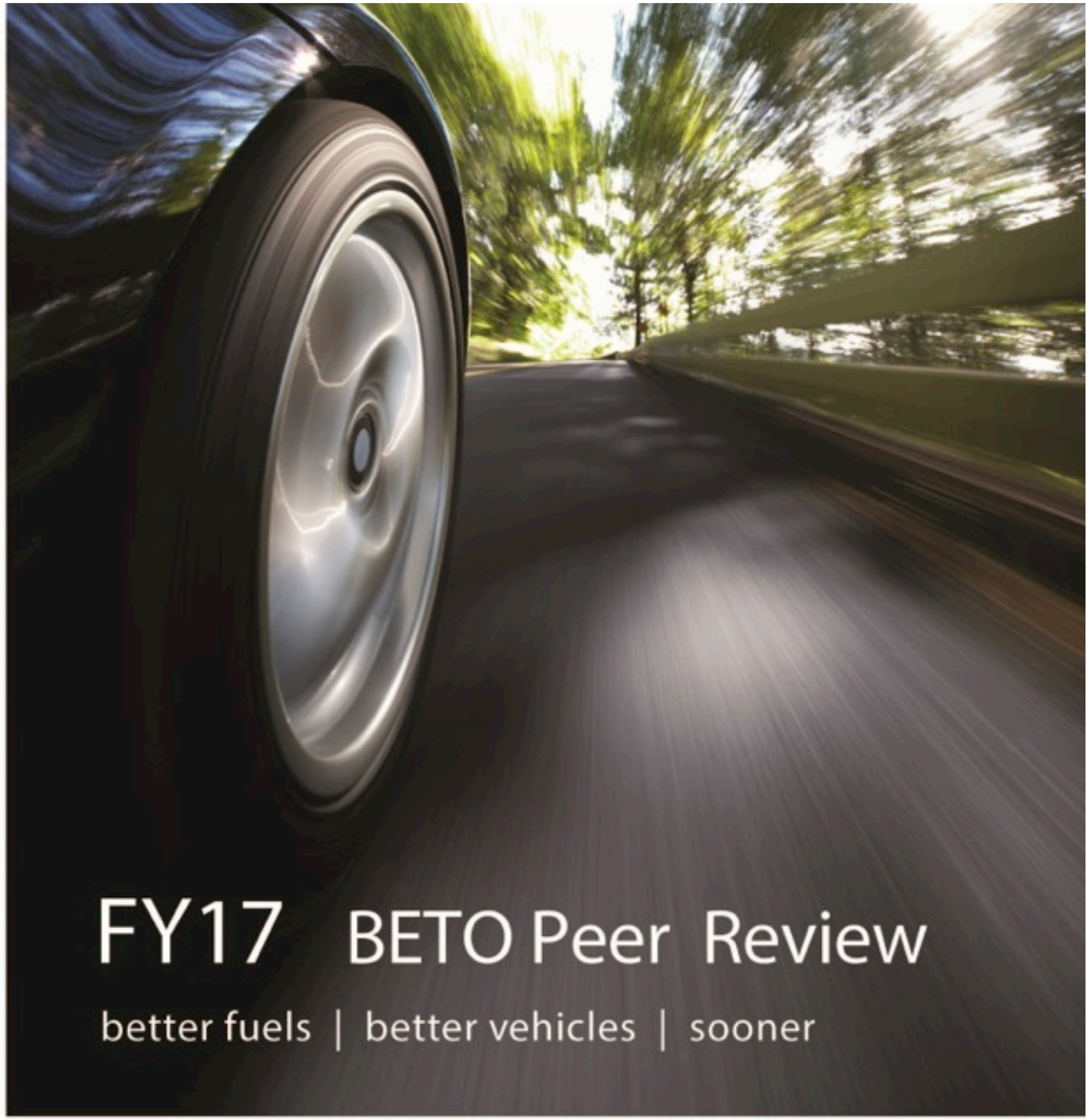
Co-Optimization of
Fuels & Engines

Introduction

John Farrell, NREL
John Holladay, PNNL

8 March 2017



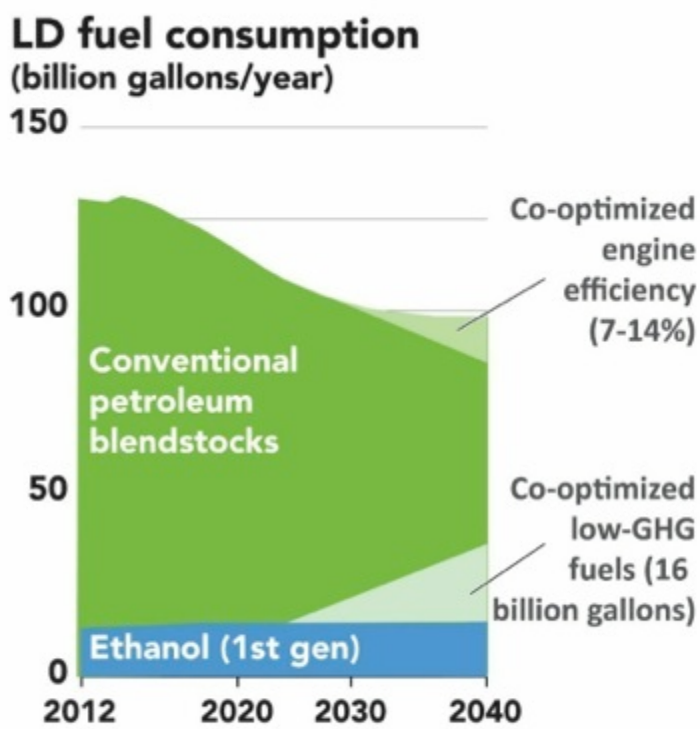
Acronym List

AED	Advanced Engine Development Team
ACI	Advanced Compression Ignition
ANL	Argonne National Laboratory
AOP	Annual Operating Plan
ASSERT	Analysis of Sustainability, Scale, Economics, Risk and Trade Team
BETO	Bioenergy Technologies Office
BOB	Blendstock for oxygenated blending
COLT	Co-Optima Leadership Team
CI	Compression Ignition (combustion)
EAB	External Advisory Council
EERE	Energy Efficiency and Renewable Energy Office
FE	Fossil Energy (content)
FP	Fuel Properties Team
FOA	Funding Opportunity Announcement
GHG	Greenhouse gas
HOV	Heat of Vaporization
HPF	High Performance Fuels Team
INL	Idaho National Laboratory
IP	Intellectual Property
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
LCA	Lifecycle Analysis
MT	Market Transformation Team
NREL	National Renewable Energy Laboratory
ORNL	Oak Ridge National Laboratory
POC	Point of Contact
PNNL	Pacific Northwest National Laboratory
R&D	Research and Development
RON	Research Octane Number
SI	Spark Ignition (combustion)
SOT	State of Technology
SNL	Sandia National Laboratory
TEA	Techno-economic analysis
TK	Tool Kit and Simulation Team
TRL	Technology Readiness Level
VTO	Vehicle Technologies Office

1 Project Overview

Goal and Outcomes

Goal: 30% per vehicle petroleum reduction through efficiency and displacement



Outcome: Market driver for biofuels

1. Science enabling targeted highly efficient combustion modes for OEMs
2. Identification of bio-blendstocks that provide the required critical fuel properties
3. Property-based specification for new fuels
4. Market viability, environmental sustainability, and job assessment for fuel-engine system
5. Scenario analysis tool that combines data, information, and assessments and weights based on stakeholder success criteria
6. Cars and trucks that operate with higher efficiency and lower emissions than possible today

Linking EERE Vehicle Technologies and Bioenergy Technologies Offices

Quad Chart

Timeline

Project Start Date: 10/1/2015
Project End Date: 9/30/2018
Percent Complete: 42%

Budget

	FY16 Budget	FY17 Budget	FY18 Budget
BETO	$14,000	$12,000	$12,000
VTO	$12,000	$12,500	$12,500
Total	$26,000	$24,500	$24,500

Partners

ANL, INL, LANL, LBNL, LLNL, NREL, ORNL, PNNL, SNL

Barriers

It-D Engines not optimized for Biofuels: Identifying fuel properties engines need and bio-blendstocks that provide those properties

Ct-I Product Finishing Acceptability and Performance: Blending studies identifying non-linear behavior and producing real samples

Im-H Awareness and acceptance of biofuels as alternative: Identifying bio-blendstocks that provide performance over petroleum (creating market pull)

Im-C Codes, standards, and approval for use: Developing property-based fuel specification, identifying UL standards, etc.

Mm-B: Inconsistent or Competing Policies: Mapping stakeholder needs to policies

At-C Data Availability across the Supply Chain and At-A Comparable, Transparent, and Reproducible Analyses: Providing transparent info across stakeholder group (value chain)

Budget by Lab (k$)*

Lab	FY16 Budget	FY17 Budget	FY18 Budget
ANL	$840	$900	$900
INL	$1,300	$540	$540
LANL	$700	$710	$710
LBNL	$1,100	$860	$860
LLNL**	$0	$0	$0
NREL	$4,100	$4,200	$4,200
ORNL	$900	$670	$670
PNNL	$3,100	$2,400	$2,400
SNL	$2,300	$1,600	$1,600
Total	**$14,000**	**$12,000**	**$12,000**

* Only funding from BETO shown; ** VTO funding only

Budget by Team (k$)*

Teams	FY16 Budget	FY17 Budget	FY18 Budget
Task A: High Performance Fuels	$9,500	$7,100	$7,100
Task B: ASSERT	$2,200	$2,200	$2,200
Task C: Market Transformation	$1,400	$1,400	$1,400
Task D: Co-Optima Leadership Team	$1,200	$1,100	$1,100
Total	**$14,000**	**$12,000**	**$12,000**

* Only funding from BETO shown

Motivation

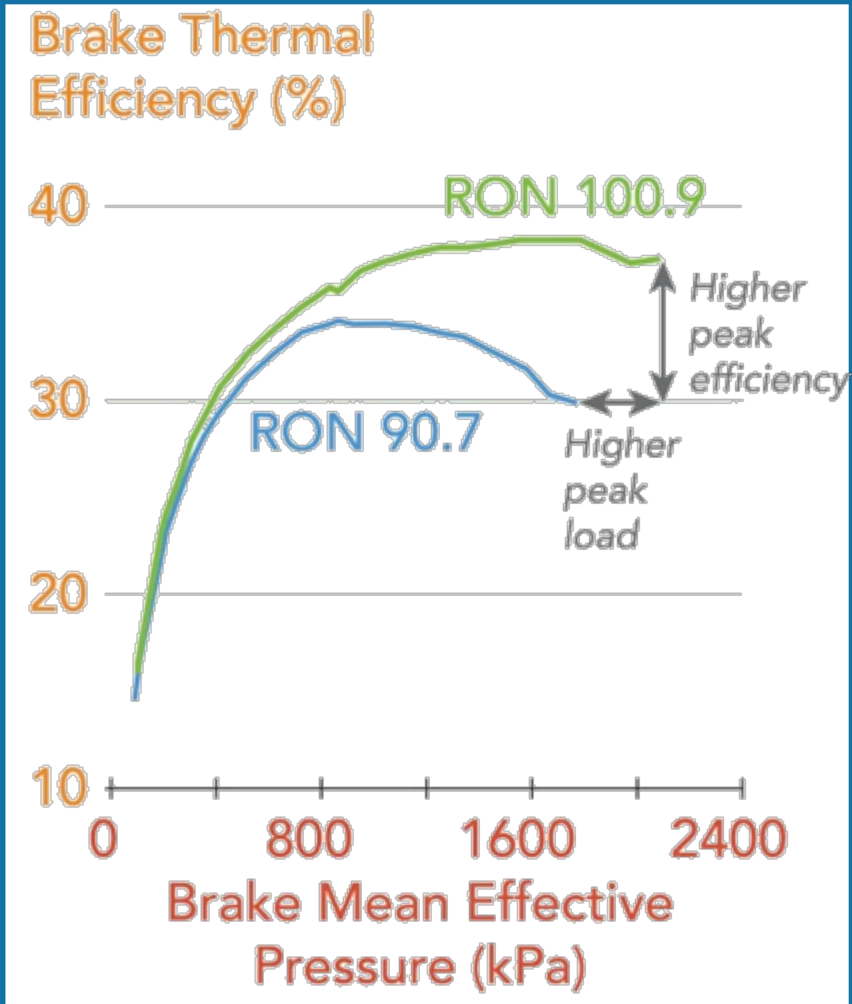
Today's fuels do not allow engines to operate at their peak efficiency

New fuels, with targeted properties, can enable significantly higher efficiency and fuel economy

Intend to exploit unique properties available from biomass-derived molecules/mixtures to produce higher-value blendstocks

"Better fuels, better vehicles, sooner"

Engine R&D **Fuel R&D**



Engine: Ford Ecoboost 1.6L 4-cylinder, turbocharged, direct-injection, 10.1 CR source: C.S. Sluder, ORNL

2 Approach (Management)

How We Are Organized

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

A formal "Roles and Responsibilities" document has been developed that is regularly updated and available on the Co-Optima team SharePoint site

Leadership

Board of Directors

Senior leadership (EERE and labs)

DOE

- Rueben Sarkar (EERE)
- Jonathan Male (BETO)
- Michael Berube (VTO)

Labs (Assoc. Lab Directors)

- Johney Green (NREL)
- Moe Khaleel (ORNL)
- Jud Virden (PNNL)
- Marianne Walck (SNL)

Leadership Team

Leaders from VTO, BETO and labs

DOE

- Alicia Lindauer (BETO)
- Kevin Stork (VTO)

Labs

- John Farrell, Lead (NREL)
- John Holladay, BETO (PNNL)
- Robert Wagner, VTO (ORNL)

External Advisory Board (EAB)

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, not individual companies
- Entire board meets twice per year; smaller groups meet on targeted issues

Six Technical Teams

HPF

High Performance Fuels

Identify promising bio-derived blendstocks, develop selection criteria for fuel molecules, and identify viable production pathway

ASSERT

Analysis of Sustainability, Scale, Economics, Risk, and Trade

Analyze energy, economic, and environmental benefits at U.S. economy-level and examine routes to feedstock production at scale through existing biomass markets

MT

Market Transformation

Identify and mitigate challenges of moving new fuels and engines to markets and engage with full range of stakeholders

Teams are staffed with world-leading experts across nine national labs to provide the diverse expertise needed to tackle broad challenges

Six Technical Teams

TK	**Modeling and Simulation Toolkit**	Extend the range, confidence, and applicability of engine experiments by leveraging high-fidelity simulation capabilities
AED	**Advanced Engine Development**	Quantify interactions between fuel properties, engine design, and operating strategies – enabling optimal design of efficient, emission-compliant engines
FP	**Fuel Properties**	Identify critical properties and allowable ranges, systematically catalogue properties, and predict fuel-blending behavior

Teams are staffed with world-leading experts across nine national labs to provide the diverse expertise needed to tackle broad challenges

Team Leads and Roles


HPF

Dan Gaspar
(PNNL)


TK

Matt McNenly
(LLNL)


ASSERT

Jennifer Dunn
(ANL)


AED

Paul Miles
(SNL)


MT

Doug Longman
(ANL)

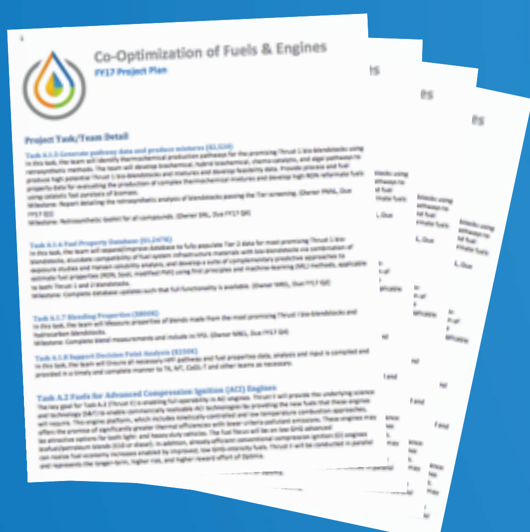

FP

Jim Szybist
(ORNL)

Roles and Responsibilities: Plan yearly AOPs, evaluate team performance, report monthly highlights and quarterly progress, communicate across teams, team-building

Project Plan and Program Management

A project plan is developed annually to organize the work of the teams across the individual labs' annual operating plans (AOPs)

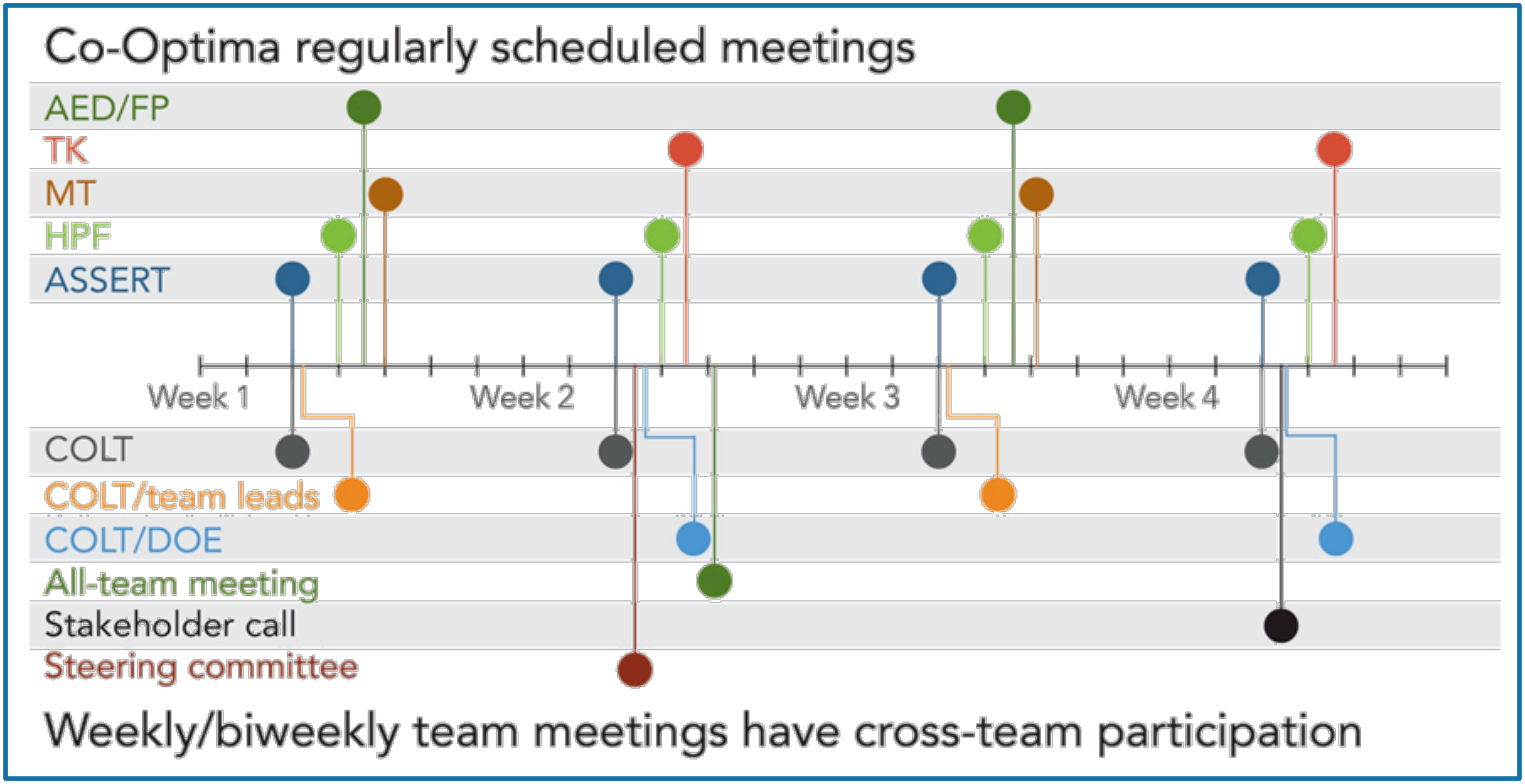


A full-time project manager is utilized to ensure task coordination and milestone completion

Hierarchy of Milestones

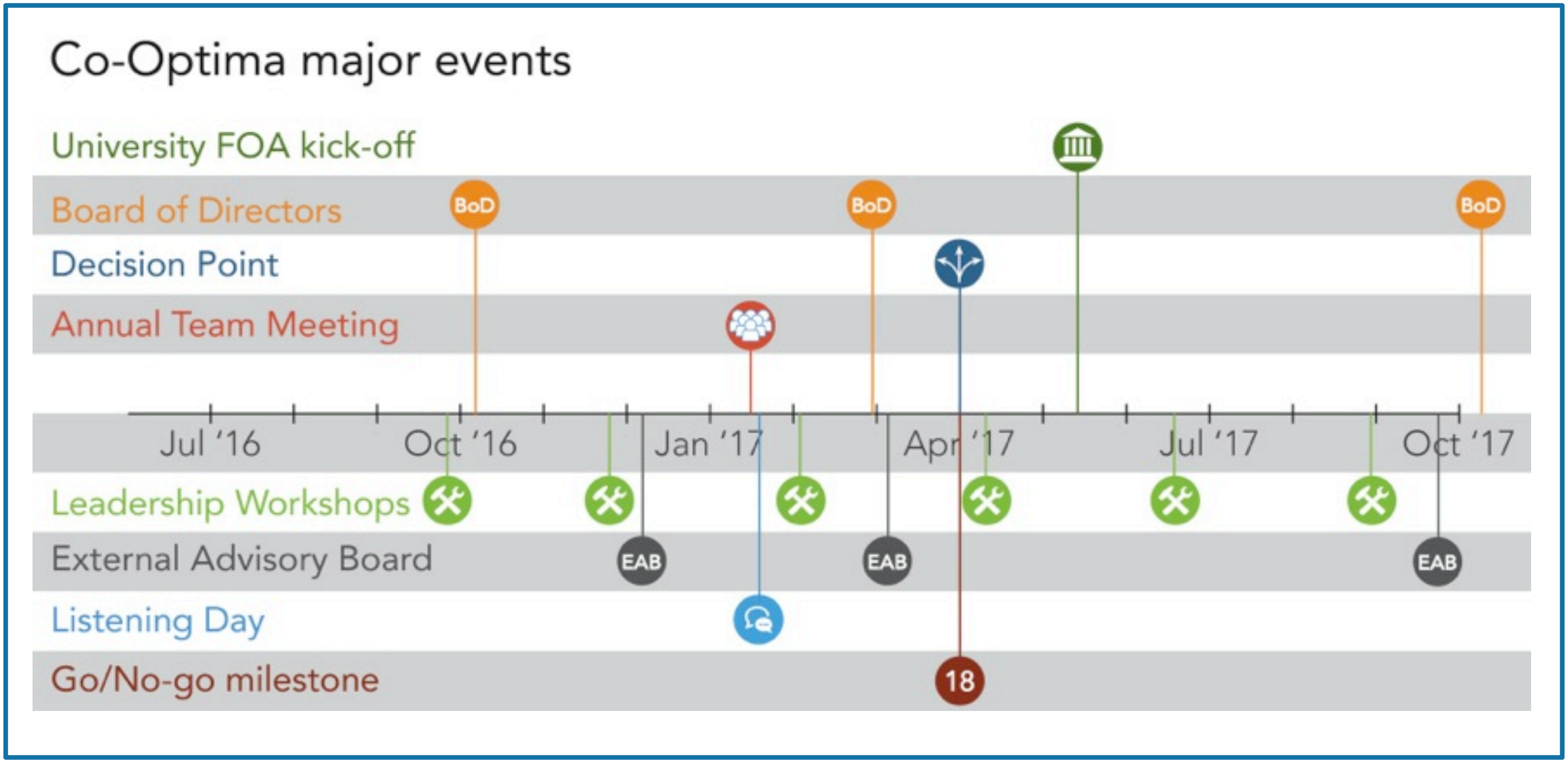
Milestone Type	FY17 count	Description	Purpose
DOE Dashboard	4	High-impact multi-lab accomplishments reported quarterly to Senior DOE Leadership	Ensure most strategic goals are being met and project is on-track at a high level
Team	28	Key multi-lab technical team accomplishments reported quarterly to Leadership Team	Facilitate coordination and progress tracking by Co-Optima Leadership Team
Task	72	Single-lab accomplishments reported quarterly to VTO/BETO technology managers	Ensure progress at the individual task level, typically in support of team milestone

Communication and Coordination



AED/FP: Advanced Engine Development/Fuel Properties; TK: Modeling and Simulation Toolkit MT: Market Transformation; HPF: High Performance Fuels; ASSERT: Analysis of Sustainability, Scale, Economics, Risk, and Trade; COLT: Co-Optima Leadership Team

Engagement and Stewardship



Go/No-Go Milestone (3/31/2017)

Milestone

1. Identify at least three bio-blendstocks that have passed Tier 2 screening as a Thrust I blend component
2. Demonstrate in an engine that a fuel blended with one of these components provides matching engine performance to a petroleum-derived fuel

Criteria

1. Demonstrate sufficient progress on Thrust I R&D to justify continued funding
2. Establish validity of the research approach
3. Determine if the project scope needs to be redefined

Decision Point (March 2017)

Purpose:
Define relative Thrust I and Thrust II research priorities

Timing coincides with end of Thrust I fuel discovery (candidate identification) and preliminary evaluation

Key questions: What essential fuel R&D is needed in Thrust I and are there candidates ready for further scale-up R&D?

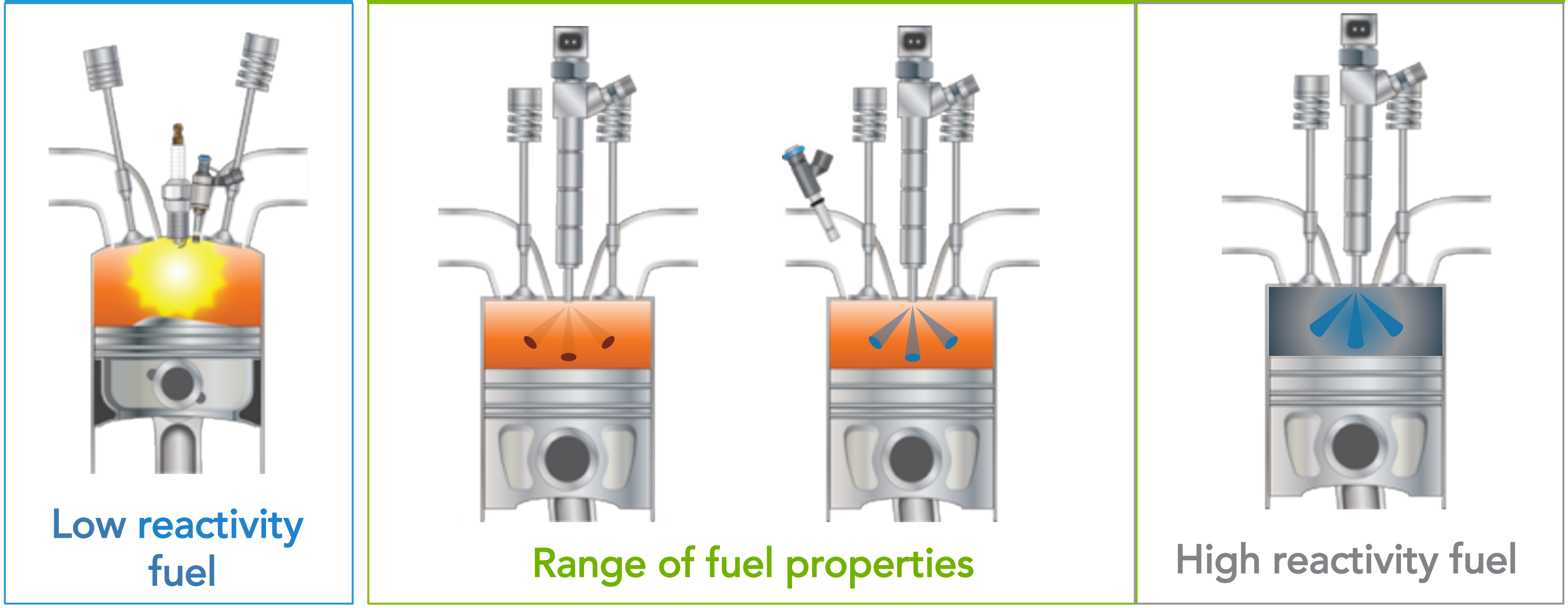
The team will have:

- Surveyed bio-blendstock options available
- Evaluated their physical and chemical properties
- Measured and/or predicted their engine performance
- Assessed their sustainability, scalability, and affordability metrics
- Evaluated infrastructure / retail barriers to their use
- Shared this information broadly with stakeholders / scientific community

2 Approach (Technical)

Two Parallel R&D Thrusts

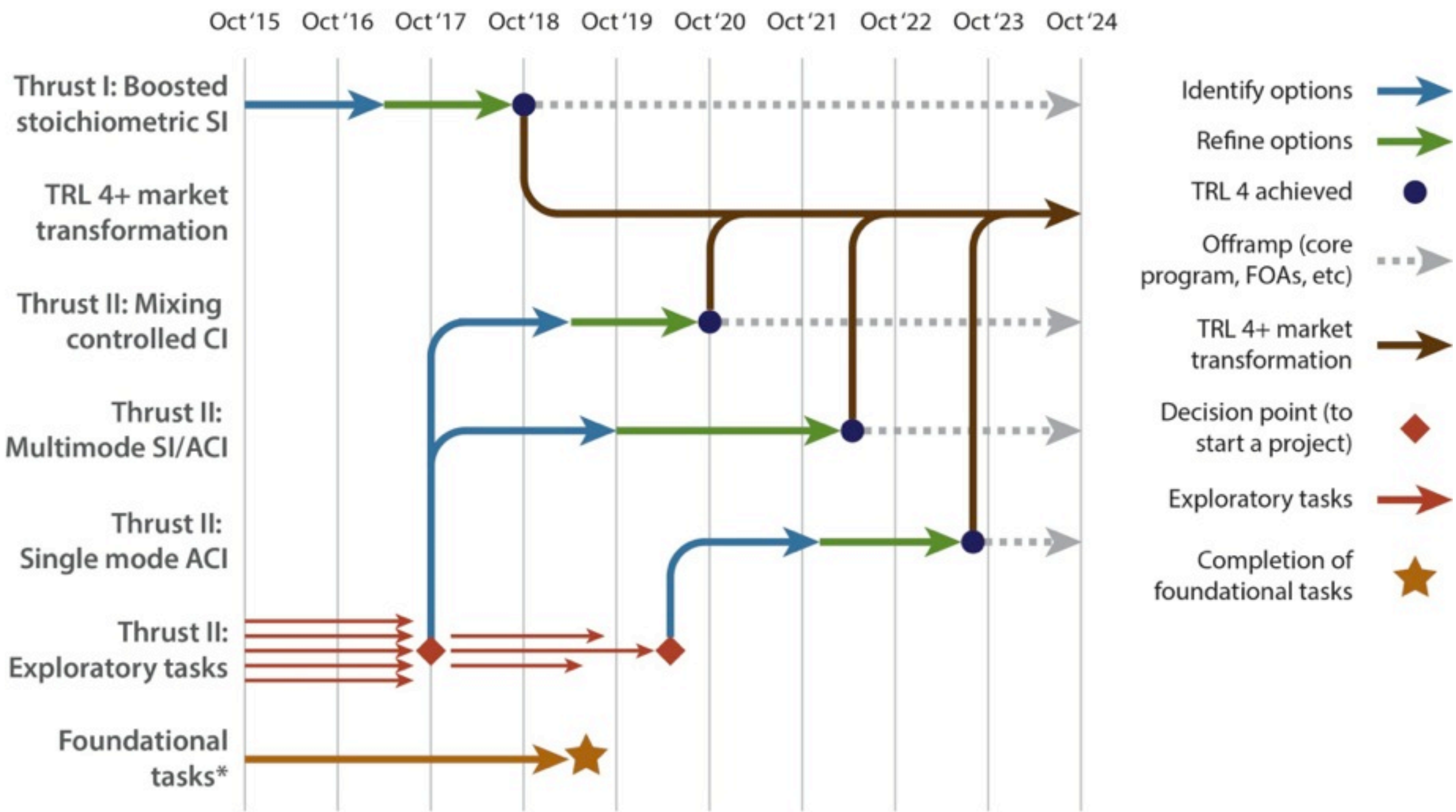
Thrust I: Spark Ignition (SI)	Thrust II: Advanced Compression Ignition (ACI) Kinetically controlled and compression-ignition combustion



Thrust I – Improve near-term efficiency of spark-ignition (SI) engines through identification of fuel properties and engine design parameters that maximize performance

Thrust II – Identify fuel properties that enable advanced compression ignition (ACI) engines, providing a longer-term, higher-impact solutions with greater engine efficiency/emissions, petroleum reduction, and biofuels market pull

Notional Timeline



* Development of fuel property database, analysis framework, co-optimizer development, fuel blending models, etc.

Governing Hypotheses

Central Engine Hypothesis

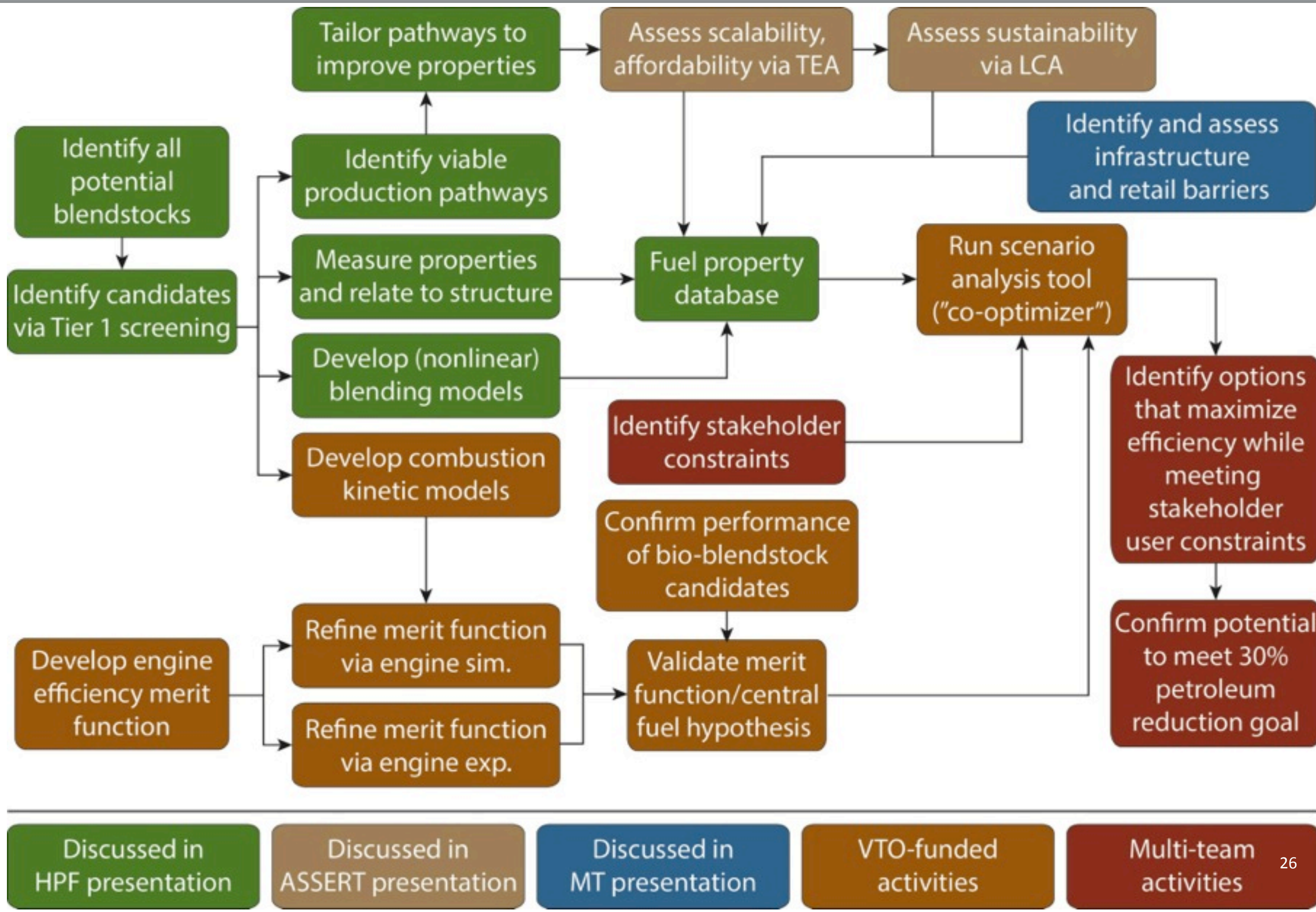
There are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range

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

The governing hypotheses provide a framework to pursue engine and fuel discovery and development research simultaneously

Technical Approach



Key Elements of Property-Based Approach

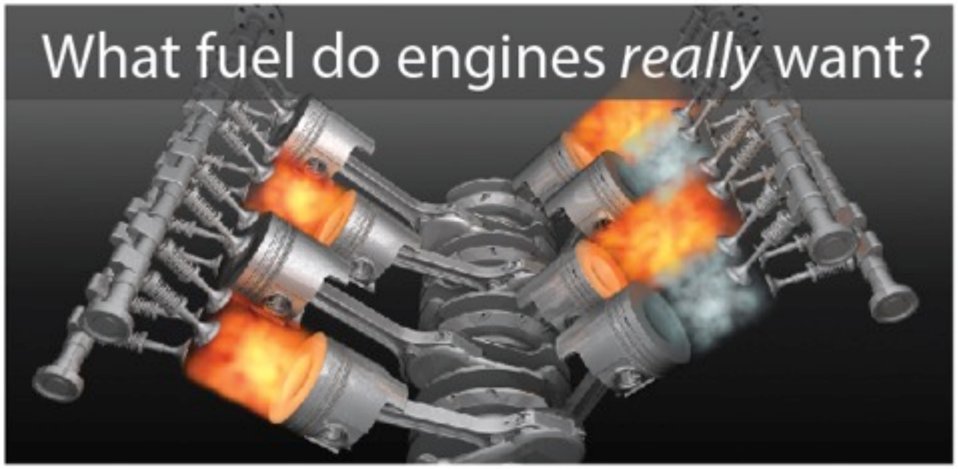
Co-Optima is focused on identifying fuel properties that optimize engine performance, independent of composition,* allowing the market to define the best means to blend and provide these fuels

* We are not going to recommend specific "recipes" for commercial use

However, at the same time, we are pursuing a systematic study of bio-derived molecules and mixtures to identify bio-blendstocks that provide preferential properties

Objective is to supplement our extensive understanding of petroleum-derived blendstocks

Primary Technical Challenges



Identifying the key fuel properties that impact efficiency for advanced spark ignition and compression ignition combustion approaches

Identifying fuel formulations that provide key fuel properties and take advantage of unique properties of bio-blendstocks

Technical Challenge 1

What fuels do engines really want?

Identify fuel properties that maximize engine performance

Efficiency Merit Function Approach

RON | Octane Sensitivity | HOV

$$\text{Merit} = \alpha \cdot [\text{RON} - 92] - \beta \cdot K \cdot [S - 10] + \gamma \cdot \text{ON} \cdot [\text{HOV} - 415] + \delta \cdot [\text{HOV} - 415]$$

$$+ \varepsilon \cdot [S_L - 46] - \text{LFV}_{150} - H(\text{PMI} - 2.0)[\zeta + 0.5(\text{PMI}-2.0)]$$

Flame Speed | Distillation | Particulate Emissions

- Research framed around "efficiency merit function" that estimates potential engine efficiency gains associated with key fuel properties
- Merit function establishes fuel property relationships in a systematic and comprehensive way that guides fuel R&D
- Approach facilitates knowledge transfer at unprecedented bandwidth and scale
- Each combustion approach will have unique merit function

VTO-funded work

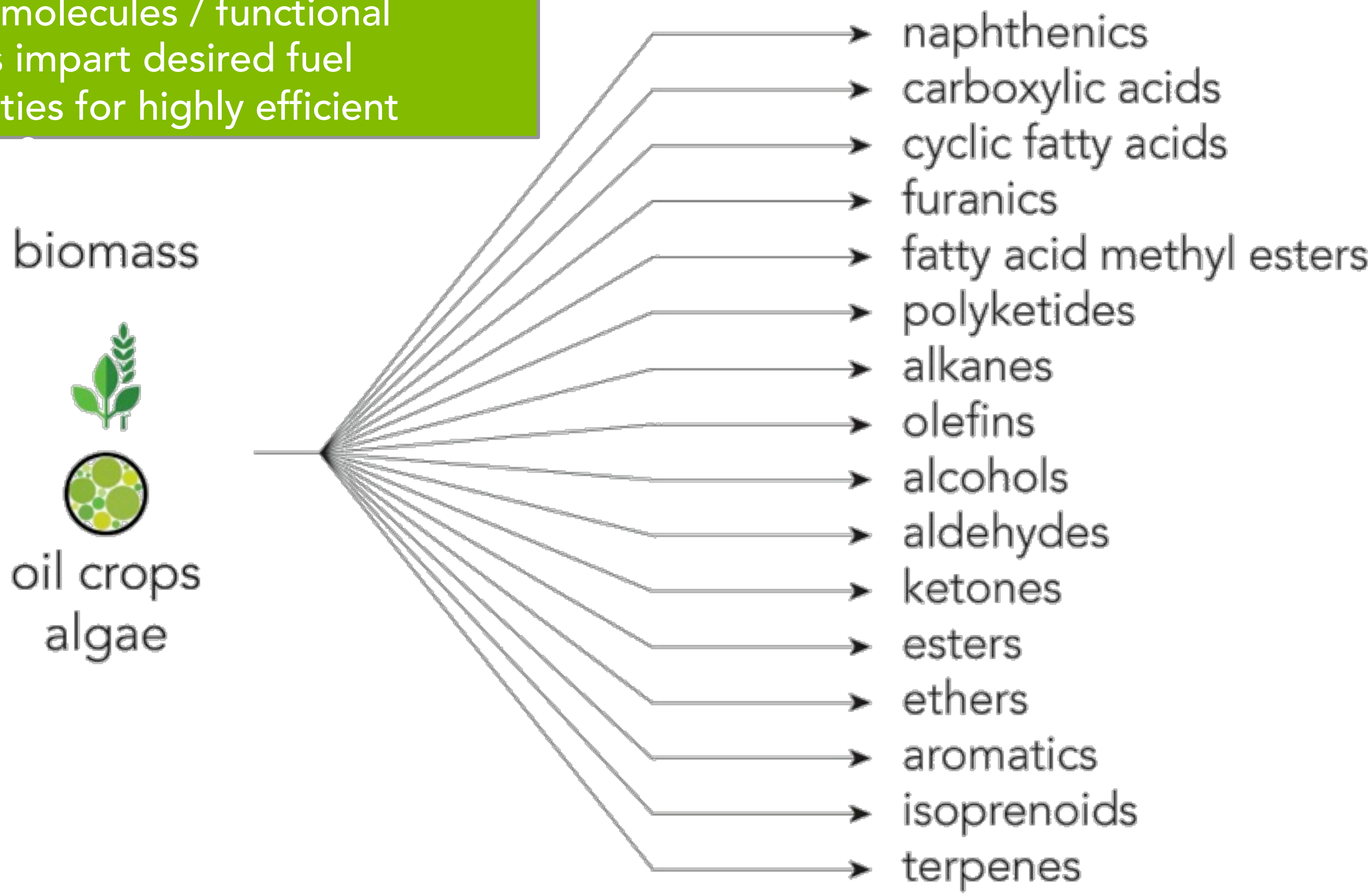
Technical Challenge 2

What fuels should we make?

Identifying blendstock options that provide key properties

Leverage BETO's Core Research

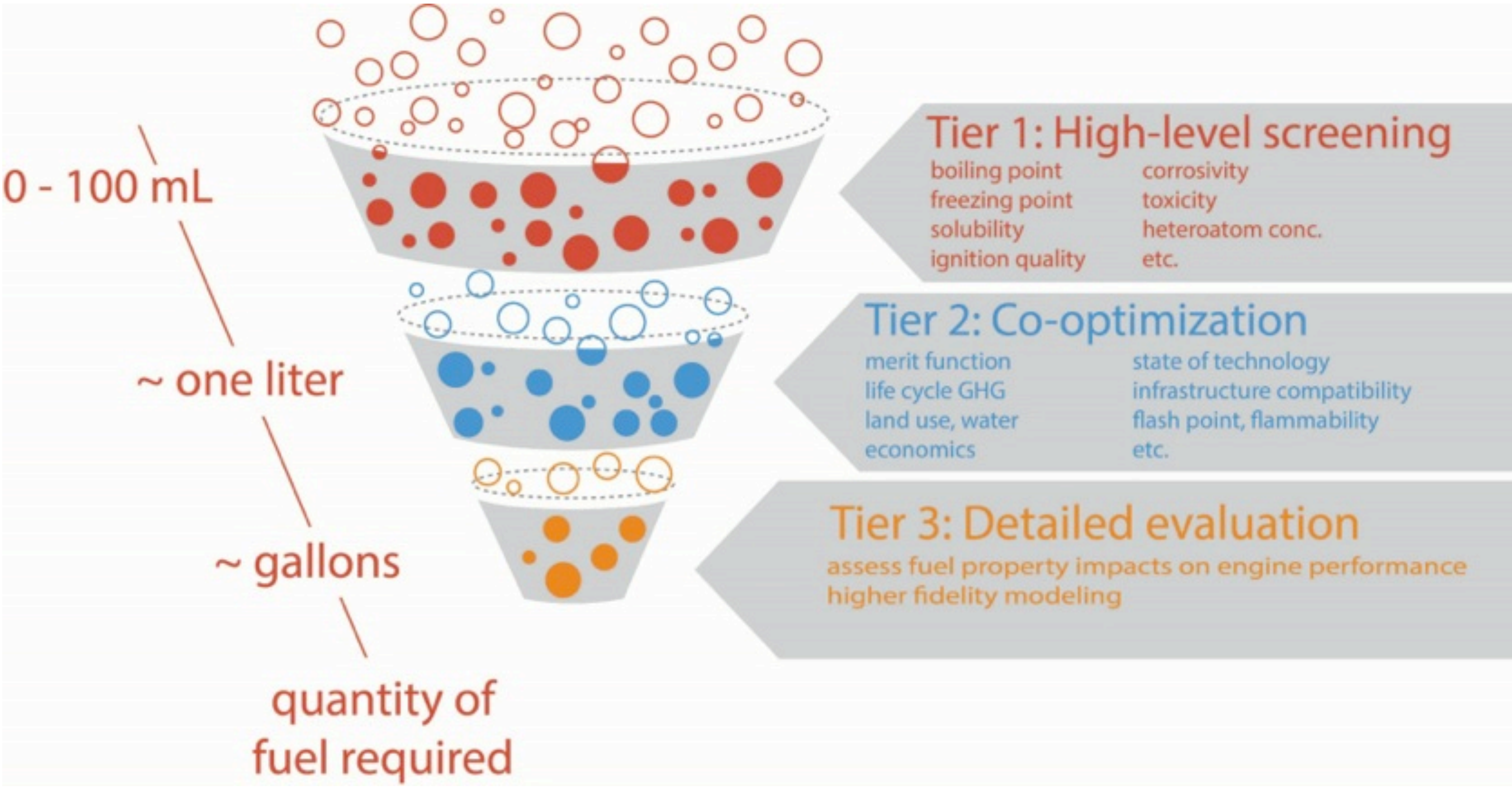
Which molecules / functional groups impart desired fuel properties for highly efficient



More details in HPF talk

Fuel Screening

"Leaky funnel" concept



More details in HPF talk

Critical Success Factors

Identifying fuel and engine options that have near-term (~ 2025+) market viability (affordable, sustainable, scalable, and compatible)

Identifying deployment scenarios with maximum market pull for all stake-holders (a "win-win" for all)

Critical Success Factor 1

What will work in the real world?

Assessing affordability, sustainability, scalability, and compatibility

Assessing Viability

Feasibility Metrics

Technology Readiness	Environmental	Economics	Market
SOT - fuel production	Carbon efficiency	Target cost	Uncertainty
SOT - vehicle use	Target yield	Needed cost reduction	Regulatory requirements
Conversion TRL level	Life cycle GHG	Co-product economics	Geographic factors
Feedstock sensitivity	Life cycle water	Feedstock cost	Political factors
Process robustness	Life cycle FE use	Alternative high-value use	Vehicle compatibility
Feedstock quality			Infrastructure compatibility
# of viable pathways			

SOT = state of technology; TRL = technology readiness level; GHG = greenhouse gas; FE = fossil energy

Candidates are being evaluated against 23 metrics to assess feasibility of technology ready for introduction in 2025–2030

More details provided in presentations by ASSERT and MT

Critical Success Factor 2

How do we co-optimize?

Identifying deployment scenarios with maximum market pull for all stake-holder groups (a "win-win" for all)

Understanding needs and value propositions for all major stakeholder groups (including consumers)

Co-Optimizer – Approach and Tool

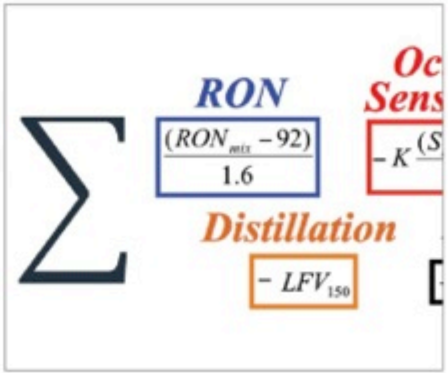
Database:
fuel properties,
sustainability,
affordability,
scalability,
infrastructure,
and retail
attributes

ΔGHG = *a*
H_2O consumption = *b*
Viable routes > *c*
Feedstock cost < *d*
Pipeline compatibility = *e*
Tech Readiness Level > *f*
Energy density > *g*
Biodegradability > *h*
⋮ ⋮ ⋮

Scenario constraints

"Co-Optimizer"

Engine/vehicle merit function



Optimal fuel blend formulation options for stakeholder consideration

The Co-Optimizer computational tool will identify fuel formulations that meet commercial fuel specifications and maximize engine efficiency, subject to various constraints

3 Technical Accomplishments, Progress, and Results

Ten Major Accomplishments, Year 1

1. Developed Central Fuel Hypothesis [1]
2. Constructed Thrust I merit function [2]
3. Refined understanding of how fuel properties affect engine combustion [2]
4. Developed and populated fuel property database with 400+ bio-blendstocks and fuel mixtures [1]
5. Identified 40+ high-potential Thrust I blendstocks via tiered screening [1]
6. Developed co-optimizer approach and methodology [2]
7. Identified key economic, environmental, & market transformation metrics for candidate evaluation [3, 4]
8. Completed cost & environmental impact analyses (LCA, TEA) of 20 promising Thrust I candidates [3]
9. Completed benefits analysis (impact of Co-Optima) [3]
10. Convened EAB and maintained extensive external stakeholder engagement [4]

[1] Covered by HPF [2] VTO funded work (not covered in BETO Peer Review)

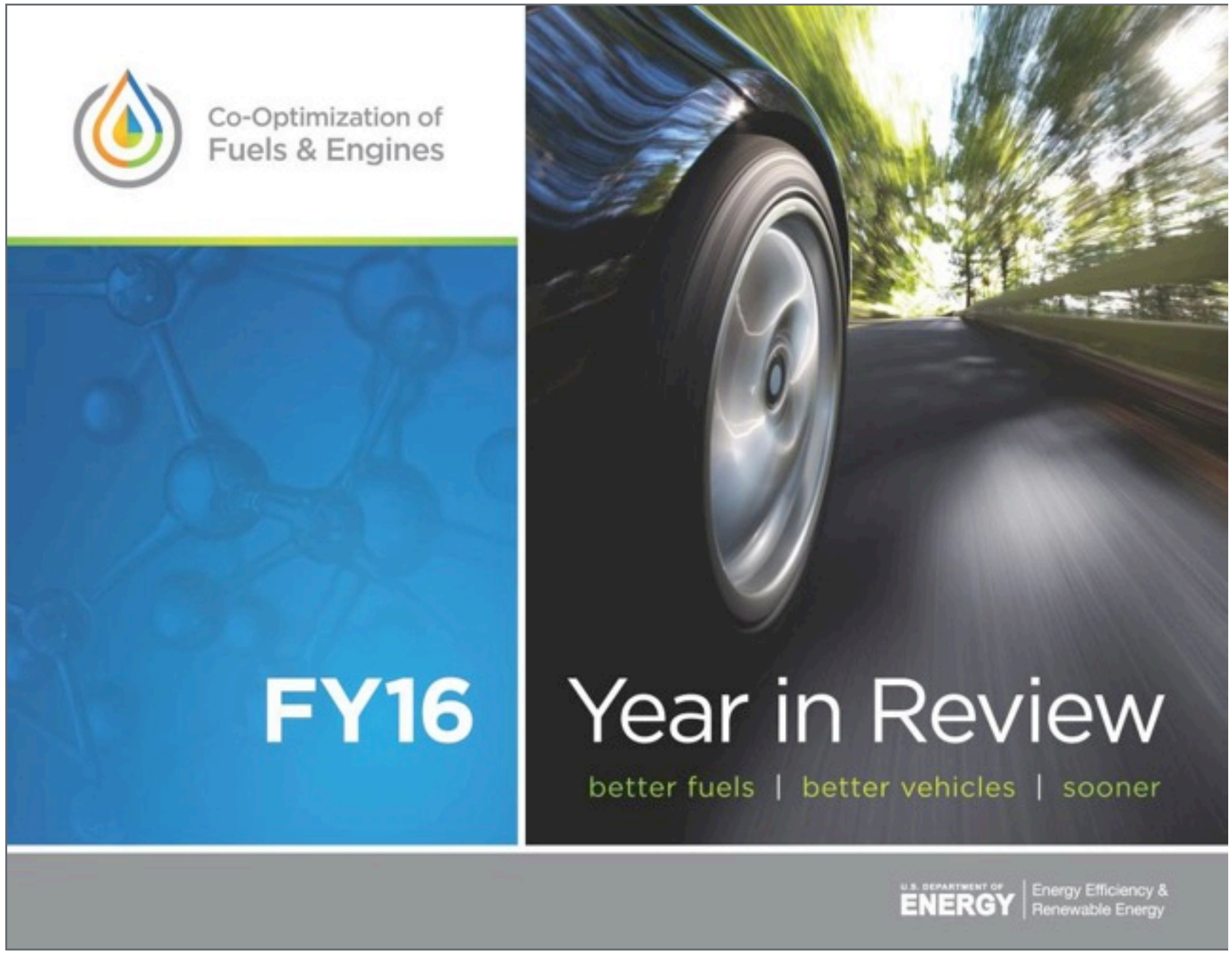
[3] Covered by ASSERT
[4] Covered by MT

FY16 Year in Review

Highlights 24 accomplishments

Distributed to wide range of stakeholders

Complements more detailed BETO & VTO reports



http://www.nrel.gov/docs/fy17osti/67595.pdf

DOE Dashboard Milestones

FY16	FY17
Q1: Identify 20 bio-derived blendstocks for evaluation as Co-Optima Thrust I blend components	Q1: Complete development of Thrust II strategy and deliver summary report document to DOE
Q2: Quantify Co-Optima benefits in terms of economy-wide energy savings, GHG reduction, and job creation	Q2: Release preliminary version of Co-Optimizer tool
Q3: Establish Co-Optima Board of Directors and External Advisory Board and hold kickoff meetings	Q3: Hold decision point review and document outcome of results
Q4: Complete preliminary TEA and LCA results for up to 20 Thrust I blendstock candidates	Q4: Complete market acceptance and implementation strategy for Thrust I fuel

HPF | ASSERT | MT | TK | Leadership Team | Multi-Team

All dashboard milestones have either been completed on-time or are on-track

4 Relevance

Co-Optima at a Glance

Goal: 30% per vehicle petroleum reduction through efficiency and displacement

Approach

1. Determine key fuel properties that enable improved engine efficiency
2. Provide key science to enable high efficiency combustion modes
3. Capitalize on unique properties available from bio-blendstocks
4. Use stakeholder input to guide analysis
5. Focus on activities that can accelerate market penetration

Outcome: Market driver for biofuels

1. Science enabling targeted highly efficient combustion modes for OEMs
2. Identification of bio-blendstocks that provide the required critical fuel properties
3. Property-based specification for new fuels
4. Market viability, environmental sustainability, and job assessment for fuel-engine system
5. Scenario analysis tool that combines data, information, and assessments and weights based on stakeholder success criteria
6. Cars and trucks that operate with higher efficiency and lower emissions than possible today

Integrate vehicle and biofuel research across the
EERE Vehicle Technologies and Bioenergy Technologies Offices

Fills a Gap in BETO Strategy

BETO 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

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 relationship)
- Provides retro-synthetic analysis that connect to BETO's pathways

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

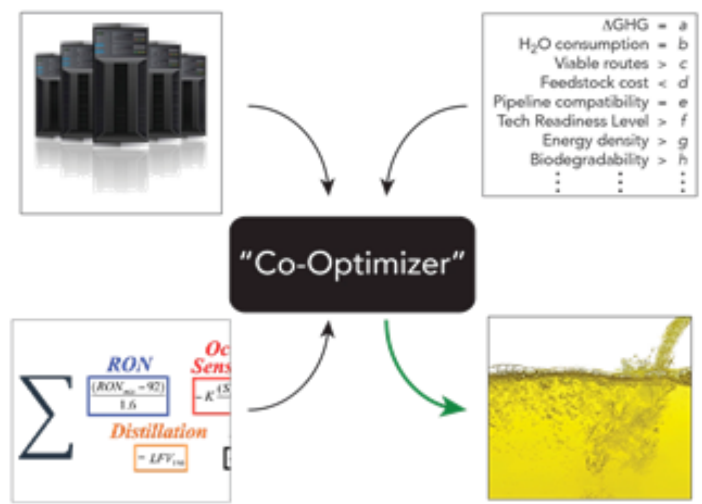
Impact: Fills a critical gap for BETO, provides options for producers in a way that does not pick winners

Informs BETO Portfolio Planning

BETO MYPP: Strategic Analysis program "provides context and justification for decisions at all levels by establishing the basis of quantitative metrics… and informing portfolio planning and management."

Co-Optima contributes to context and justification for decisions based on science-driven models and tools working with broad stakeholder group

- ASSERT model output (TEA, LCA, Benefits Analysis)
- Market transformation output
- Co-Optimizer Tool (scenario modeling balancing stakeholder drivers)
- Provides targets for BETO core programs and future FOAs



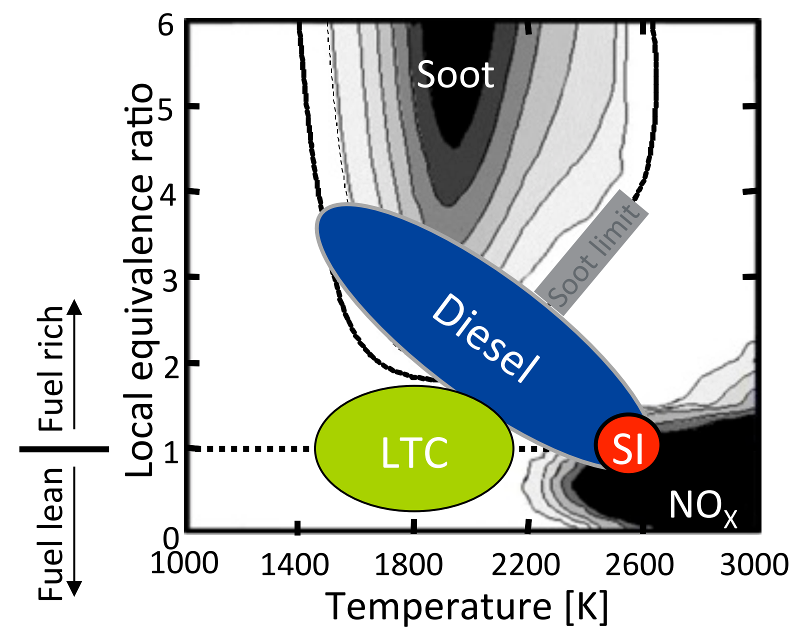
Impact: More robust BETO and VTO strategies

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 bio-blendstock 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

Higher Efficiency and Performance

From strategic plan "Co-optimization of fuels and engines offers the potential to significantly improve vehicle engine efficiency, maximize engine performance and carbon efficiency, … through accelerating the widespread deployment of improved fuels and engines."

Co-Optima is developing science that provides new value propositions and supports market pull

- Assessing how fuel properties extend the range of efficiency across the speed-load drive cycle
- Targeting bio-blendstocks that offer improvements over petroleum-derived fuels

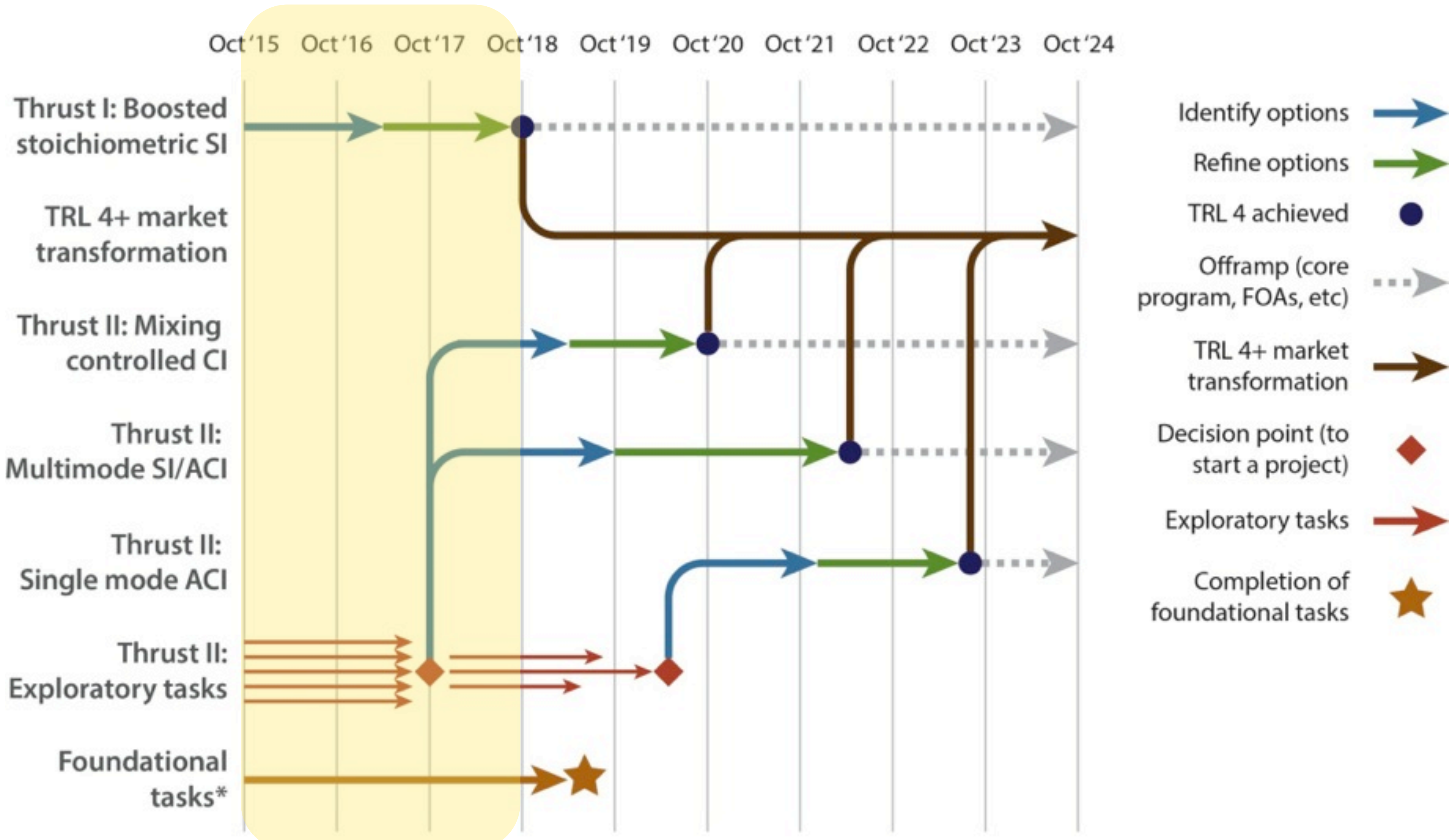
Co-Optima is addressing fuel deployment

- Determining the blending behavior of the bio-blendstocks within a petroleum matrix
- Understanding impact on infrastructure (engines, fuel transport and storage
- Producing property-based fuel specifications

Impact:
market pull

5 Future Work

Look Ahead at Next 18 Months



* Development of fuel property database, analysis framework, co-optimizer development, fuel blending models, etc.

Thrust I – Thrust II Rebalance and Budget

Decision Point at 18 months

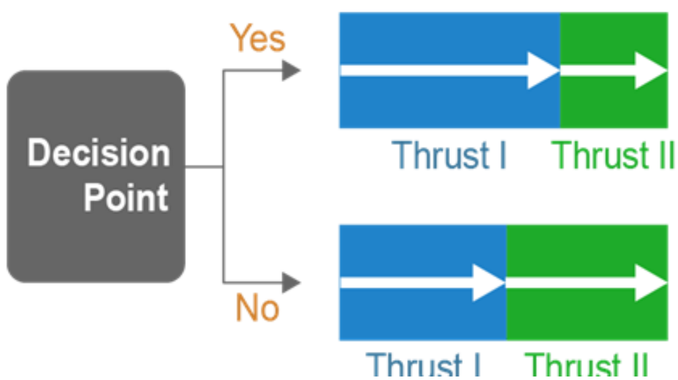
- Determines relative effort toward Thrust I and Thrust II for each team

Options

- Hand-off to BETO Core or FOA
- Continue co-optimization

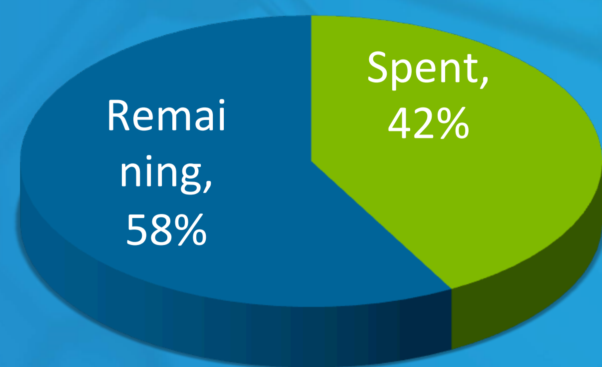
Steps

- Completed draft document of team-by-team work scope following rebalance
- Present to External Advisory Board and Board of Directors



Budget is sufficient to

- Complete Thrust I work
- Initiate Thrust II diesel (mixing controlled CI)
- Initiate Thrust II multimode SI/ACI (fuel properties definition strongly leverages Thrust I efforts)



Completing Thrust I

Thrust I Activities
Completion at 36 months

Engine: Boosted stoichiometric spark ignition
Fuel: high octane

Action	Outcome	Relevance
Develop blending models	Understand non-linear blending behavior	Establishes fuel property-based specification
Assess fuel–component compatibility	Expanded compatibility testing	Determines fit into today's infrastructure
Determine combustion and emission profiles	Understand emission clean-up requirements	Clean burning and high efficiency
Validate merit function in engines with biofuels	Improved Merit Function (at load)	Establishes approach
Expand co-optimizer tool	Balance stakeholder needs	Create market pull

Future Work: Key Milestones

	FY17		FY18
Project	Decision Point- rebalance I & II	Form Thrust II multi-team project	Confirm ability to meet 30% target
HPF/FP/AED	Complete series of blend measurements	Screen >200 diesel-like candidates	Measure blending behavior of 10 candidates
	Retrosynthetic toolkit for all compounds	Establish engine emission (2 fuels)	Determine blending behavior in more BOBs
	Determine missing pathway data	Establish pathways	Determine infrastructure compatibility (2-5 fuels)
ASSERT	Infrastructure costs & envir. impacts	Thrust II TEA, LCA, benefits	Business case
MT	Scenario analysis	Stakeholder engagement	Develop fuel property specification

Thrust I | Thrust II | I & II

Summary

Goal: Develop fuel chemistry–engine performance relationships and scenario analyses that provide new fuel and combustion options for more efficient engines with lower harmful emissions, resulting in market pull for the transport sector.

Approach	Accomplishments	Relevance	Future Work
Multi-discipline, multi-office effort	Developed engine efficiency merit function	Provides technical basis for evaluating bio-blendstocks	Thrust I and Thrust II rebalance
Hypothesis-driven fuel property-based approach	Provided a publicly accessible fuel property database (400 compounds)	Identifies key bio-blendstocks that enable engines to operate cleanly and efficiently	Establish performance improvements offered by promising Thrust I candidates
Constrain combustion options and co-optimize renewable fuel blendstocks	Identified promising Thrust I candidates	Identifies what fuels engines want and compliments BETO pathway approach	Identify promising Thrust II options
Two thrusts (I nearer term, SI; II longer-term, ACI)	Measured blending behavior of chemically diverse bio-blendstocks in two base fuels	Developing performance and pathway to enable technical analyses	Improve pathway technical and market barrier analysis
Output informs industry stakeholders	Completed initial life-cycle analysis of 20 bio-blendstock options		Develop merit function for two Thrust II options

Additional Slides

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