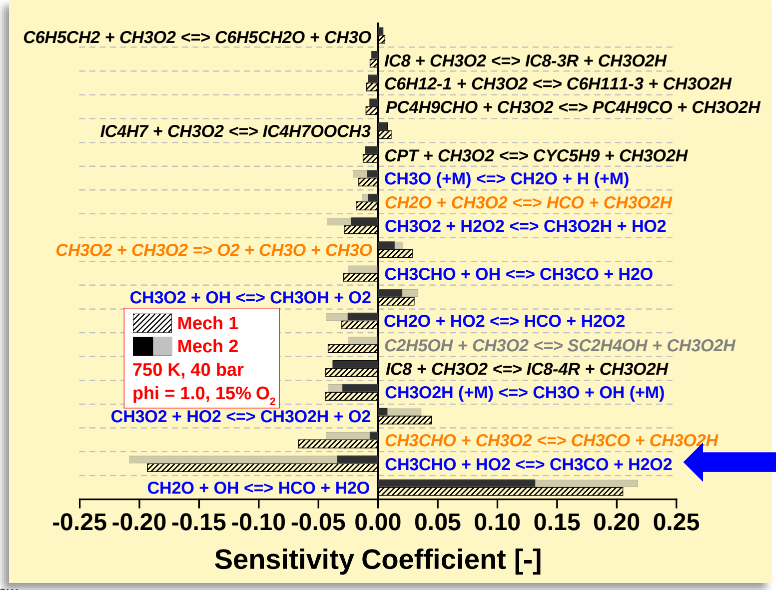
GPR model estimates local error, which is less than 6% (95% CI) at the resolution saved in the database (512 points)

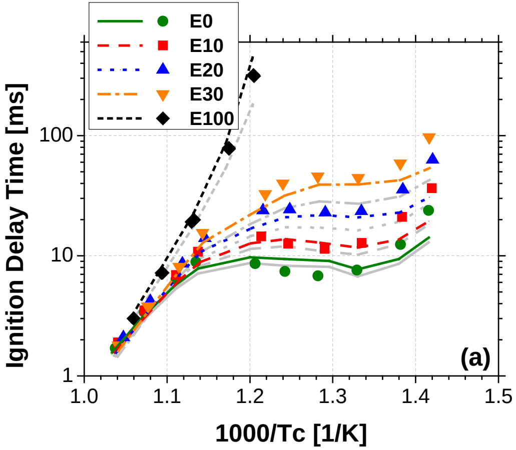
- Rapid evaluation time allows many metrics to be tested and compared: 2.5 µs versus 11 s per point.

PI: Matt McNenly, LLNL

RCM Kinetic Mechanism Development

- Developed novel computational approach to investigate fuel blending effects—identifying important controlling chemistry
- Demonstrated technique using gasoline/ethanol blends where critical intermolecular interactions were highlighted, and missing chemistry inferred, with significant improvements to LLNL's Co-Optima model compared against RCM database.



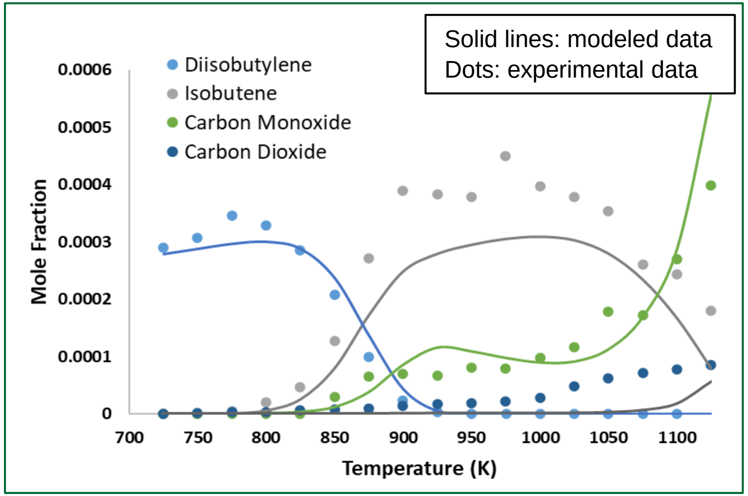


PI: S. Scott Goldsborough, ANL

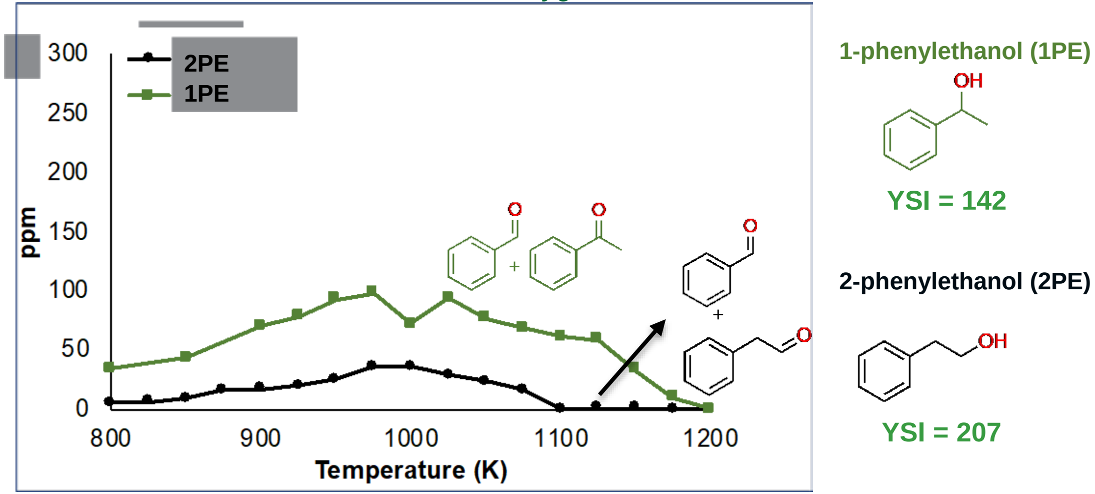
Flow Reactor Autoignition Kinetic Mechanism Development and Validation

Flow reactor studies validate kinetic and soot precursor formation mechanisms

Diisobutylene Autoignition Species Profiles



Soot Precursor Formation: Validation of Oxygenated Aromatics Formation

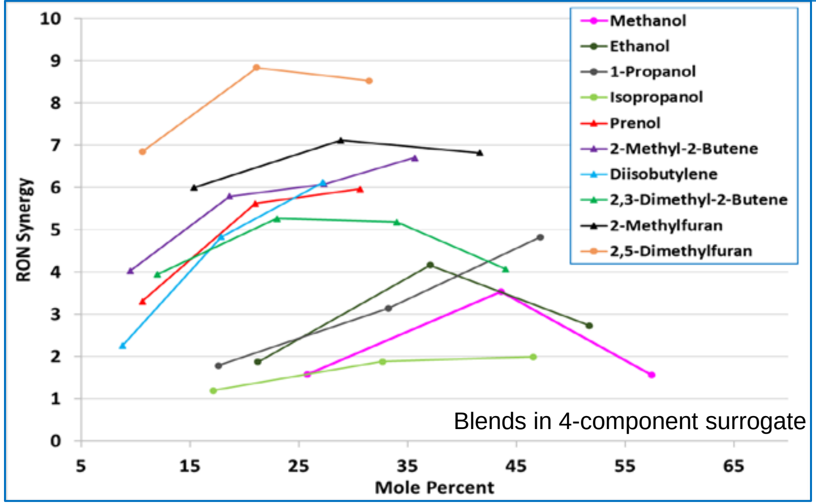


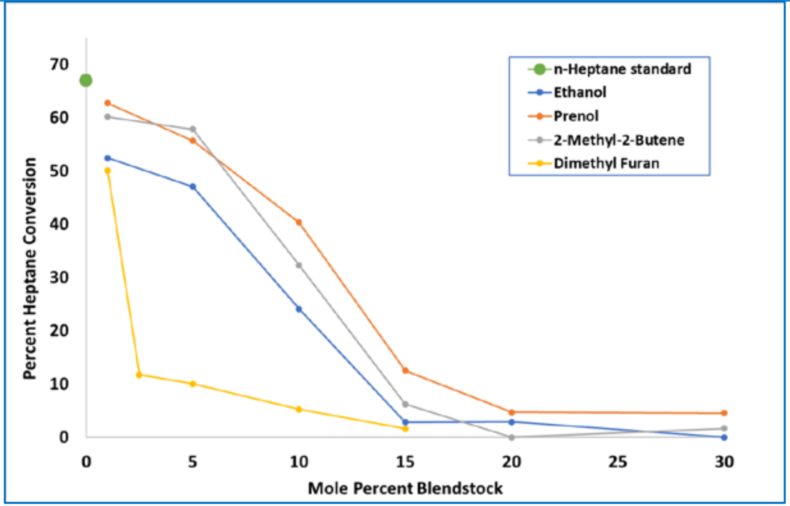
- Provided species profiles from flow reactor to validate kinetic mechanisms in collaboration with LLNL
  - Diisobutylene isomers and the three isomers of methyl-butenes data utilized to improve kinetic models
- Utilized quantum mechanical (QM) calculations from Seonah Kim's group in conjunction with flow reactor experiments to explain differences in sooting tendency of different isomers of phenyl ethanols and ethyl phenols.

Impact: A simple yet powerful tool for validating kinetic simulations and soot precursor mechanisms that can be rapidly applied to a wide range of systems

Mechanistic Basis Low and Intermediate Temperature Autoignition

Flow reactor studies allow for understanding of the chemical basis for nonlinear blending effects





Flow reactor conditions:
600 K
6-second residence time
$\phi = 0.25$

RON Synergy = D2699 measured RON – RON linear blending model

- Implemented new RON synergy metric to describe nonlinear blending behavior of various blendstocks
- Utilized flow reactor to investigate RON synergy observations and to examine intermediate species responsible for nonlinear blending trends-added FTIR to quantitate aldehyde species
- Currently working with simulations team at NREL to understand how blendstocks are affecting radical species concentrations
- Working to upgrade flow reactor to observe radical species to provide full picture of nonlinear blending behavior.

Impact: Flow reactor allows for observation of intermediate species responsible for nonlinear blending behavior

Selected Publications and Presentations (1 of 4)

Selected Publications:

1. Mueller, J., Kim, N., Lapointe, S., McNenly, M., Sjoberg, M., and Whitesides, R., “Optimization of fuel formulation using adaptive learning and artificial intelligence,” In J. Badra, P. Pal, Y. Pei, and S. Som (Eds.) *AI and Data Driven Optimization Techniques for Internal Combustion Engines,* Elsevier, 2021 *(in review).*
2. Dong, S., Aul, C., Gregoire, C., Cooper, S. P., Mathieu, O., Petersen, E. L., Rodriguez, J., Mauss, F., Wagnon, S. W., Kukkadapu, G., Pitz, W. J., and Curran, H. J., "A Comprehensive Experimental and Kinetic Modeling Study of 1-Hexene," *Combustion and Flame*, accepted, 2021.
3. Wang, M., Kukkadapu, G., Fang, R., Pitz, W.J., and Sung, C.-J., “Autoignition Study of iso-Cetane/Tetralin Blends at Low Temperature,” *Combustion and Flame*, accepted, 2021.
4. Pitz, W. J., Liang, J., Kukkadapu, G., Zhang, K., Conroy, C., Bugler, J., and Curran, H. J., "A Detailed Chemical Kinetic Modeling and Experimental Investigation of the Low- and High-Temperature Chemistry of n-Butylcyclohexane," *International Journal of Chemical Kinetics* 53(3), 2021.
5. Lokachari, N., Wagnon, S. W., Kukkadapu, G., Pitz, W. J., and Curran, H. J., "An Experimental and Kinetic Modeling Study of Cyclopentane and Dimethyl Ether Blends," *Combustion and Flame* 225: 255-271, 2021.
6. Nagaraja, S. S., Kukkadapu, G., Panigrahy, S., Liang, J., Lu, H., Pitz, W. J., and Curran, H. J., "A Pyrolysis Study of Allylic Hydrocarbon Fuels," *International Journal of Chemical Kinetics*, 2020 https://doi.org/10.1002/kin.21414.
7. Cheng, S., Kang, D., Fridlyand, A., Goldsborough, S. S., Saggese, C., Wagnon, S., McNenly, M. J., Mehl, M., Pitz, W. J., and Vuilleumier, D., "Autoignition Behavior of Gasoline/Ethanol Blends at Engine-Relevant Conditions," *Combustion and Flame* 216, 369-384, 2020 https://doi.org/10.1016/j.combustflame.2020.02.032.

Link to Co-Optima Publications Database: https://www.energy.gov/eere/bioenergy/co-optima-publications-library

Selected Publications and Presentations (2 of 4)

8. Mergulhão, C. S., Carstensen, H.-H., Song, H., Wagnon, S. W., Pitz, W. J., and Vanhove, G., "Probing the Antiknock Effect of Anisole through an Ignition, Speciation and Modeling Study of Its Blends with Isooctane," *Proceedings of the Combustion Institute* 38(1): 739-748, 2021, https://doi.org/10.1016/j.proci.2020.08.013.
9. Zhang, K., Capriolo, G., Kim, G., Almansour, B., Terracciano, A. C., Vasu, S. S., Pitz, W. J., and Konnov, A. A., "Experimental and Kinetic Modeling Study of Laminar Burning Velocities of Cyclopentanone and Its Binary Mixtures with Ethanol and n-Propanol," *Energy & Fuels* 34(9): 11408-11416, 2020.
10. Lokachari, N., Panigrahy, S., Kukkadapu, G., Kim, G., Vasu, S. S., Pitz, W. J., and Curran, H. J., "The Influence of Iso-Butene Kinetics on the Reactivity of Di-Isobutylene and Iso-Octane," *Combustion and Flame* 222: 186-195, 2020.
11. Kwon, H., Lapointe, S., Zhang, K., Wagnon, S. W., Pitz, W. J., Zhu, J., McEnally, C. S., Pfefferle, L. D., and Xuan, Y., "Sooting Tendencies of 20 Bio-Derived Fuels for Advanced Spark-Ignition Engines," *Fuel* 276: 118059, 2020.
12. Luecke, J. and Zigler, B. T., “Rapid prediction of fuel research octane number and octane sensitivity using the AFIDA constant-volume combustion chamber,” *Fuel*, 2021 (accepted).
13. Abel, R.C., Luecke, J., Ratcliff, M.A., and Zigler, B.T., “Comparing Cetane Number Measurement Methods,” ASME ICEF2020-3017, Proceedings of the ASME 2020 Internal Combustion Engine Fall Technical Conference, 2020.
14. Boehman, Andre L., Luecke, Jon, Fouts, Lisa, Ratcliff, Matthew, Zigler, Brad, and McCormick, Robert, “Ignition Delay Measurements of Four Component Model Gasolines Exploring the Impacts of Biofuels and Aromatics,” *Proceedings of the Combustion Institute* 38(4): 5549-5555, 2021.
15. Messerly, Richard, Rahimi, Mohammad J., St. John, Peter C., Luecke, Jon H., Park, Ji-Woong, Huq, Nabila A., Foust, Thomas D., Lu, Tianfeng, Zigler, Bradley T., McCormick, Robert L., and Kim, Seonah, “Towards quantitative prediction of ignition-delay-time sensitivity on fuel-to-air equivalence ratio,” *Combustion and Flame* 214: 103-115, 2020. doi:10.1016/j.combustflame.2019.12.019.

Selected Publications and Presentations (3 of 4)

16. Cheng, S., Goldsborough, S. S., Saggese, C., Wagnon, S., and Pitz, W. J., "New Insights into Fuel Blending Effects: Intermolecular Chemical Kinetic Interactions Affecting Autoignition Times and Intermediate-Temperature Heat Release," *Combustion and Flame,* 2021 (accepted).
17. Yeonjoon, K., Etz, B.D., Fioroni, G.M., Hays, C.K., St. John, P.C., Messerly, R.A., Vyas, S., Beekley, B.P., Guo, F., McEnally, C.S., Pfefferle, L.D., McCormick, R.L., and Kim, S., "Investigation of structural effects of aromatic compounds on sooting tendency with mechanistic insight into ethylphenol isomers," *P. Combust. Inst.* https://doi.org/10.1016/j.proci.2020.06.321.
18. Etz, B.D., Fioroni, G.M., Messerly, R.A, Rahimi, M.J., St. John, P.C., Robichaud, D.J., Christensen, E.D., Beekley, B.P., McEnally, C.S., Pfefferle, L.D., Xuan, Y., Vyas, S., Paton, R.S., McCormick, R.L., and Kim, S., "Elucidating the chemical pathways responsible for the sooting tendency of 1 and 2-phenylethanol," *P. Combust. Inst.* https://doi.org/10.1016/j.proci.2020.06.072.
19. Johnson, M.S., Nimlos, M.R., Ninnemann, E., Laich, A., Fioroni, G.M., Kang, D., Bu, L., Khanniche, S., Goldsborough, S.S., Vasu, S., and Green, W.H, "Oxidation and pyrolysis of methyl propyl ether," *Int. J. Chem. Kinet.* https://doi.org/10.1002/kin.21489.

Selected Publications and Presentations (4 of 4)

Selected Presentations

1. M. McNenly, “Virtual Fuel Property Exploration: Optimizing BOBs and Discovering the Origins of Phi-Sensitivity,” presented at the Advanced Engine Consortium (AEC) Program Review Meeting, Aug. 2020.
2. N. Killingsworth, M. McNenly, M. Sjoberg, N. Kim, R. Vijayagopal, S. Sarvaiya, and J. Mueller, “Fuel Effects on Fuel Economy for a Vehicle with a Multimode Engine – a Progress Update,” presented at the Advanced Engine Consortium (AEC) Program Review Meeting, Feb. 2021.
3. Chiara Saggese, “Experimental and kinetic modeling study of ignition and combustion behavior of n-pentanol,” American Chemical Society Virtual Spring Meeting, April 2021.
4. Chiara Saggese, “An improved detailed chemical kinetic model for C3-C4 linear and iso-alcohols and their blends with gasoline at engine-relevant conditions,” 38th International Symposium of Combustion, Jan. 2021.