Co-Optimization of
Fuels & Engines

Introduction

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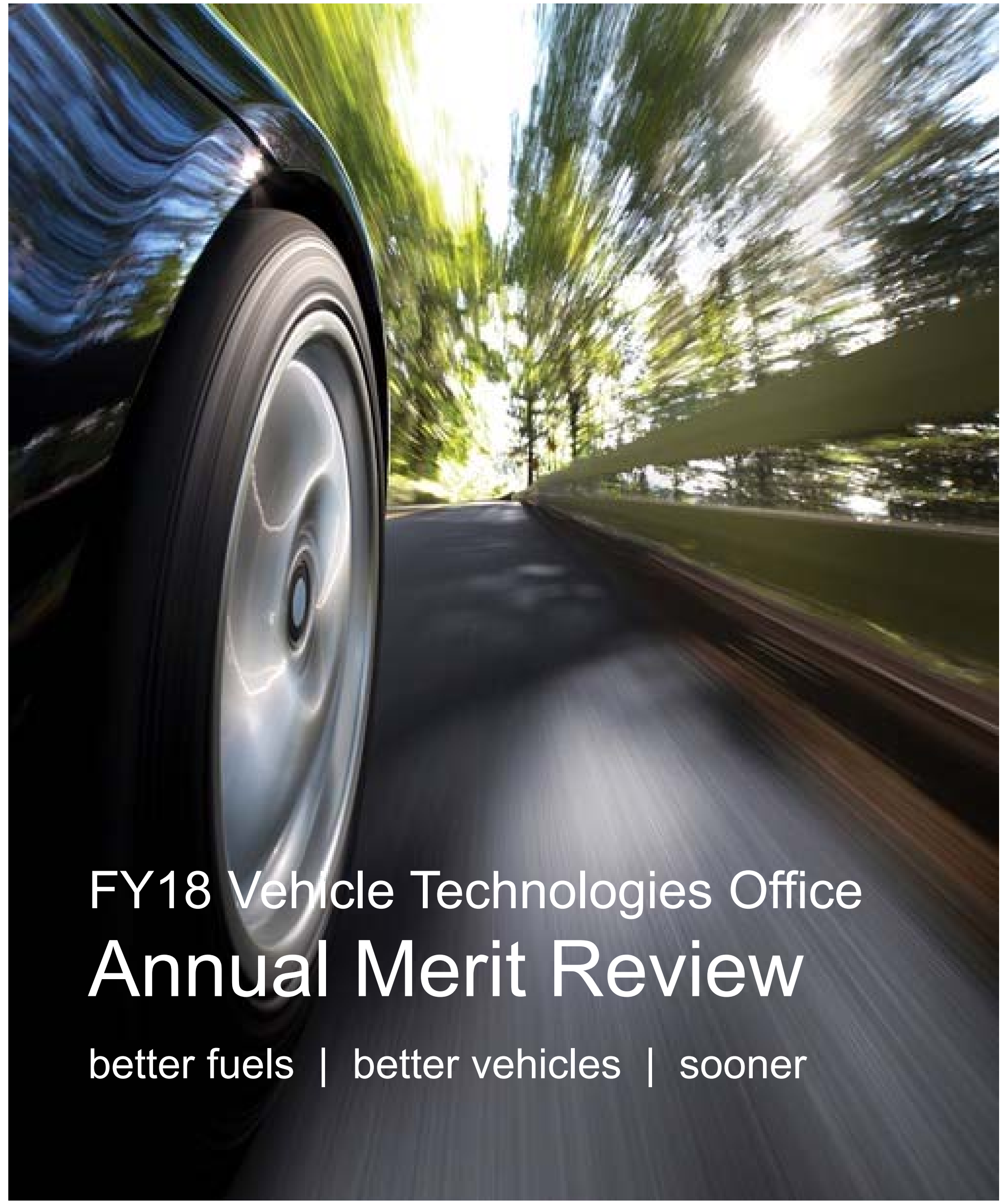
Project # FT037

June 20, 2018



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

VTO Program Managers: Gurpreet Singh, Kevin Stork, & Michael Weismiller

Goals and Outcomes

Light-duty

10% fuel economy (FE) improvement* from boosted SI and multi-mode SI/ACI

Heavy-duty

Up to 4% FE improvement (worth $5B/year)*

Potential lower cost path to meeting next tier of criteria emissions regulations

Fuels

Diversifying resource base

Providing economic options to fuel providers to accommodate changing global fuel demands

Increasing supply of domestically sourced fuel by up to 25 billion gallons/year

Cross-cutting goals

Stimulate domestic economy

Adding up to 500,000 new jobs

Providing clean-energy options

* Beyond projected results of current R&D efforts; 2030 target. The team is actively engaging OEMs, fuel providers, and other key stakeholders to refine goals and approaches to measuring FE improvements

Overview

Timeline

- Project start date: 10/1/2016
- Project end date:* 9/30/2018
- Percent complete: 88%

Budget

	FY16 Budget	FY17 Budget	FY18 Budget***
VTO	$12,000	$12,500	$8,100
BETO	$14,000	$12,000	$6,400
Total	$26,000	$24,500	$14,500

* Start/end dates refer to three-year life cycle of DOE lab-call projects. Co-Optima has proposed for an additional three-year cycle to begin at start of FY19

*** As of April 2018 (funding under FY18 continuing resolution

Barriers**

Lack of robust high-dilution stoichiometric and lean-burn combustion technology/controls

Inadequate fundamental knowledge base for clean diesel combustion and emissions processes

Determine factors limiting low temperature combustion (LTC) and develop methods to extend limits

Understanding impact of likely future fuels on LTC and whether LTC can be more fully enabled by fuel specifications different from gasoline and diesel fuel

Partners

Partners include nine national labs, 13 universities, external advisory board, and stakeholders (145 individuals from 86 organizations)

**https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf

Overview: Budget by Presentation

Topic	Presenter	FY16 ($K)	FY17 ($K)	FY18 ($K)
Overview (Project Management)	Farrell	1,000	1,000	700
Fuel property characterization and prediction	Fioroni	1,300	1,300	480*
Fuel kinetics and simulation	McNenly	1,500	1600	1,435
Boosted SI and Multimode SI/ACI Combustion, Part 1 (boosted SI and fuel effects)	Sluder	1,400	1,300	1,655
Boosted SI and Multimode SI/ACI Combustion, Part 2 (mostly boosted SI and fuel effects)	Kolodziej	1,200	1,300	855
Boosted SI and Multimode SI/ACI Combustion, Part 3 (mostly multi-mode)	Curran	1,700	1,900	1,435
MCCI and ACI Combustion; Sprays	Mueller	2,300	2,300	1,010
Emissions, Emission Control, and Merit Function	Pihl	1,600	1,800	980*
Total		12,000	12,500	8,550*

*Includes relevant BETO Funded work

Overview: Co-Optima Organization

Board of Directors

(Labs and DOE)

Approve direction and changes in focus

Steering Committee

POC for each lab, communications, IP

Operations

Project management, project integration, and strategic consulting

Leadership Team

(Labs and DOE)

Establish vision, define strategy, integrate work plan, oversee execution, evaluate performance, engage stake holders, and team build

External Advisory Board

Advise on technology and direction, provide recommendations, bridge to stakeholders

Technical Team Leads

Plan projects, evaluate team performance and gaps, report monthly highlights and quarterly progress, communicate across teams to minimize silos

Overview: External Advisory Board

USCAR
David Brooks

American Petroleum Institute
Bill Cannella

Fuels Institute
John Eichberger

Truck & Engine Manufacturers Assn
Roger Gault

Advanced Biofuels Association
Michael McAdams

Flint Hills Resources
Chris Pritchard

EPA
Paul Machiele

CA Air Resources Board
James Guthrie

UL
Edgar Wolff-Klammer

University Experts
Ralph Cavalieri (WSU, emeritus)
David Foster (U. Wisconsin, emeritus)

Industry Expert
John Wall (Cummins, retired)

- EAB advises National Lab Leadership Team
- Participants represent industry perspectives
- Entire board meets twice per year

Relevance

- Internal combustion engines will dominate the fleet for decades and their efficiency can be increased significantly
- Research into better integration of fuels and engines is critical to accelerating progress towards economic development, energy security, and emissions goals
- Improved understanding in several areas is critical for progress:
  - Fuel structure – property relationships
  - How to measure and predict key fuel properties
  - The impact of fuel properties on engine performance and emissions
- Research focused on key barriers to LD SI/multi-mode, MD/HD diesel, and ACI combustion approaches
- Research addresses VTO program plan knowledge gaps surrounding advanced combustion engine regimes and predicting the impact of fuel properties

LD = light duty; MD = medium duty; HD = heavy duty; SI = spark ignition; ACI = advanced compression ignition

Relevance: Overall Objectives

- Identify engine parameters and fuel properties that can significantly increase fuel economy across light, medium, and heavy duty fleets
  - Focus is on precompetitive, early stage research
  - We are not looking to define or recommend commercial solutions
- Conduct comprehensive and consistent blendstock survey to identify broad range of options that can be blended into petroleum base stocks and yield target values of key properties
- Demonstrate blendstock candidates that can be produced from renewable domestic biomass feedstocks that are affordable, scalable, sustainable, and compatible
- Identify implications to the refueling infrastructure for the various blendstock options
- Develop tools that allow us to do the work faster/more efficiently

Milestones

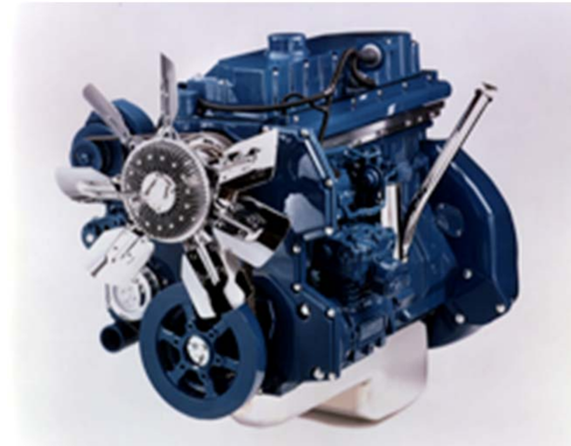
Month / Year	Description of Milestone or Go/No-Go Decision	Status
Mar 2018	Define suite of pathways with high carbon efficiency that can produce high cetane blendstocks needed for efficient Mixing-Controlled CI; provide report to DOE that will inform decision point on identifying promising fuel candidates Mixing Controlled CI.	Complete
Sep 2018	Review impact of at least 3 Co-Optima blendstocks for boosted spark ignition including considerations towards blending, refinery upgrading, and impact on refinery economics. Then provide Briefing to DOE that describes how Co-Optima focused pathways could address gasoline and diesel demand and defines key properties that can improve/drive market pull.	On track

- Table reflects high-level “dashboard” milestones
- Overall effort has 80 milestones
- Many milestones discussed in following presentations

Approach: Governing Hypotheses

Central Engine Hypothesis

There are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range



Central Fuel Hypothesis

If we identify target values for the critical fuel properties that maximize efficiency and emissions performance for a given engine architecture, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance

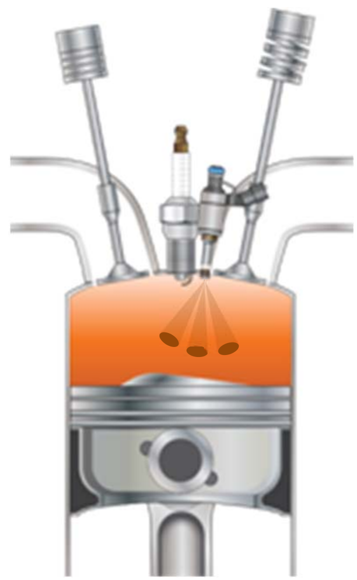
Approach: Two Parallel R&D Projects

Light-Duty

Boosted SI

Higher efficiency via downsizing

Near-term

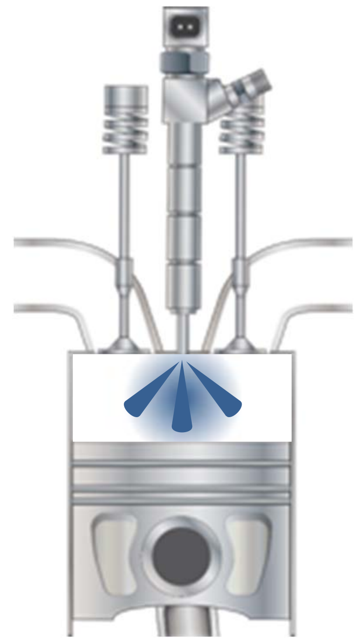


Multi-mode SI/ACI

Even higher efficiency over drive cycle

Mid-term

Medium/Heavy-Duty



Mixing Controlled

Improved engine emissions

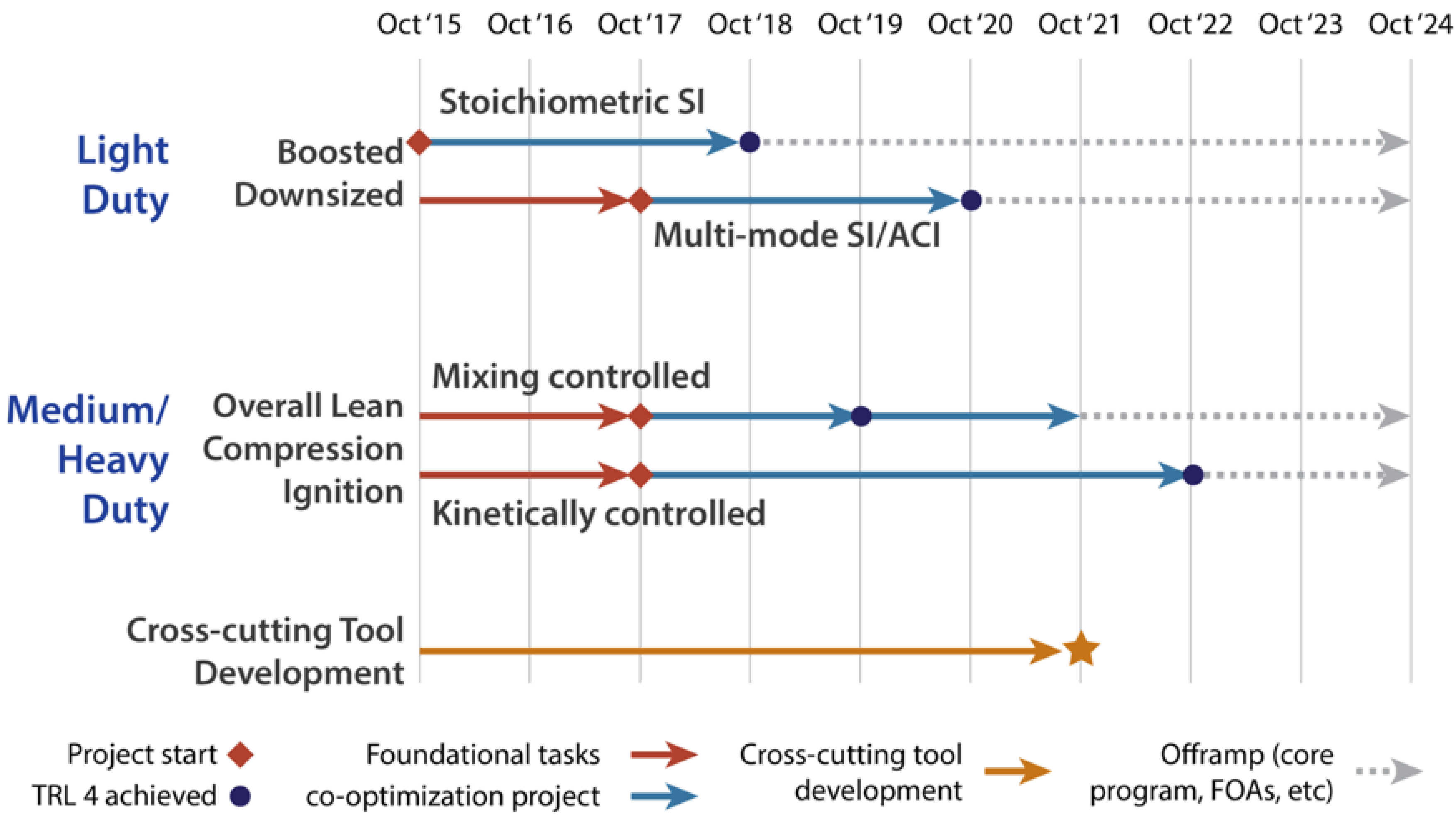
Near-term

Kinetically Controlled

Highest efficiency and emissions performance

Longer-term

Approach: Timeline



Approach: Main Elements

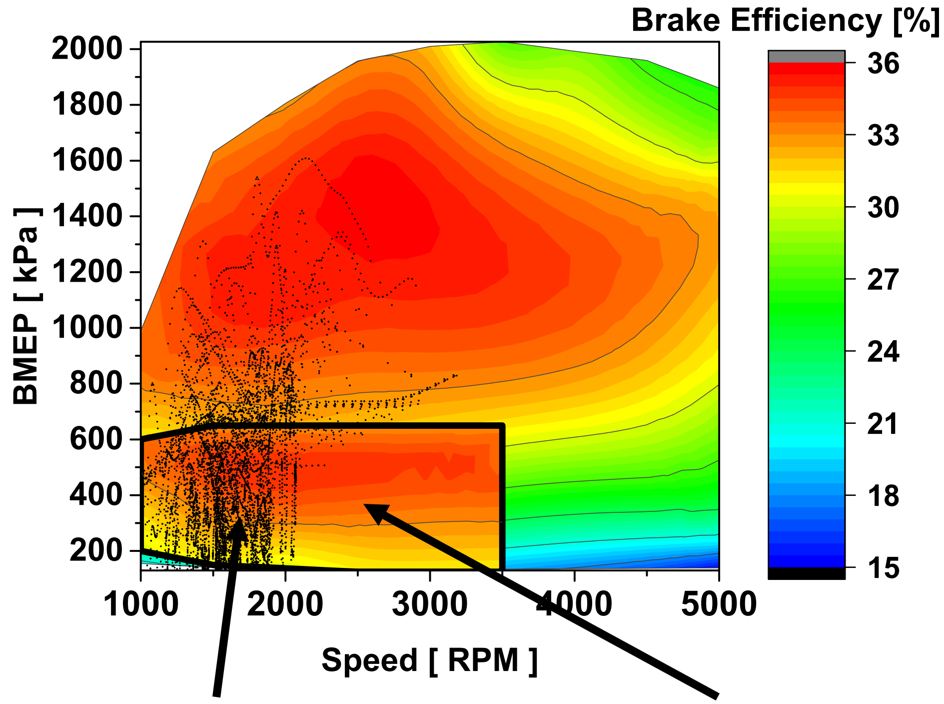
- Identify key fuel properties that impact efficiency for advanced combustion approaches (SI, ACI, MCCI, KC)
- Identify engine parameters that impact engine efficiency, operable range, and emissions
  - Address other key barriers such as transient control, cold operation, combustion noise, high HC and CO emissions, cold exhaust temperature, mode switching, complexity, cost, etc
- Apply systematic tiered screening approach to identify blendstock options that provide key fuel properties
- Develop fundamental understanding of fuel structure-property relationships to guide blendstock identification
- Analysis
  - Identify barriers to widespread commercial introduction related to cost, scale, sustainability, and compatibility
  - Focus on options with viable routes to near-term commercial use (petroleum- or bio-based)
  - Identify blendstocks providing value when produced from biomass
- Leverage capabilities/results from VTO core combustion programs

SI = spark ignition; ACI = advanced compression ignition; MCCI = mixing controlled compression ignition; KC = kinetically controlled

Approach: LD Multimode Research

- Light duty multi-mode efforts combining SI and ACI combustion
  - ACI used at part-load (where engine operates most frequently during drive cycle) for increased efficiency
  - SI used at high load/speed
- Approach maintains power density/ efficiency gains achieved through downsizing and downspeeding

Efficiency Contours



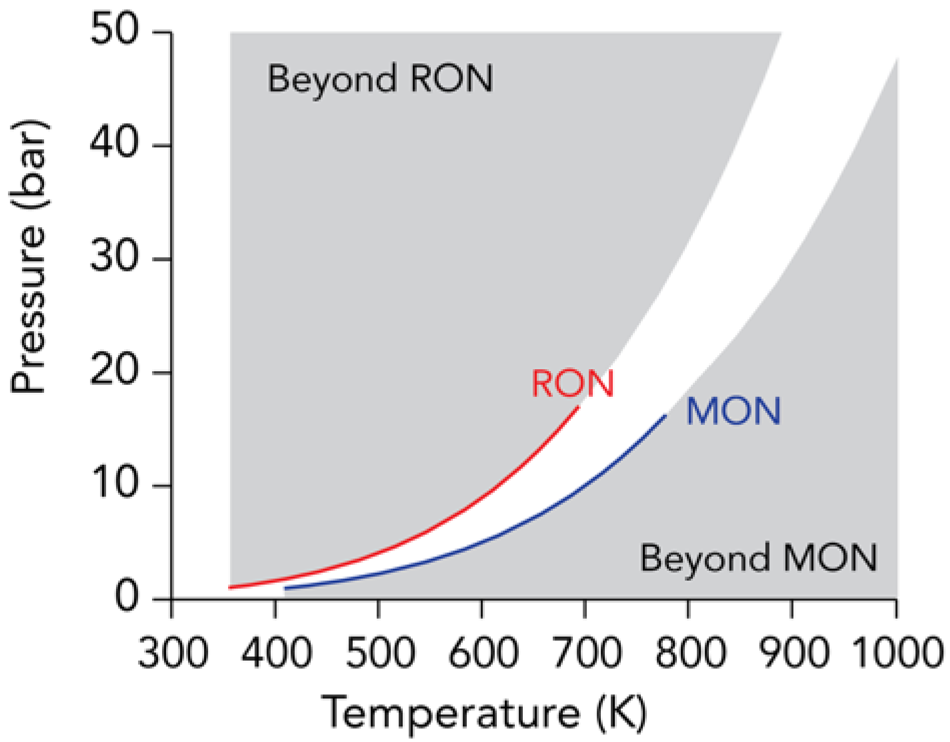
Data from UDDS "City" drive cycle

ACI Multimode With Co-Optima

Approach: Conceptual Foundation

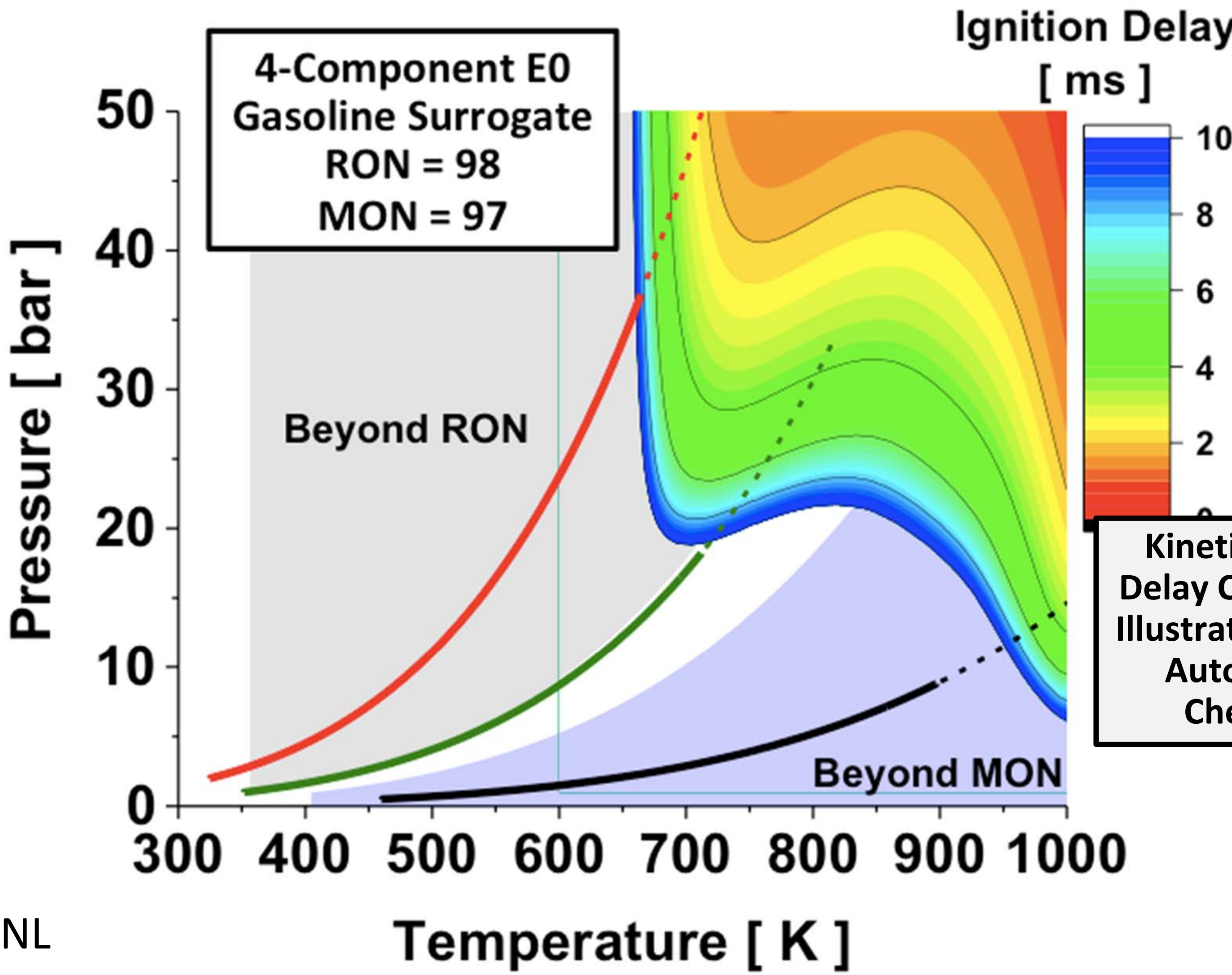
- Most fuel property and engine parameter “knobs” used to control SI and ACI combustion either promote or retard fuel autoignition

- Time history of fuel/air mixture starting with compression stroke fundamentally determines when mixture will autoignite



Approach: Overlay Ignition Kinetics on P,T Trajectory

Initial In-Cylinder Conditions Determine P-T Trajectory
Autoignition Chemistry Depends on Trajectory

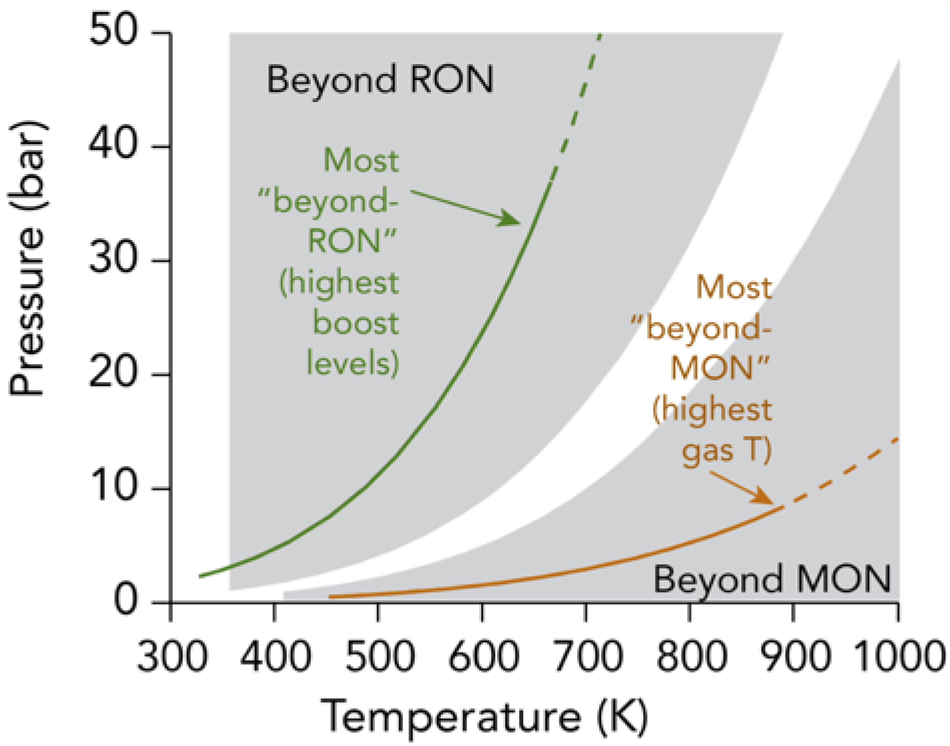


Kinetic Ignition Delay Calculations Illustrate Changing Autoignition Chemistry

Szybist, ORNL

T,P Framework Relevant for SI, ACI, and KC

1. Identify "bookend" P-T trajectories bound most highly boosted SI operation & most aggressive ACI approach
   i. Need to also account for ϕ, EGR, and other key parameters
2. Identify engine experiments that operate at "bookends"; select intermediate conditions; collect data on fuel property and engine parameter impacts
3. Develop simulations that reproduce data across this broad range of conditions
4. Use global sensitivity analysis to identify most important fuel/engine interactions



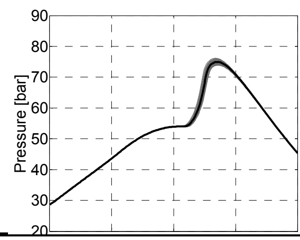
T,P Trajectory Framework Relevant for SI, ACI, and KC

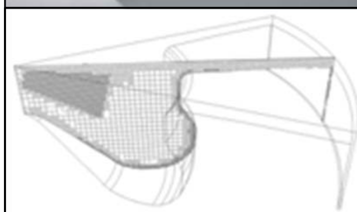
The primary difference between multi-mode ACI and KC is that the former research is constrained to simultaneously allow boosted SI operation at high load; KC is free from this constraint and has opportunity to utilize much wider range of fuel properties

Approach: Global Sensitivity Analysis

- Production GM 1.9 L diesel engine run on gasoline compression ignition mode (GCI)
- CFD used to optimize combustion using CONVERGE
- Global Sensitivity Analysis (GSA) on fuel properties
- 5 fuel-related inputs perturbed
- 400K cells, 8000 cores, 128 cases run in 5 days on Mira

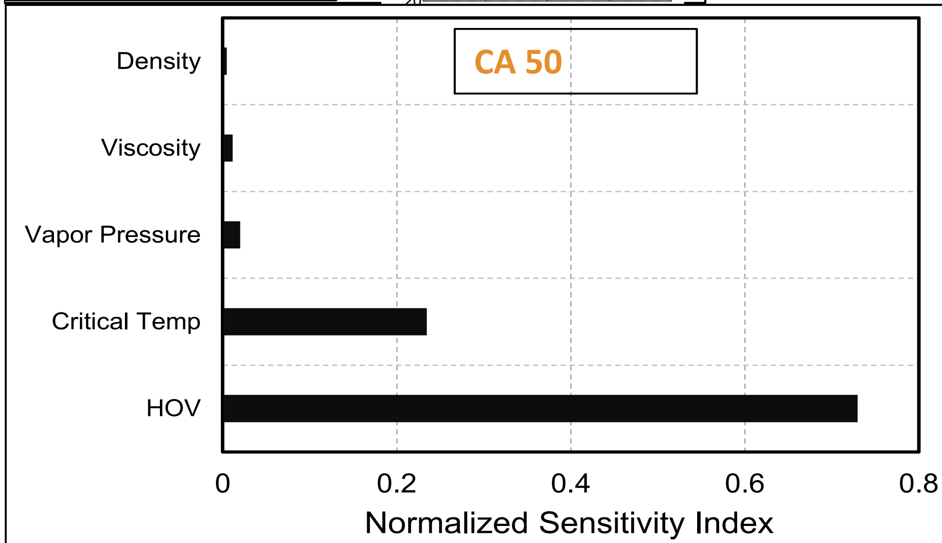
Co-Optima Presentation:
2016 VTO AMR talk
FT040

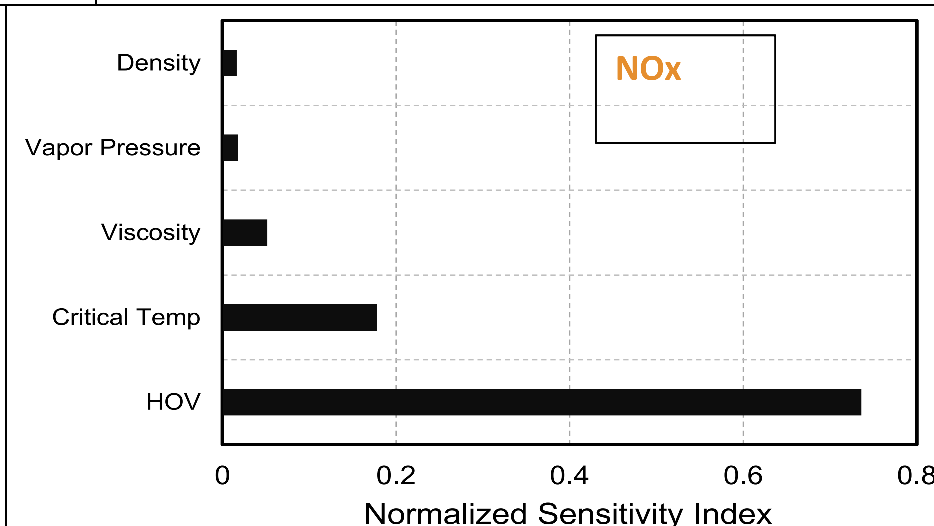




variable	description	baseline	min	max
$T_{(f,crit)}$	fuel critical temperature	540K	530K	550K
Density	fuel density	1.00	0.95	1.05
HOV	fuel heat of vaporization	1.0	0.9	1.1
VP	fuel vapor pressure	1.0	0.9	1.1
Viscosity	fuel viscosity	1.0	0.7	1.3

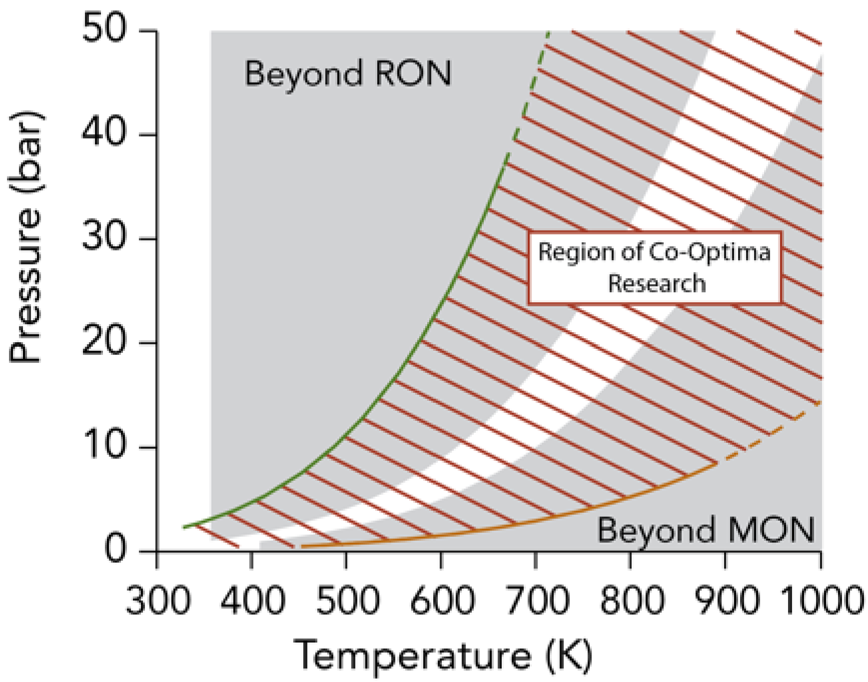
- Fuel properties varied (Monte Carlo)
- Fuel properties have significant influence on CA50



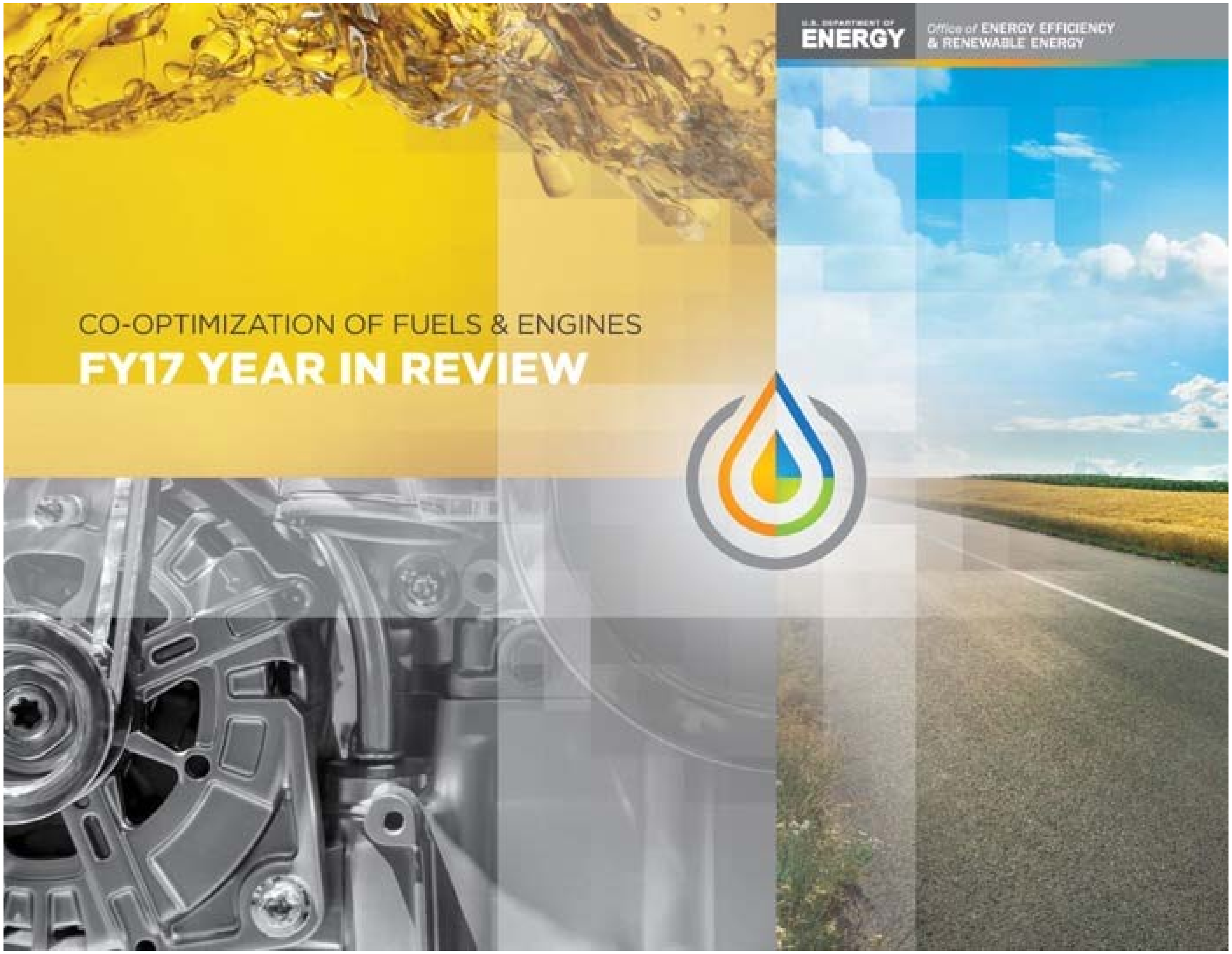


Summary of Approach for SI, ACI, and KC

- Co-Optima LD emphasis shifting from standalone boosted SI to multimode
- Framework developed to identify fuel property/engine parameter impacts across multidimensional thermodynamic and operating space
  - Engine experiments will identify fuel property and engine parameter impacts across P-T space
  - Simulations will be validated against data & used to identify properties/ parameters with strongest impact on efficiency and operability
- Output will be information on efficiency/operability relevant to wide variety of part-load ACI approaches



Major FY17 Accomplishments



https://www.energy.gov/sites/prod/files/2018/04/f50/Co-Optima_YIR2017_FINAL_Web_180417_0.pdf

Major FY17 Accomplishments

1. Established improved merit function quantifying fuel property impacts on boosted SI engine efficiency
2. Screened wide range of blendstocks to assess compatibility with vehicles and infrastructure
3. Determined relationships that describe how chemical structure impacts key fuel properties
4. Conducted preliminary assessment of fuels identified during boosted SI research for compatibility with multimode operation
5. Completed functional group analysis of chemical families for mixing-controlled compression ignition blendstocks
6. Developed improved surrogate kinetic models for gasoline and diesel range fuels
7. Developed new numerical algorithms and computational tools that accelerate R&D
8. Completed integrated, systems-level analyses of blendstocks in relation to economic, technological, market, and environmental factors [1]

[1] Reflects work predominantly funded by BETO and not covered in today's AMR presentations

Response to Previous Year Reviewers' Comments

"The reviewer wondered why this project considers renewable fuels only, and explained that blendstock for oxygenated blending (BOB), which will consist of at least 70% of the future fuels, should also be included in the Co-Optima program. *Co-Optima is focused on identifying blendstocks with the properties needed for advanced LD engines, irrespective of their source (renewables or petroleum). A significant part of our LD work has focused on petroleum BOBs and their blending behavior with candidate blendstocks.*

"The reviewer commented that, if the Governing Hypothesis is used as a surrogate for the approach, it assumes that higher engine efficiency is needed for some of the advanced combustion regimes. The reviewer questioned whether really impressive efficiencies had not already been demonstrated for several advanced combustion regimes with market fuels. The reviewer suggested that the barriers to those concepts were limited operating range, transient control, cold operation, combustion noise, high hydrocarbon (HC) and carbon monoxide (CO) emission, cold exhaust temperature, mode switching, complexity, cost, and other factors. The reviewer stated that from this overview presentation one does not get the impression that Co-Optima will focus on these barriers, but instead will continue to pursue high engine efficiencies, primarily while expanding operating range." *We agree that the barriers highlighted by the reviewer are significant impediments to market viability of advanced combustion approaches, and these barriers are indeed the focus of Co-Optima research. We will emphasize the importance of these in future communications.*

The reviewer commented that working more closely with energy companies and refining stakeholders would enable the team to look for more value-added pathways. For instance, some of the fuels being looked at could be co-produced in the refinery and be a win-win for the auto and oil companies. *We agree and have taken efforts to increase our engagement with energy companies and refiners to identify opportunities to co-produce blendstocks and improve their economic viability*

Collaboration/Coordination with Other Institutions

- Collaboration across nine national laboratories and two DOE offices
- Eight university teams joined initiative in FY17
  - University/national lab efforts are being tightly integrated
  - Each team assigned a national lab “mentor” to facilitate integration and coordination
- Industry FOA issued April 2018
  - Intent is to integrate FOA activities with national lab and university efforts
- Stakeholders (145 individuals from 86 organizations)
  - External advisory board (advising national labs, not DOE)
  - Monthly telecons with technical and programmatic updates
  - One-on-one meetings and conference presentations

Remaining Challenges and Barriers

- Formally complete boosted SI work; ensure results inform external debate on new fuels/engines
- Developing fundamental autoignition understanding for blendstocks of diverse composition under full boosted SI operating pressure range
- Developing combined experimental/ modeling approach to identifying fuel property/engine parameter impacts for wide array of ACI approaches
- Identifying ability of new MCCI blendstocks to reduce PM and reduce cost/complexity of emission control systems
- Identifying extent of fuel property effects on ducted fuel injection (DFI)
- Identifying key fuel properties/engine parameters that provide efficiency, power density, and wide operability for kinetically controlled combustion
- Developing effective control strategies effective aftertreatment capable of low-temperature NOx/PM control
- Developing high-fidelity, computationally efficient kinetic and fluid dynamic models and high quality experimental data to validate
- Developing improved analysis tools that assess process economics, refinery integration of new blendstocks, technology readiness, sustainability, and infrastructure compatibility to guide R&D efforts
- Maintaining strong stakeholder engagement

Proposed Future Research

- Identify/define (new) fuel properties that impact engine performance under ACI operation
- Identify fuel property/engine parameters that:
  - Improve ACI operability (simplify transient control/mode switching, expand speed/load range, improve cold start/low load performance)
  - Reduce ACI combustion noise and engine-out emissions
- Develop more fundamental understanding of non-linear fuel blending effects
- Reduced HD engine-out NOx and PM emissions (including cold start) while preserving high efficiency
- Identifying MCCI blendstocks that significantly reduce emissions while maintaining (or improving) other key properties
- Identify fuel property/engine parameters that expand speed and load range of KC regime while reducing engine-out HC/CO emissions and combustion noise

Much more detail will be presented in subsequent presentations

Summary

Relevance

- Better integration of fuels and engines research critical to accelerating progress towards economic development, energy security, and emissions goals

Approach

- Focused on identifying fuel property/engine parameters that improve efficiency, operability, and emissions performance
- Integrate fuels (BETO) and engines (VTO) R&D: combine experiment, modeling, analysis

Technical Accomplishments

- Major accomplishments span light-duty (boosted SI and multimode) and medium/heavy-duty research projects (experiment, modeling, simulation, analysis).
- Many additional accomplishments will be discussed in detail in subsequent presentations

Proposed Future Research

- Identify fuel property/engine parameters that improve ACI operability and reduce combustion noise/engine-out emissions for LD multimode applications
- Reduce HD engine-out NOx/PM emissions (including cold start) while preserving high efficiency

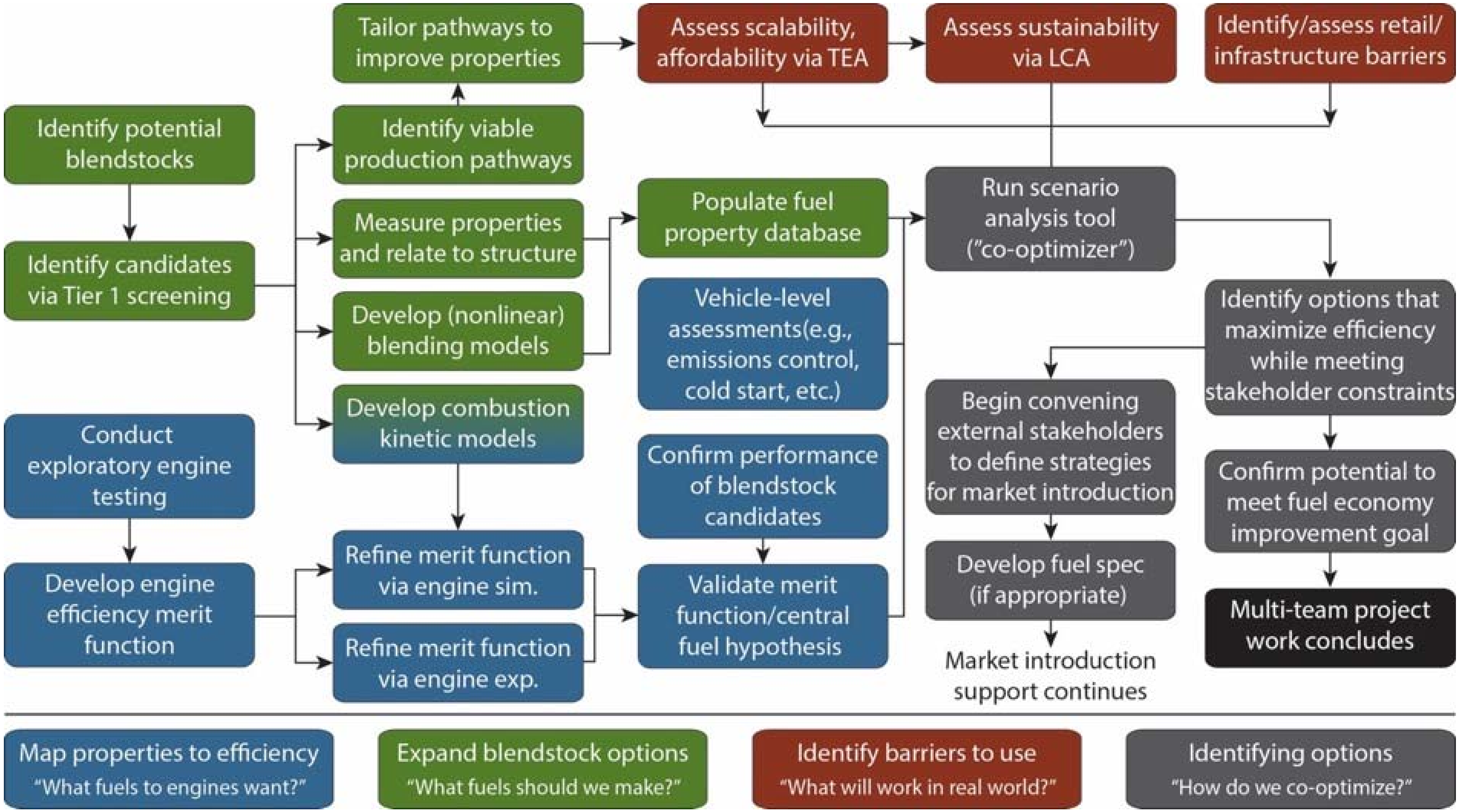
Collaborations

- Strong industry engagement including industry-led external advisory board, monthly stakeholder phone calls, and annual team meeting
- Collaboration across nine national laboratories, two DOE offices, and thirteen universities

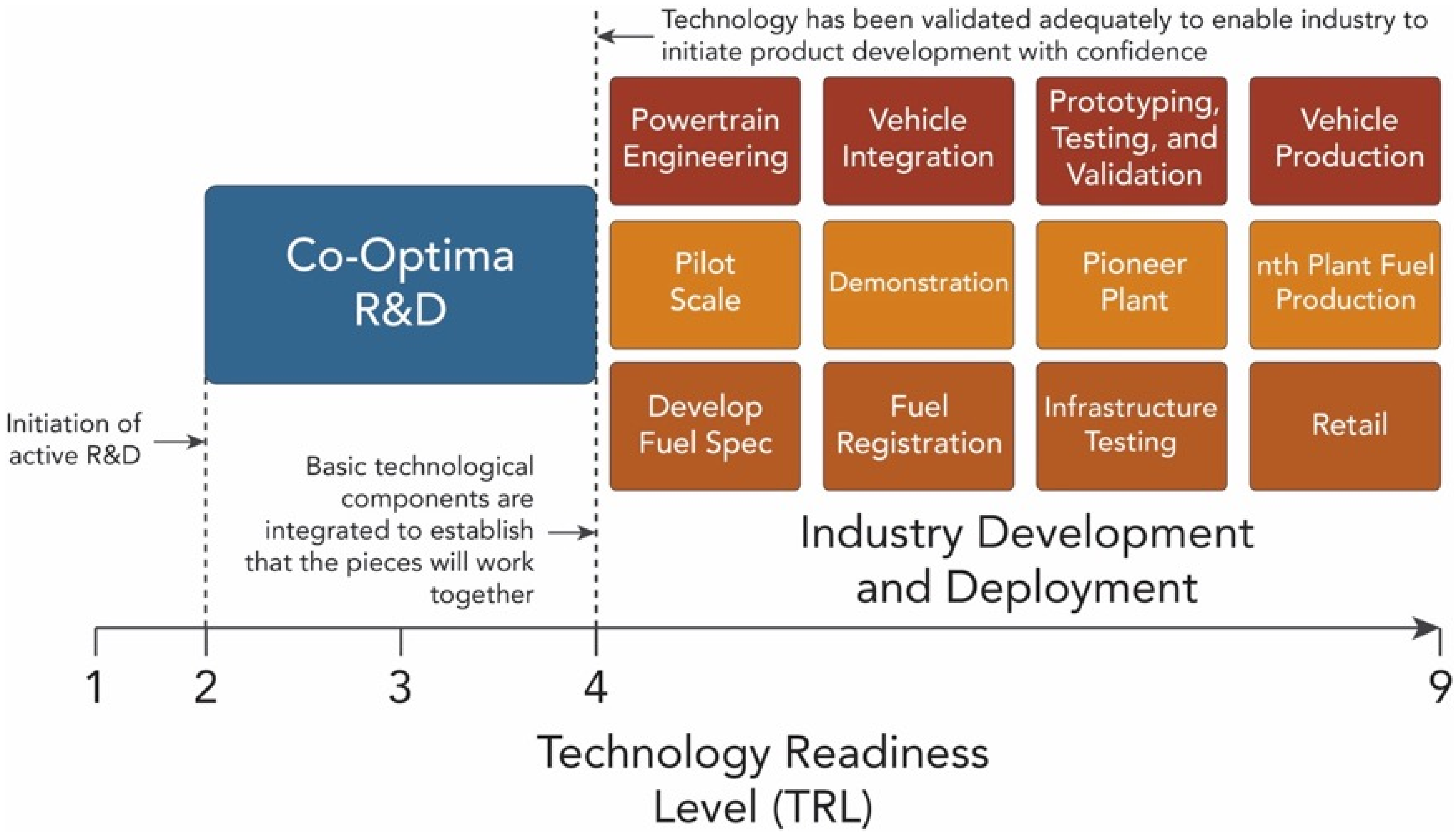
Technical Back-Up Slides

(Include this “divider” slide if you are including back-up technical slides **[maximum of five]**. These back-up technical slides will be available for your presentation and will be included in the USB drive and Web PDF files released to the public.)

Technical Approach



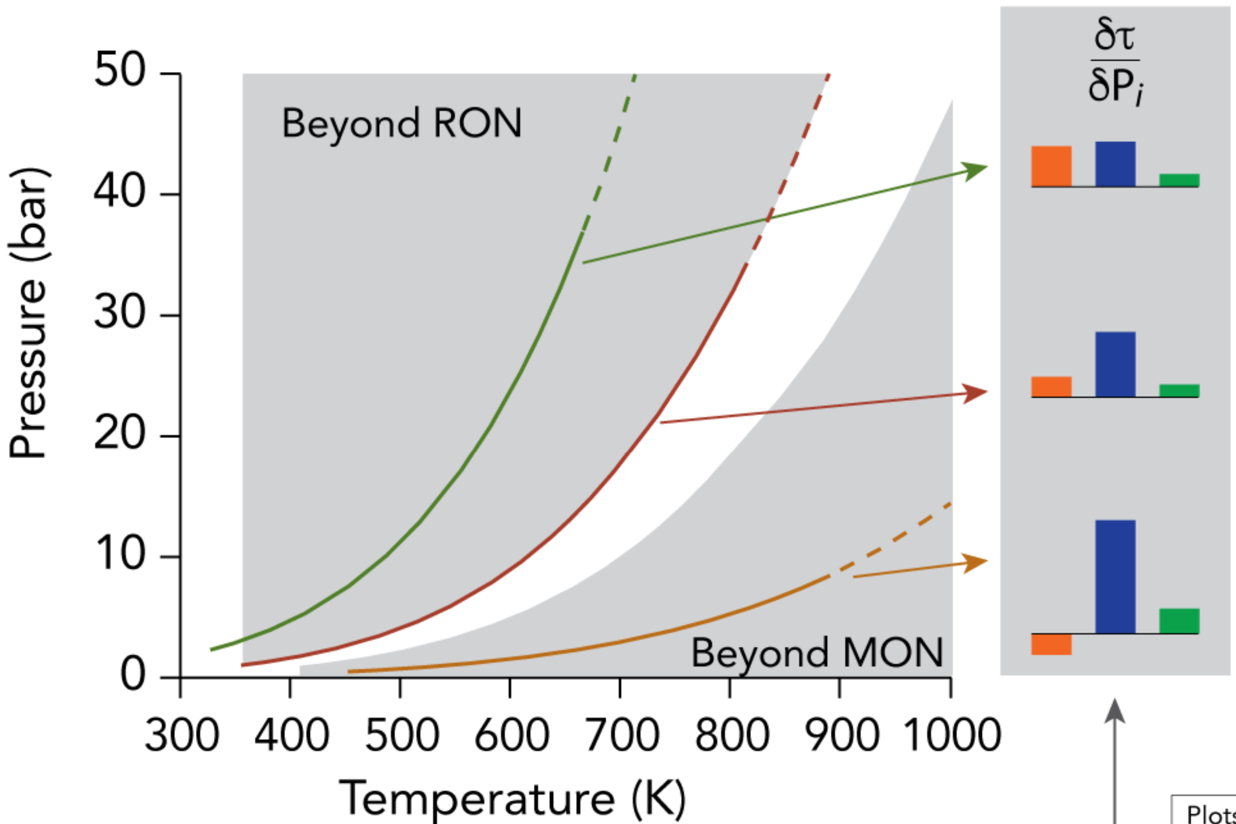
Engagement with Industry



Partners – University Teams

1. Yale Univ./Penn State Univ.
   Measure sooting tendencies of various biofuels and develop emission indices
2. Univ. Michigan
   Engine combustion model simulating combustion duration, flame speed, and pressure development
3. Louisiana State Univ./Texas A&M/Univ. Connecticut
   Models and metrics for predicted engine performance
4. Univ. Alabama
   Combustion properties of biofuels and blends under realistic (ACI) engine conditions
5. Cornell University/UC San Diego
   Combustion characteristics of several diesel/biofuel blends
6. MIT/Univ. Central Florida
   Detailed kinetic models for several biofuels
7. Univ. Michigan-Dearborn/Oakland Univ.
   Miniature ignition screening rapid compression machine
8. Univ. Central Florida
   Measure and evaluate fuel spray atomization, flame topology, volatility, viscosity, soot/coking, and compatibility

Approach: Identifying Fuel/Engine Impacts



Validated simulations and computational approaches will be used to identify impacts of fuel properties and engine parameters on variables such as ignition timing (e.g,. CA50).

These impacts will vary with PT trajectory and other fuel variables (ϕ, dilution, etc) and engine parameters (CR, turbulence, etc)

Combined experimental and simulation approach provides consistent framework to identify fuel and engine impacts and tradeoffs on key metrics such as efficiency, operability, etc.

Plots represent impact of key variables τ (e.g., CA50 timing) on fuel properties P_i (e.g., RON, S, HOV) and engine parameters (e.g., turbulence intensity, CR, etc)