Co-Optimization of Fuels & Engines

MM: Fuel Kinetics

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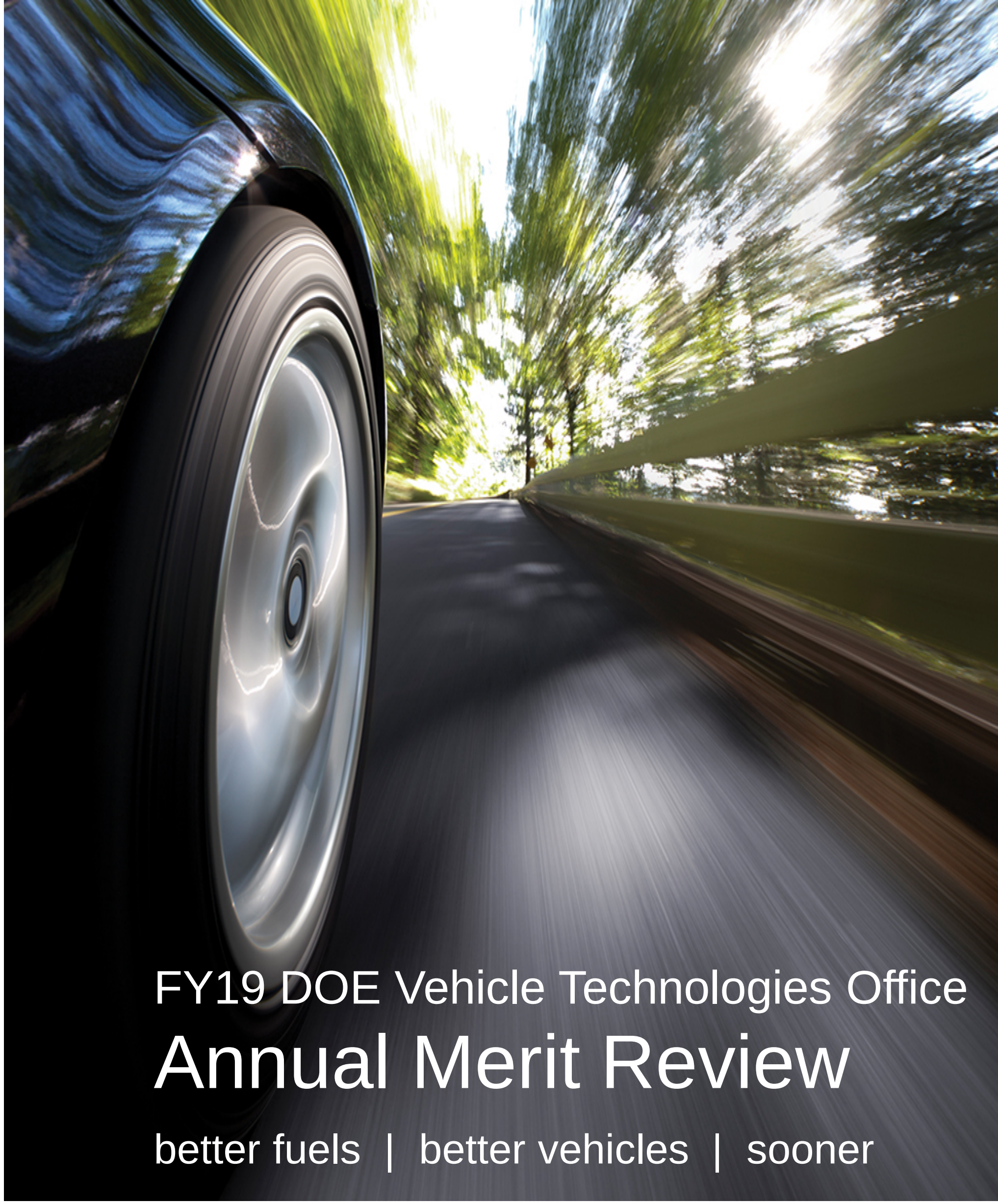
Project # FT075



FY19 DOE Vehicle Technologies Office

Annual Merit Review

better fuels | better vehicles | sooner

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

Overview

Timeline

Project start date: 10/1/2015

Project end date: 9/30/2021*

Percent complete: 18%*

Budget

Task	FY18	FY19
F.2.2.2 LLNL Pitz	$800K	$707K
F.1.2.3 LLNL Pitz	$65K	$30K
F.2.2.4 LLNL Pitz	$157K (Q4)	to F.2.2.2
F.2.2.5 LLNL Pitz	$60K (Q4)	to F.2.2.2
F.2.2.3 ANL Goldsborough	$185K	$180K
F.2.3.1 ANL Goldsborough	Not funded	$115K

Barriers

Lack of fundamental knowledge about the fuel kinetics impact on multi-mode, mixing controlled compression ignition, and advanced compression ignition engine performance:

- Dilute Gasoline Combustion
- Low-Temperature Combustion
- Clean Diesel Combustion

Partners

One industry awardee

External advisory board

Nine national labs

20+ universities

80+ stakeholder organizations

120+ researchers

*Start and end dates refer to the two three-year life cycles for DOE lab-call projects. Progress reflects the current three-year cycle.

Relevance: Barriers

"… robust lean-burn and EGR-diluted combustion technology and controls, especially relevant to the growing trend of boosting and down-sizing engines."

"… understanding of the impact of likely future fuels on LTC…"

"Soot formation and oxidation processes … are not well enough understood to develop robust soot models for computational fluid dynamics (CFD)."

Barriers from the Advanced Combustion and Emission Control Roadmap, March 2018

Relevance: Objectives

Overall Co-Optimization of Fuels and Engines objective:

Deliver foundational science to develop fuel and engine technologies that will work in tandem to achieve efficiency, environmental, and economic goals

Task objectives

Kinetic mechanism development

Develop an understanding of the controlling chemical kinetics for blendstocks and their blends with base fuels at conditions relevant to advanced combustion strategies

Fuel property blending model

Predict important fuel properties at conditions relevant to multimode, medium- and heavy-duty ACI, and mixing controlled compression ignition

Development/application of multimode/ACI fuel quality metric

Rank autoignition behavior of fuels in lieu of existing metrics which have limitations

ACI: advanced compression ignition

Milestones

Month, Year	Description of Milestone or Go/No-Go Decision	Status	Lab
March, 2019	F.2.2.3: Complete measurement of top tier fuels	Completed	ANL
~~March, 2019~~ June, 2019	F.2.2.2: Develop/improve kinetic models for 2-3 blendstocks for multimode, ACI and MCCI	Delayed, on target	LLNL
June, 2019	F.1.2.3: Predict blending behavior of MCCI blendstocks into base diesel (sooting propensity)	On target	LLNL
~~March, 2019~~ September, 2019	F.2.3.1: Complete formulation / RCM testing for higher ϕ-stratified conditions	Delayed, on target	ANL
September, 2019	F.2.2.3: Measurement of fuels + research-grade full boiling range fuel	On target	ANL
September, 2019	F.2.2.2: Develop/improve kinetic models for 3-4 blendstocks for multimode, ACI and MCCI	On target	LLNL

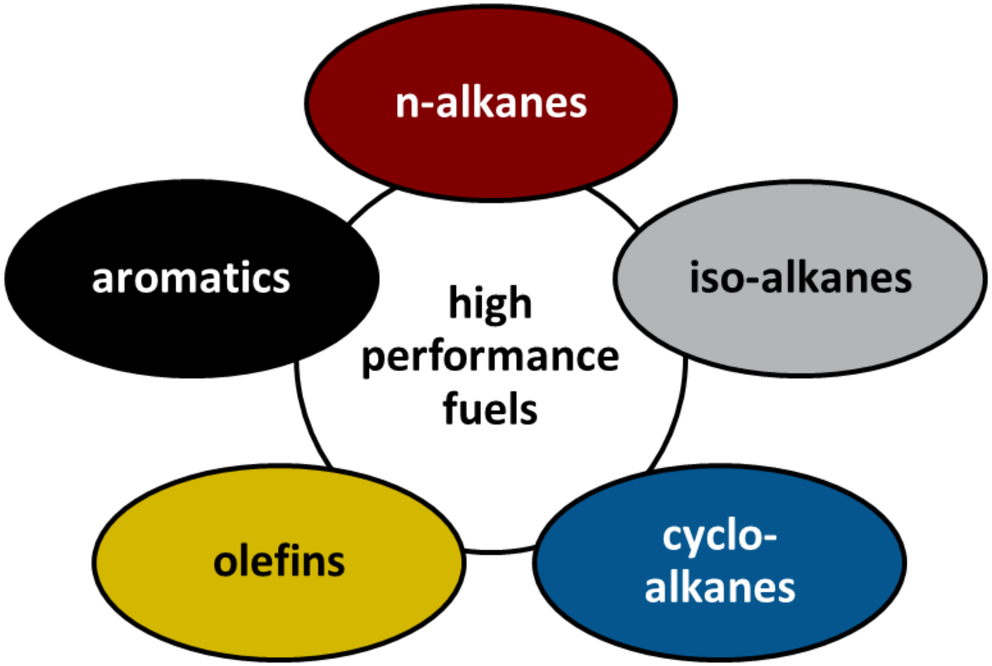
Approach

Kinetic mechanism development

F.2.2.2 LLNL Pitz and F.2.2.3 ANL Goldsborough

LLNL
- Develop and validate chemical kinetic mechanisms for high performance fuels (HPFs) and their blends with base fuels (BOBs).
- Validate and verify PAH/soot model for HPFs and blends of interest.

ANL
- Acquire rapid compression machine datasets that can be used to provide insight into chemical kinetic effects of fuel performance in engines



Approach

Fuel property blending model

F.1.2.3 LLNL Pitz

- Predict key behavior of fuel properties identified in merit functions.
- Validate predicted blending behavior using available fuel property measurements.

Development/application of multimode/ACI fuel quality metric

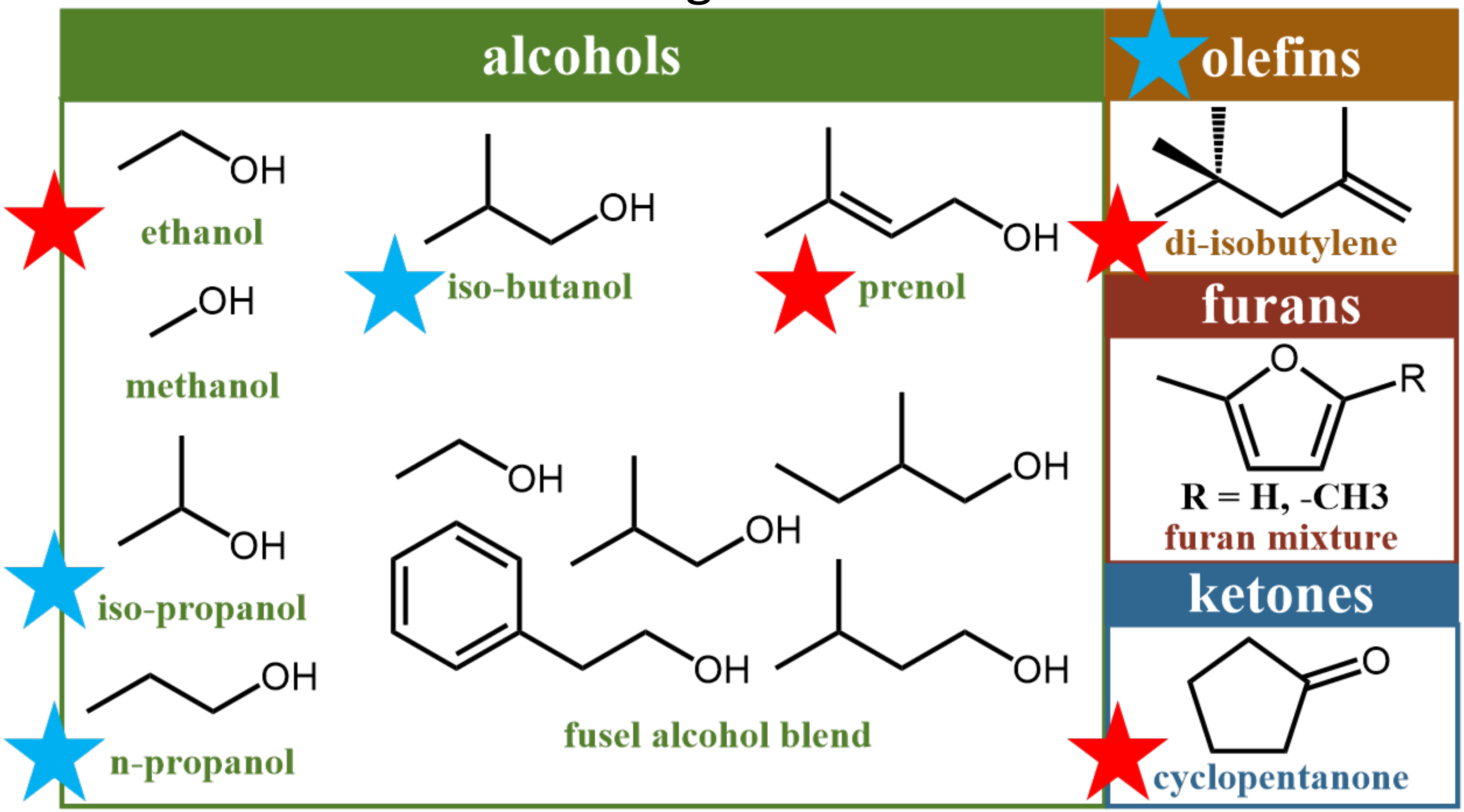
F.2.3.1 ANL Goldsborough

- Quantify relative reactivities at engine relevant time scales in a rapid compression machine to rank fuels, assess sensitivities (ϕ, EGR), identify control methodologies to expand ACI operating region.

Developed and improved kinetic models for fuels on the top 10 fuel list

Technical accomplishments and progress

Blendstocks with highest merit function score

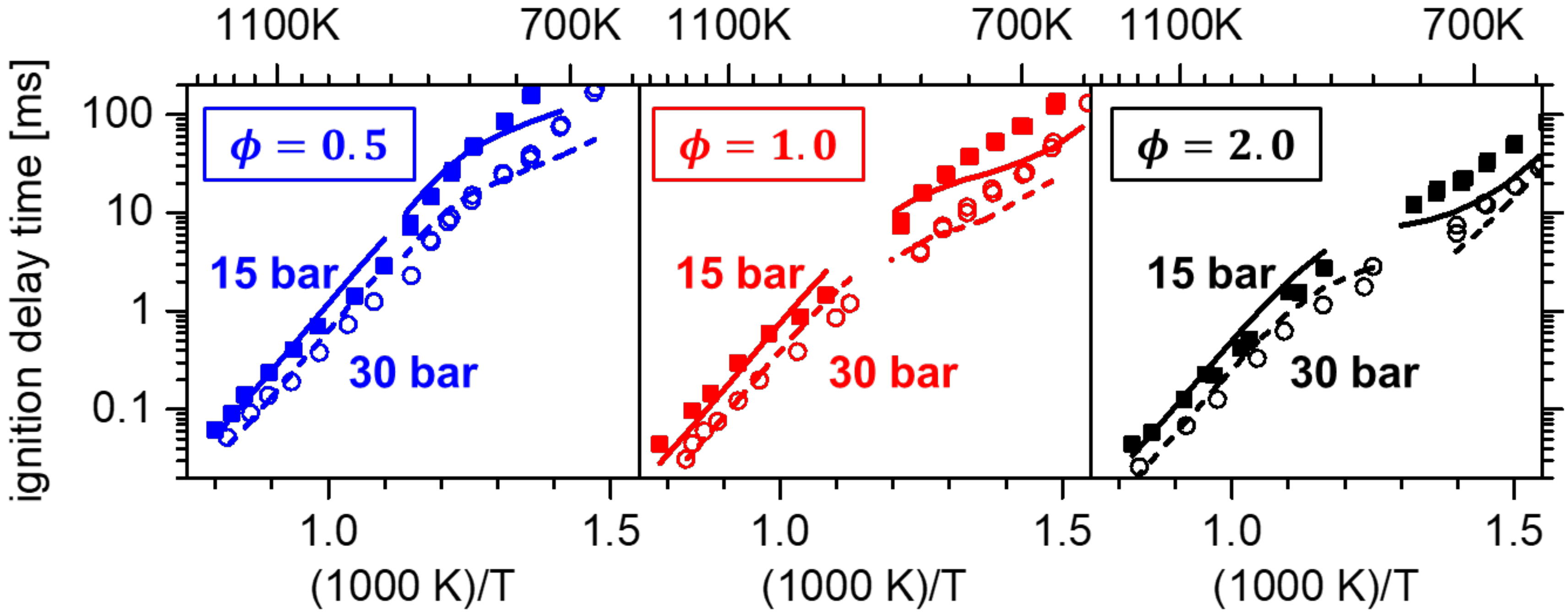


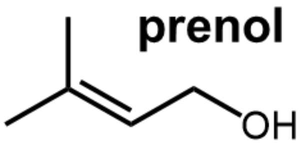
<u>Since the last DOE Annual Merit Review</u>

- ★ Four new or improved kinetic models
- ★ Four new rapid compression machine datasets

Developed kinetic models for prenol & iso-prenol which exhibit synergistic blending[1]

F.2.2.2 (Pitz): Develop/improve kinetic models for blendstocks for multimode (SI/ACI)





Symbols: New NUI-Galway experiments

Lines: LLNL kinetic model

Collaborations with SNL, NREL, NUIG, & UCF to collect flow reactor, shock tube, rapid compression machine, and flame speed data

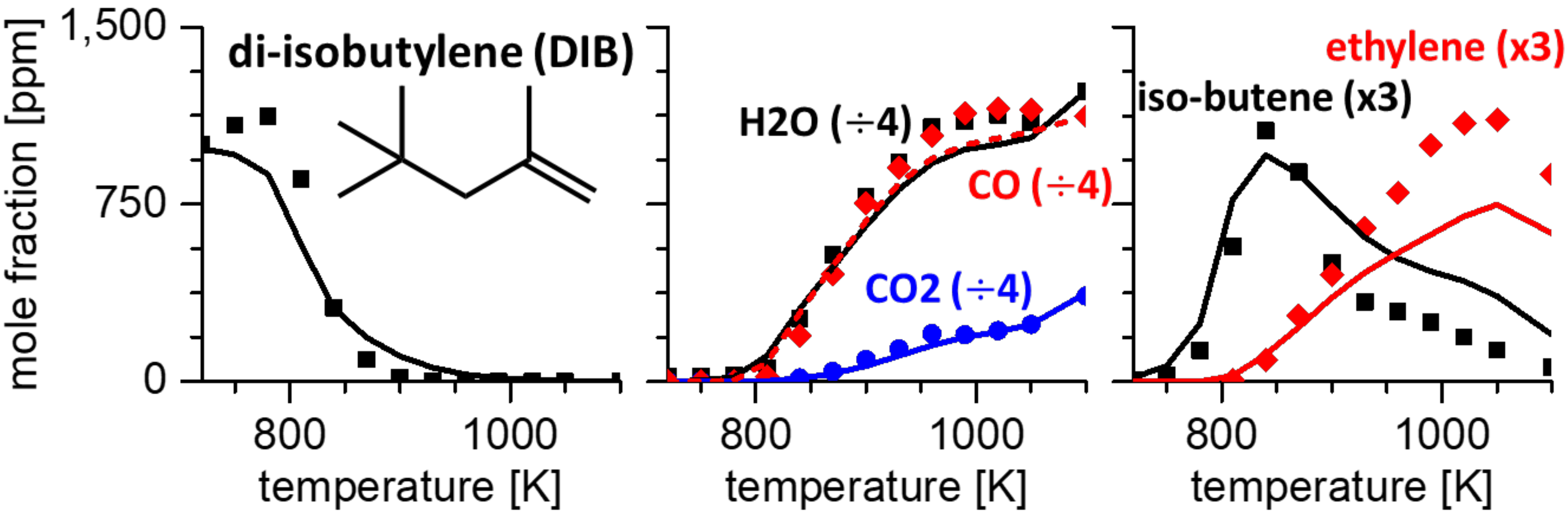
[1]Monroe, Gladden, Albrecht, Bays, McCormick, Davis, George. Fuel 239 (2019) 1143

Improved DIB model using JSR data, RCM ignition data, and flame speed data

Technical accomplishments and progress

F.2.2.2 (Pitz): Develop/improve kinetic models for blendstocks for multimode (SI/ACI)

Oxidation in a jet-stirred reactor (JSR) at 10 atm, ϕ = 1



Symbols: New CNRS Orleans experiments   Lines: LLNL kinetic model

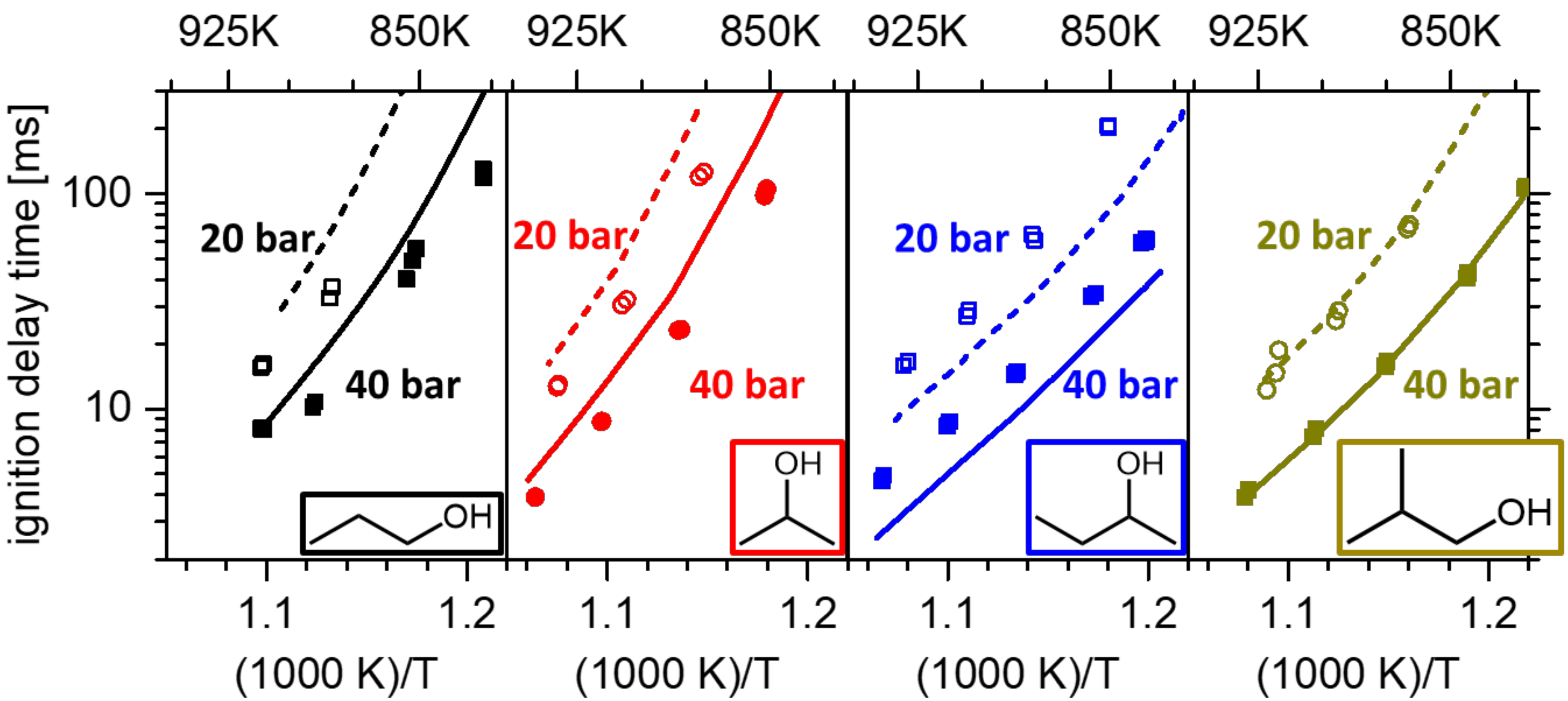
Collaborations with NREL, NUIG, & UCF to collect flow reactor, shock tube, rapid compression machine, and flame speed data

Acquired new autoignition data for fuels on the top 10 fuel list

Technical accomplishments and progress

F.2.2.3 (Goldsborough): Complete measurement of top tier fuels

Rapid compression machine (RCM) experiments at dilute, stoichiometric conditions



Symbols: New ANL experiments

Lines: LLNL kinetic model

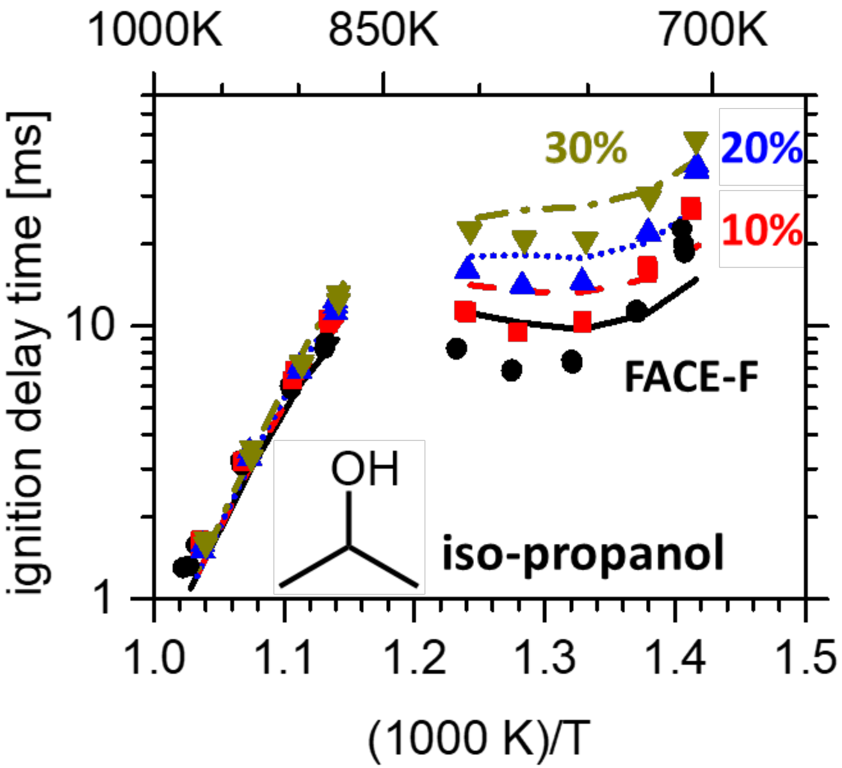
RCM measurements of “neat” fuels provide additional validation targets for updated, refined kinetic model

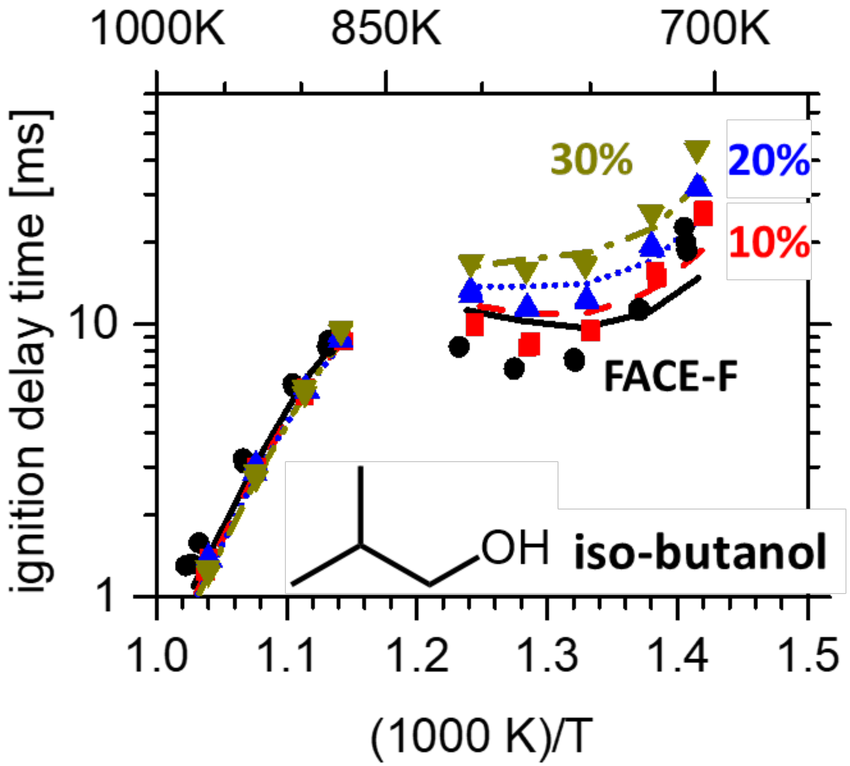
Acquired new autoignition data for top 10 fuels blended with research-grade gasoline

Technical accomplishments and progress

F.2.2.3 (Goldsborough): Measurement of fuels + research-grade full boiling range fuel

Rapid compression machine (RCM) experiments at 40 bar





Symbols: New ANL experiments Lines: LLNL kinetic model

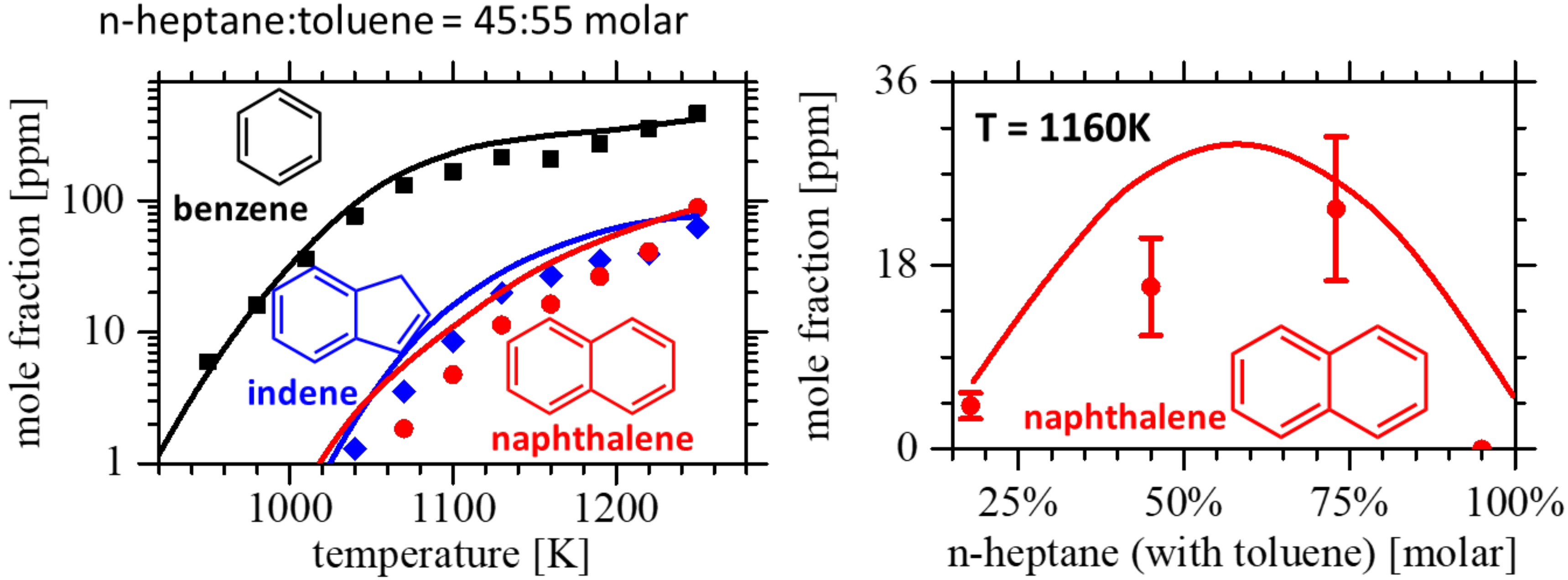
RCM measurements of blends with full boiling-range gasoline quantify perturbative effects of iso-alcohols: ignition retarded at lower temperatures

Developed & validated new kinetic model for PAHs to enable soot predictions

Technical accomplishments and progress

F.1.2.3 (Pitz): Predict blending behavior of blendstocks into base fuels (sooting propensity)

Pyrolysis of binary blends in a jet-stirred reactor



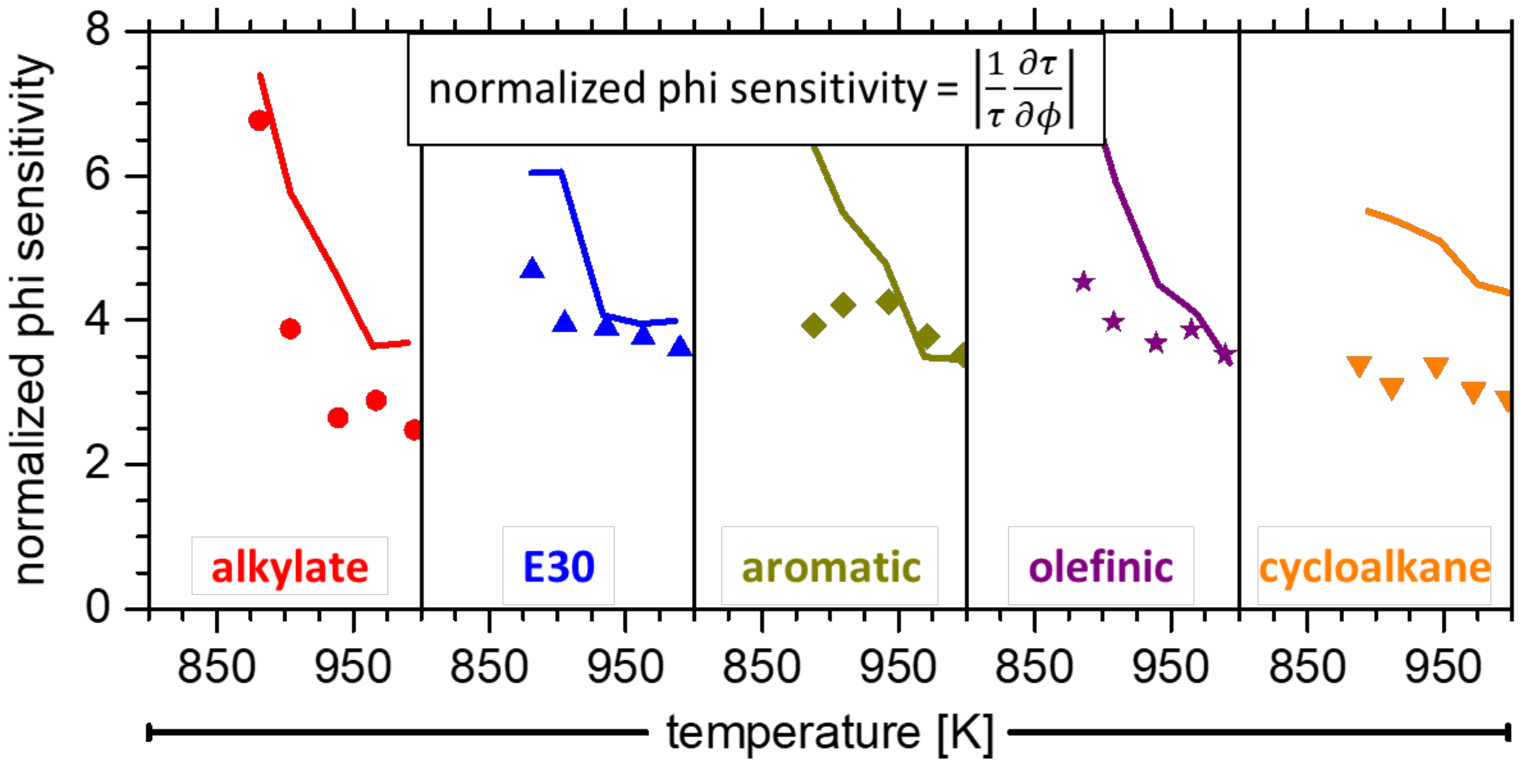
Symbols: New KAUST experiments   Lines: LLNL kinetic model

Model predicts polycyclic aromatic hydrocarbon (PAH) formation for binary and more complex blends. Blends can lead to higher PAH formation than expected from linear blending.

Developed methodologies to experimentally quantify fuel properties relevant to MM

Technical accomplishments and progress

F.2.3.1 (Goldsborough):
Complete formulation / RCM testing for higher ϕ-stratified conditions



<u>Symbols</u>: New ANL experiments

<u>Lines</u>: LLNL kinetic model

RCM measurements of Co-Optima core fuels demonstrating a path to quantifying fuel properties relevant to MM and ACI combustion schemes

Response to previous year reviewers' comments

"[consider] developing a merit function for ACI/SI multimode combustion"

F.2.3.1 is a new task this year to assist development of a multimode (SI/ACI) merit function

"kinetic mechanism reduction, and CFD simulations in actual SI, ACI, and diesel engine conditions."

Collaborations with Simulation Toolkit teams and industry to apply reduced mechanisms in CFD simulations

"consider further strengthening the interactions with OEMs… [and] develop closer coordination with the Co-Optima experimental teams on ACI and diesel combustion activities"

Collaborations with: ANL, NREL, ORNL, SNL, GM, Convergent Science

Collaboration and coordination with other institutions

Collaboration with seven national laboratories ANL, LLNL, NREL, ORNL, PNNL, SNL
Goldsborough; Som; Lapointe; McNenly; Pitz; Whitesides; Fioroni; McCormick; Splitter; Szybist; Bays; Dec; George; Hansen; Mueller; Pickett; Sjoberg; Skeen

Four Co-Optima university partners

Massachusetts Institute of Technology > Model development; theoretical calculations
Pennsylvania State University > YSI predictions using kinetic models
University of Central Florida > Experiments for kinetic model validations
Yale University > YSI measurements

One subcontract by LLNL

University of Connecticut (by LLNL) > Experiments for kinetic model validations

Four outside VTO collaborations

King Abdullah University of Science and Technology > Experiments; calculations
National University of Ireland – Galway > Experiments; modeling; calculations
Politecnico di Milano > Modeling
University of Michigan > Experiments

Industry

Advanced Engine Working Group
Coordinating Research Council
General Motors

Coordination

Monthly team and stakeholder meetings
Quarterly leadership planning meetings
Annual all-hands meeting

Remaining challenges and barriers

Validating chemical kinetic models over wider pressure ranges, equivalence ratios, EGR dilution levels, and blends

Experimental measurements of EGR mixtures, including NOx

Studies that expand our knowledge of particulate matter precursor formation and ability to predict soot formation

Modeling and measurements of research grade fuels for multi-mode (SI/ACI), mixing controlled compression ignition, and medium- and heavy-duty advanced compression ignition operation

Proposed future research*

For multi-mode, MD/HD ACI, and MCCI modes:

Acquire necessary experimental data and develop kinetic models for Co-Optima fuel blends that can be used to accurately predict combustion behavior at different engine operating modes including the effects of dilution, equivalence ratio, EGR, pressure, and temperature.

Develop PAH/soot models that predict the formation and oxidation of PAH/soot.

Develop kinetic models that accurately predict the promotion effect of NO to ensure accurate simulation of autoignition.

Refine and validate fuel metrics for MM, MD/HD ACI combustion modes.

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

MD/HD: medium- and heavy-duty
ACI: advanced compression ignition
MM: multi-mode

MCCI: mixing controlled compression ignition

Summary

Kinetic Mechanism Development

F.2.2.2 LLNL Pitz and F.2.2.3 ANL Goldsborough

Impact Chemical kinetic models and measurements of highly ranked fuels enable accurate predictions and projections of combustion behavior at MM (SI/ACI), MCCI, and MD/HD ACI operation for a wide range of stoichiometries, pressures, temperatures, and EGR levels

Fuel Property Blending Model

F.1.2.3 LLNL Pitz

Impact Accurate predictions of key properties for blended fuels at MM (SI/ACI), MCCI, and MD/HD ACI operation

Development/Application of Multimode/ACI Fuel Quality Metric

F.2.3.1 ANL Goldsborough

Impact A new fuel quality metric capable of ranking autoignition behavior of proposed fuels

MD/HD: medium- and heavy-duty
ACI: advanced compression ignition
MM: multi-mode

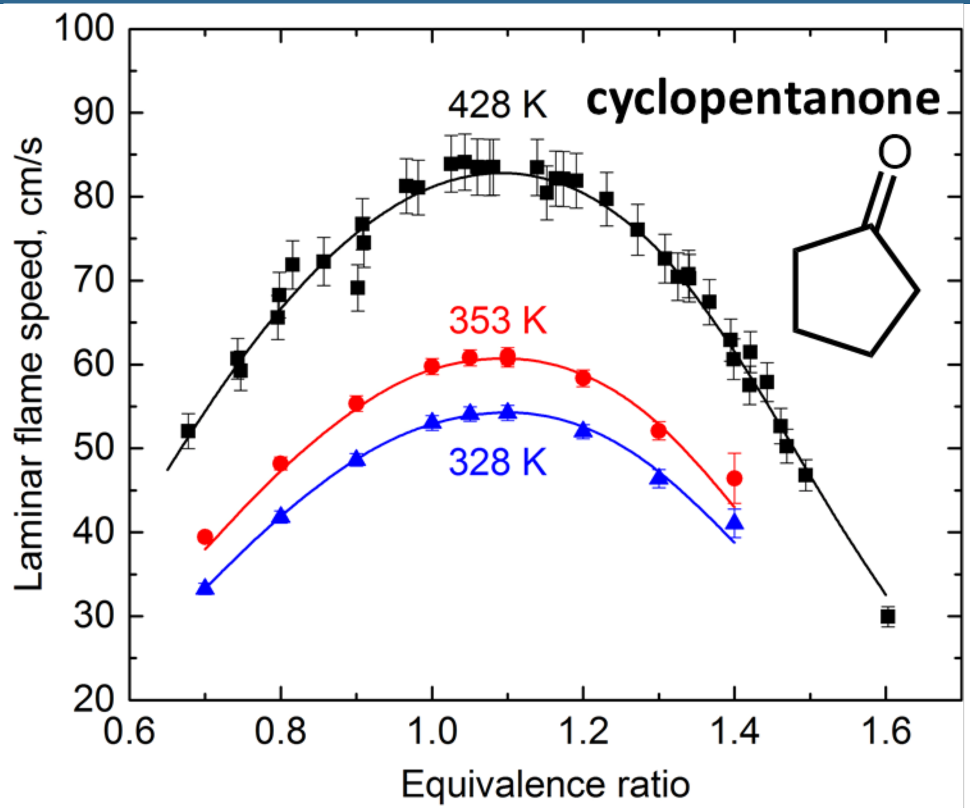
SI: spark ignition
MCCI: mixing controlled compression ignition

Technical Back-Up Slides

Improved kinetic model of cyclopentanone with MIT calculations and flame speed data

Technical accomplishments and progress (back-up)

F.2.2.2 (Pitz): Develop/improve kinetic models for blendstocks for multimode (SI/ACI)



Symbols: New UCF experiments

Lines: LLNL kinetic model

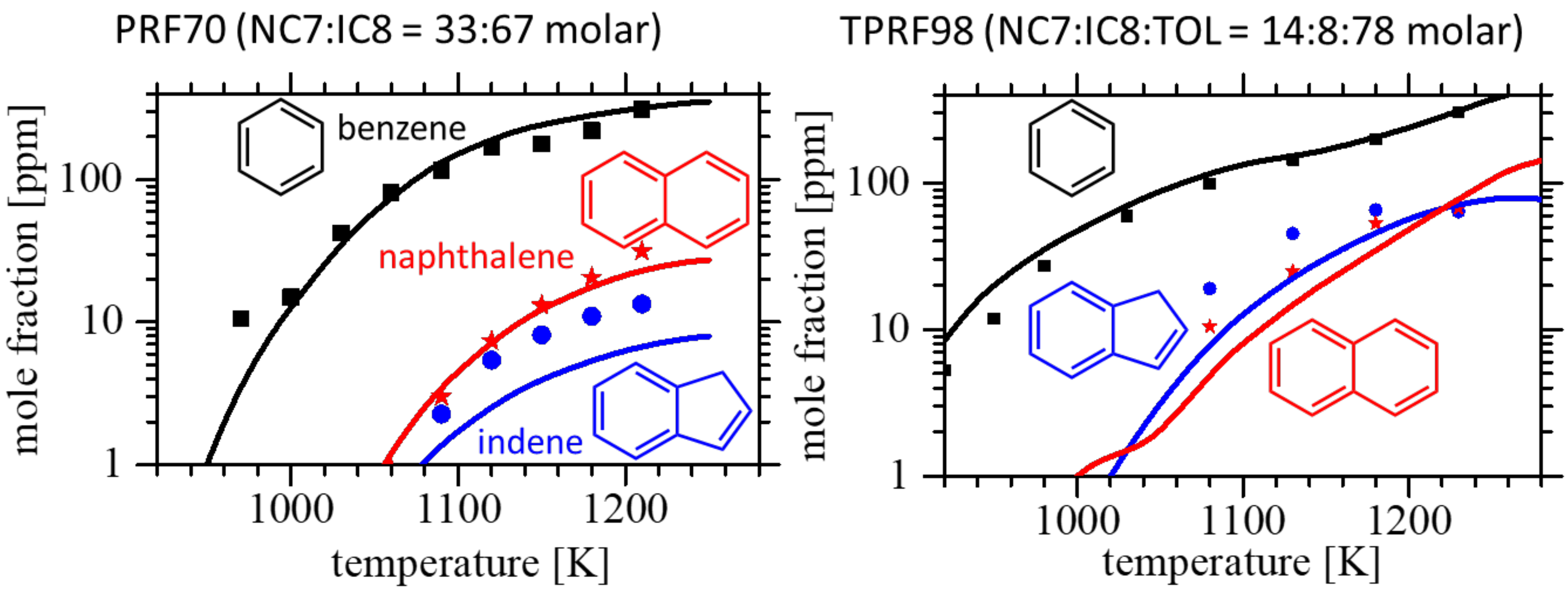
Validated simulations of cyclopentanone's high flame speeds are a step toward co-optimization of fuels and engines for multimode (SI/ACI)

Developed & validated new kinetic model for PAHs to enable soot predictions

Technical accomplishments and progress (back-up)

F.1.2.3 (Pitz): Predict blending behavior of MCCI blendstocks into base diesel (sooting propensity)

Pyrolysis of blends in a jet-stirred reactor

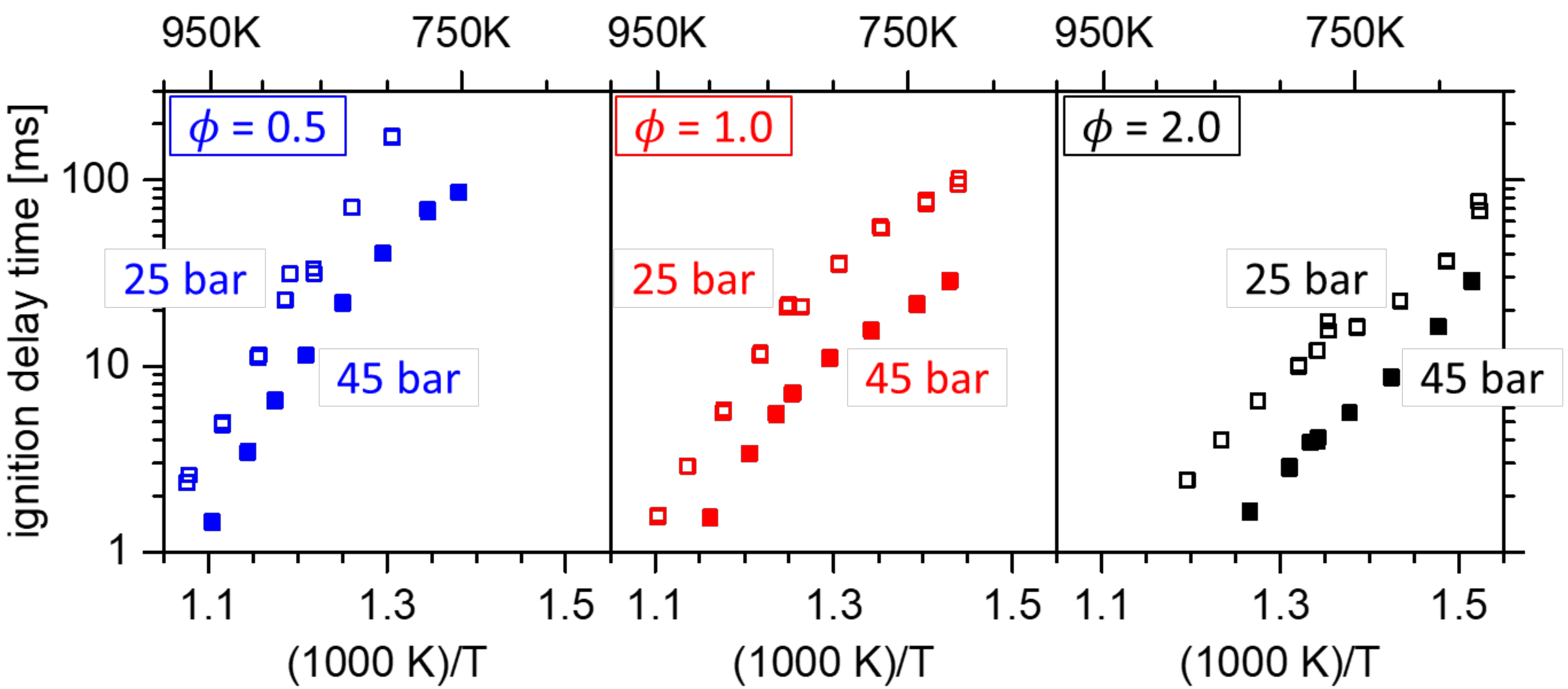


Symbols: New KAUST experiments   Lines: LLNL kinetic model

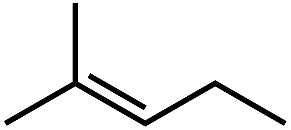
Model predicts PAH formation for PRF70 and more complex blends which will enable accurate predictions of in-cylinder soot

Extended experimental database of branched-olefins for development of robust kinetic model

F.2.2.3 (Goldsborough): Improve kinetic models for BOBs for multimode, ACI and MCCI



Symbols: New ANL experiments of 2-methyl-2-pentene



RCM measurements of “neat” branched-olefins are critical for formulating consistent rate rules used in development of kinetic model of gasoline-representative alkenes.