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Co-Optimization of Fuels and Engines (Co-Optima) Overview

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A quick aside on format and content...

Because of the large size of this project, the Co-Optima review extends across four presentations:

FT037: Co-Optima Overview (this presentation)

FT038: Fuel properties, chemical kinetics, and Thrust I engine projects

FT039: Thrust II engine projects and sprays/emission controls

FT040: Modeling and Simulation

This presentation will cover:

- Relevance, Approach/Strategy, Collaborations and Coordination, and Remaining Challenges and Barriers for the Co-Optima project

- High-level overview of select BETO-funded Co-Optima tasks for context

Detailed discussions of VTO-funded tasks will be covered in **FT038-040**

Co-Optima Overview

Timeline

- **Project start date:** **FY16**
- **Project end date:** **FY19***
- **Percent complete:** **20%**

Barriers and Challenges

- **Complexity:** *Introduction of new fuels and vehicles into the market involves large number of stakeholders with competing value propositions*
- **Timing:** *Schedule for completing R&D and achieving market impact is extremely ambitious*

Budget

- **Funding for FY16:** **$26M**
  - **VTO funding:** **$12M**
  - **BETO funding**:** **$14M**

Partners

- **External Advisory Board:**
  - USCAR
  - Advanced Biofuels Association
  - EPA
  - Dave Foster (U. Wisc)
  - Truck & Engine Manufacturers Association
  - API
  - Fuels Institute
  - CARB
  - UL
  - Joe Norbert (U.C. Riverside)
- **Stakeholders:**
  - 85 individuals representing 46 organizations

*End date for Thrust I (spark ignition R&D); Thrust II (advanced compression ignition) R&D will continue
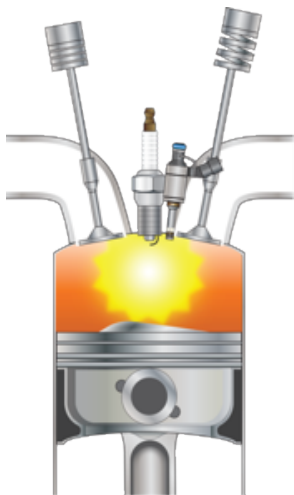**BETO – Bioenergy Technologies Office

Relevance: Why Co-optimize?

1. Internal combustion engines will continue to dominate the fleet and contribution to transportation GHG emissions for decades

2. Better integration of fuels and engines research critical to accelerating progress toward ambitious climate goals

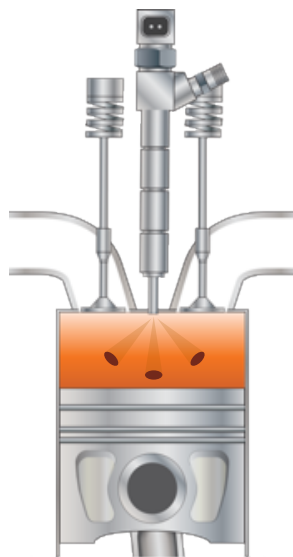3. An "end-to-end" R&D program is essential for maximum impact in the shortest timeframe
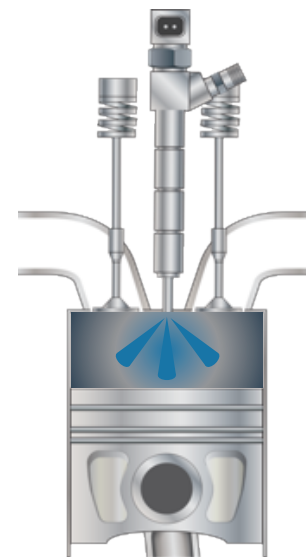
Approach/Strategy
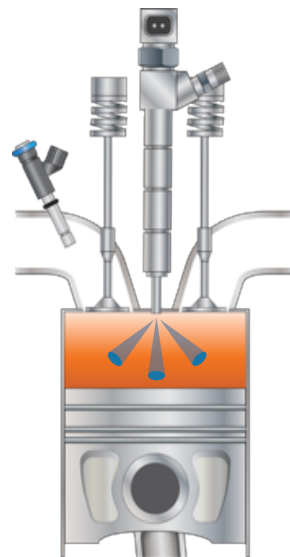
Thrust I: Spark Ignition (SI)	Thrust II: Advanced Compression Ignition (ACI) kinetically-controlled and compression-ignition combustion

Low reactivity fuel | **Range of fuel properties TBD** | **High reactivity fuel**

Approach/Strategy

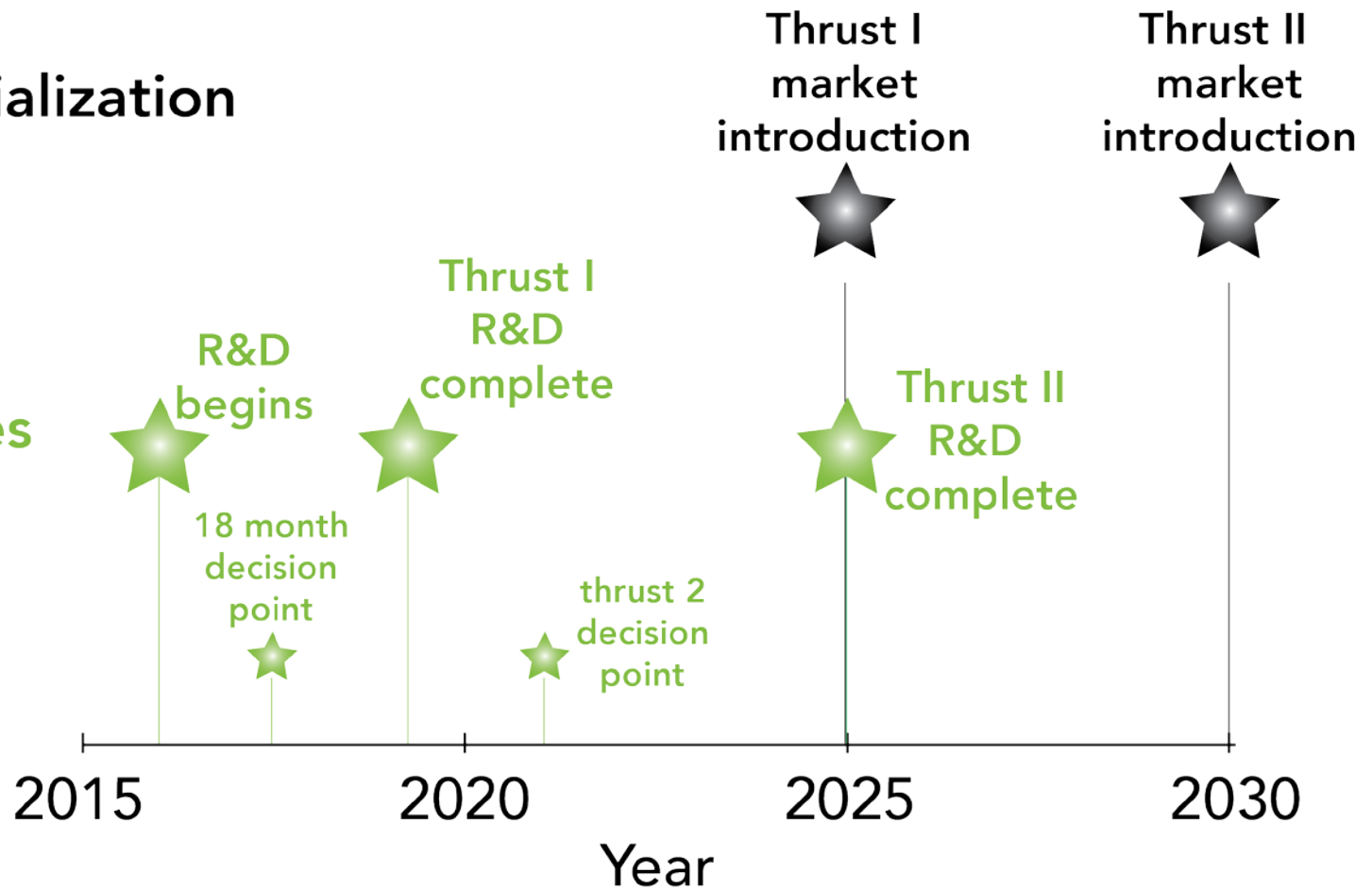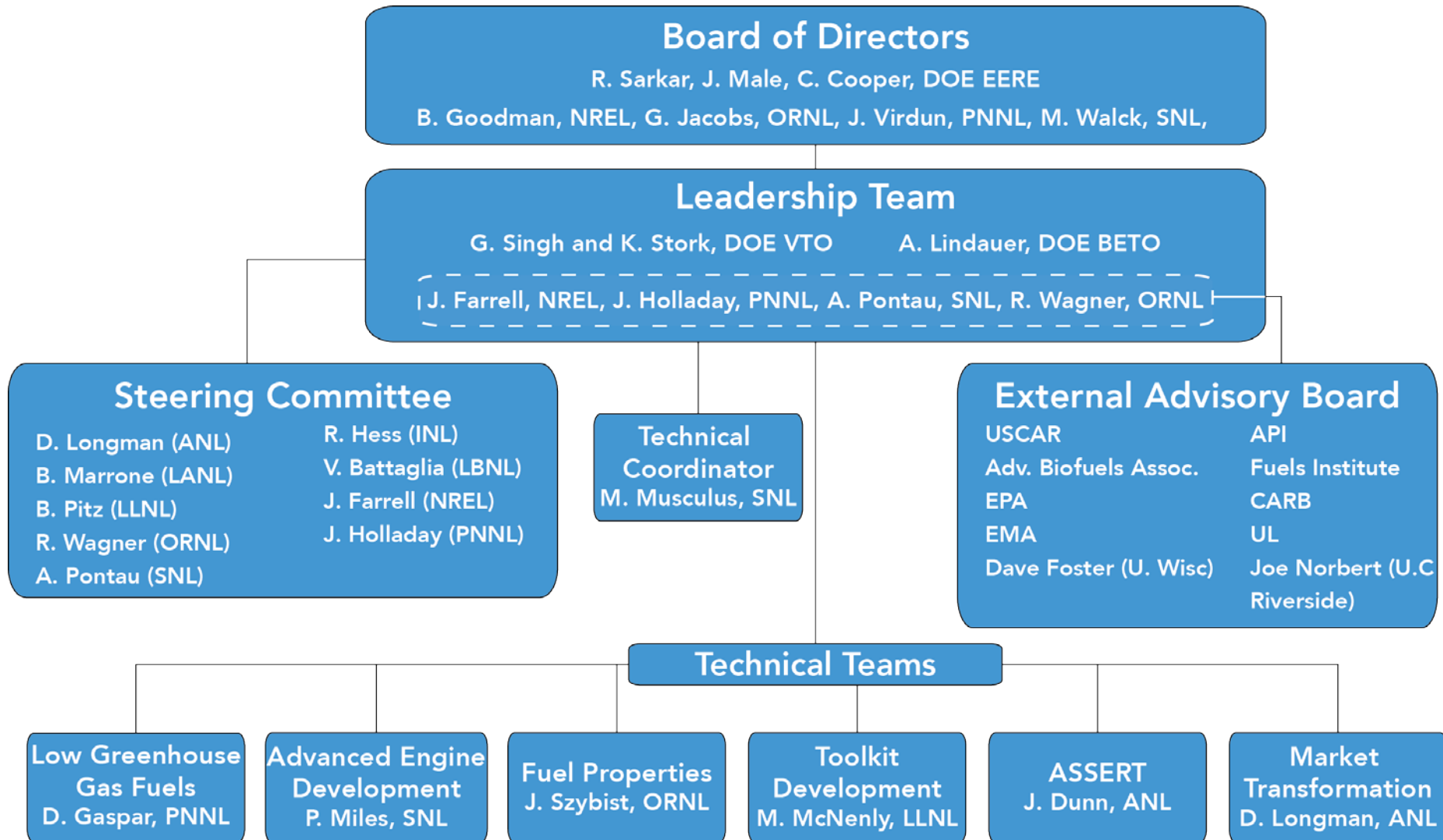Applicable to **light, medium, and heavy-duty** engines and **hybridized and non-hybridized** powertrains

Approach/Strategy: Organizational Structure

Approach/Strategy: Six Integrated Teams

Advanced Engine Development

Quantify interactions between fuel properties and engine design and operating strategies – enable optimal design of efficient, emission-compliant engines

Fuel Properties

Identify critical properties and allowable ranges, systematically catalogue properties, and predict fuel blending behavior

Modeling and Simulation Toolkit

Extend the range, confidence and applicability of engine experiments by leveraging high-fidelity simulation capabilities

Low Greenhouse Gas Fuels

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

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

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

Market Transformation

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

Approach/Strategy: Six Integrated Teams

Advanced Engine Development

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VTO-led tasks and deliverables will be discussed in following presentations

Approach/Strategy: Six Integrated Teams

BETO-led tasks are performed in close collaboration with VTO-led tasks to ensure critical knowledge discovery for "end-to-end" decision making

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Market Transformation

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

Low Greenhouse Gas Fuels Tasks

Team	Lead PI (Lab)
Low Greenhouse Gas Fuels	
Development of Thrust I fuel screening criteria*	McCormick (NREL), Gaspar (PNNL), Szybist (ORNL), Miles (SNL)
Physical and chemical analysis of Tier 2 candidates	Foust (NREL); McCormick (NREL), Albrecht (PNNL), George (SNL), Pray (LBNL), Sutton (LANL)
Measure full suite of fuel properties of 20 Thrust I fuel blend components	McCormick (NREL), Albrecht (PNNL), George (SNL), Pray (LBNL), Sutton (LANL), Gaspar (PNNL)
Measure blending fuel properties of 5 bio-blendstocks at 3 blending levels in 2 base fuels.	McCormick (NREL), Albrecht (PNNL), George (SNL), Pray (LBNL), Sutton (LANL), Gaspar (PNNL)
Provide 5 fuels for multicylinder engine testing	Foust (NREL), Albrecht (PNNL)
Determine whether promising low-GHG blendstocks/ fuels have been identified that merit further fuel development/scale-up efforts	McCormick (NREL), Albrecht (PNNL), George (SNL), Pray (LBNL), Sutton (LANL), Gaspar (PNNL), Li (INL), West (ORNL)

* Task Complete

ASSERT Tasks

Team	Lead PI (Lab)
Analysis of Sustainability, Scale, Economics, Risk, and Trade (ASSERT)	
Develop downselect metrics, definitions, guidance related to sustainability, economics, scale, and feedstocks*	Dunn (ANL), Biddy (NREL), Jones (PNNL), Searcy (INL)
Quantify benefits of Co-Optima (economy-wide energy savings, GHG reduction, job creation)*	(Dunn ANL), Newes (NREL), Brooker (NREL)
High-level TEA, LCA, feedstock implication analyses for 20 candidate blendstocks (4Q)	Biddy (NREL), Jones (PNNL), Dunn (ANL)
Combined feedstock supply system analysis and risk and trade/opportunity analysis (4Q)	Lamers/Searcy (INL)

* Task Complete

Market Transformation Tasks

Team	Lead PI (Lab)
Market Transformation	
Guidance document on previous fuel/vehicle introductions (4Q)	West (ORNL)
Guidance document on fuel/vehicle distribution (4Q)	Mintz (ANL)
Guidance document on laws and incentives for biofuel and new vehicle market introduction (4Q)	Alleman (NREL)
Mitigate market acceptance barriers with SAE, focus on misfueling (4Q)	Sluder (ORNL)
Guidance document on fuel infrastructure barriers (4Q)	Moriarty (NREL)
Guidance document on feedstock market evolution (4Q)	Shirk (INL)
Develop MT evaluation metrics related to infrastructure compatibility, market acceptance, etc. (3Q)	Longman (ANL)
Stakeholder Engagement - monthly teleconferences, individual visits, Listening Days, etc	Longman (ANL)

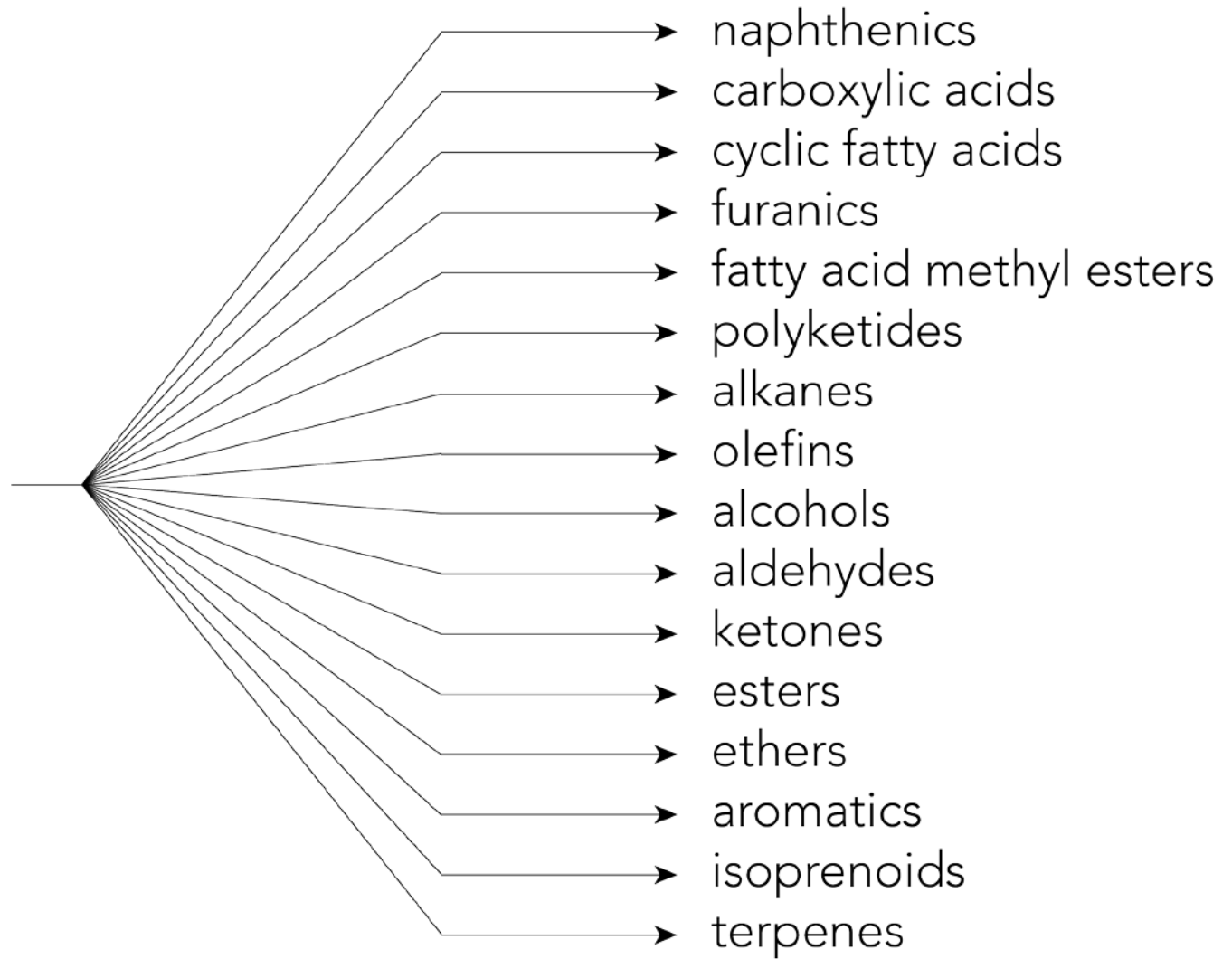What fuels can we make?

biomass

oil crops
algae
oleaginous
yeast

naphthenics
carboxylic acids
cyclic fatty acids
furanics
fatty acid methyl esters
polyketides
alkanes
olefins
alcohols
aldehydes
ketones
esters
ethers
aromatics
isoprenoids
terpenes

none   hundreds

~ one liter   ~ 20

~ gallons   ~ 5

quantify of   number of
fuel required   candidates

Tier 1: high-level screening
boiling point   corrosivity
freezing point   toxicity
solubility   heteroatom conc.
ignition quality   etc.

Tier 2: candidate selection
fuel merit function *   state of technology
life cycle GHG   infrastructure compatibility
land use, water   flash point, flammability
economics   etc.

Tier 3: candidate evaluation
evaluate promising candidates in engine tests

Thrust I decision tree results

Hydrocarbons
  Normal paraffins
  Iso-paraffins
  Cycloparaffins
  Aromatics
  Multi-ring aromatics
  Olefins
Carbonyls
  Ketones
  Aldehydes
Esters
  Simple/volatile fatty acid esters
  Fatty esters
Carboxylic Acids
Alcohols
Ethers
  Cyclic/furanics
  Linear

YES
Normal paraffins
Iso-paraffins
Cycloparaffins
Olefins
Alcohols

YES FOR SOME
Aromatics
Ketones
Simple/volatile fatty acid esters
Cyclic ethers/furanics
Linear ethers

NO
Multi-ring aromatics
Aldehydes
Fatty esters
Carboxylic acids
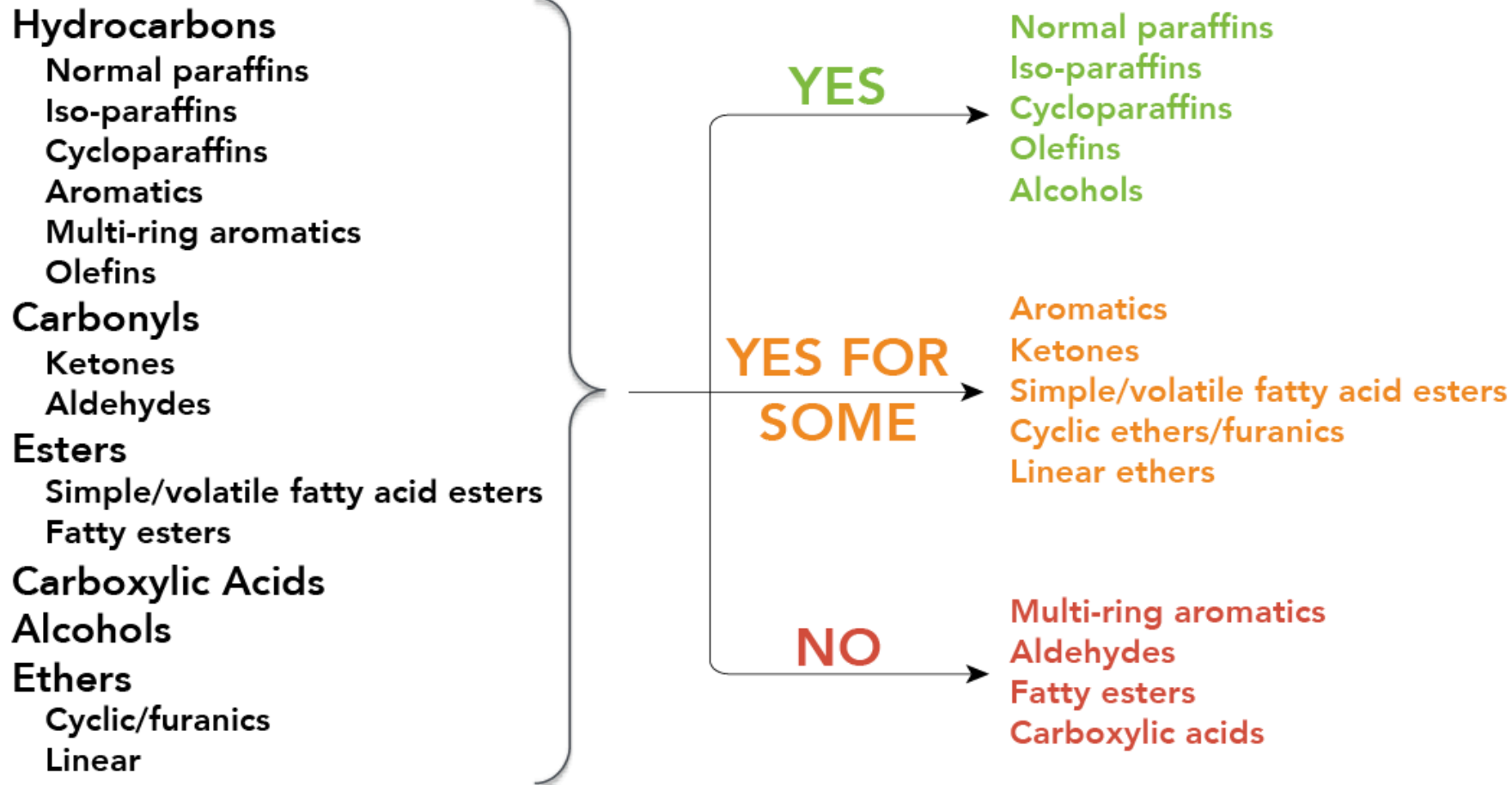
Cost and environmental impact analyses

High-level LCA, TEA,*

feedstock availability analyses

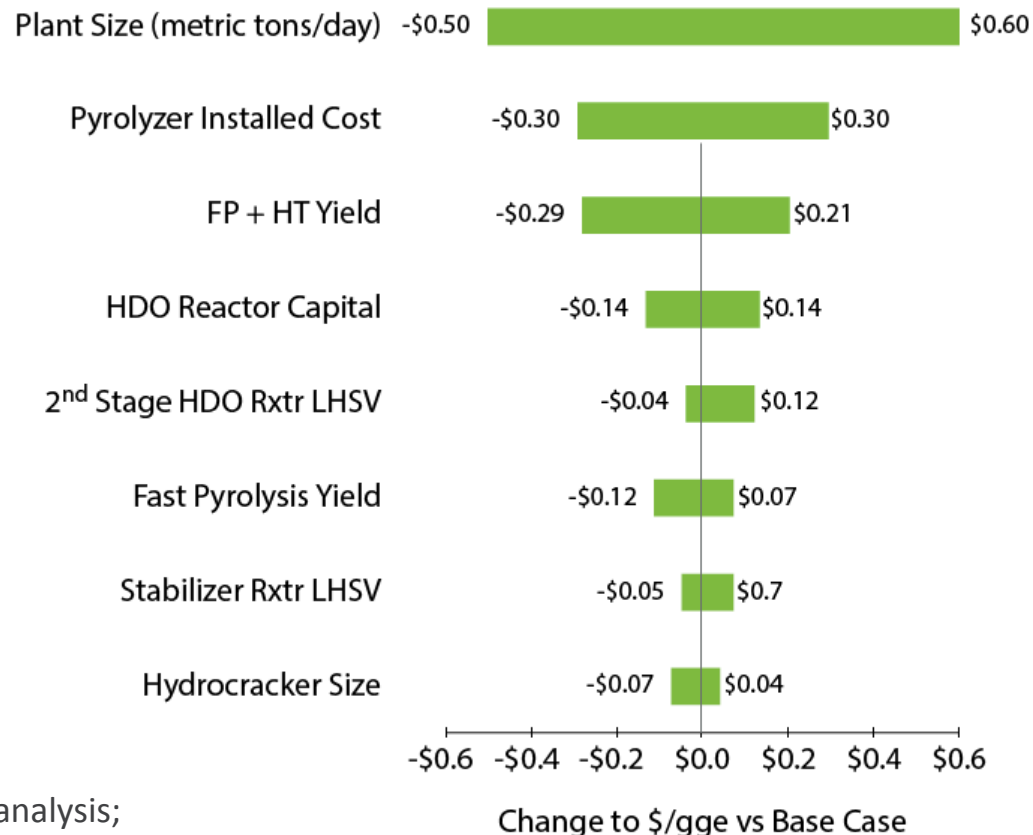Identify cost/environmental/scale attributes

Fifteen key metrics identified

GHG, water, economics, TRL
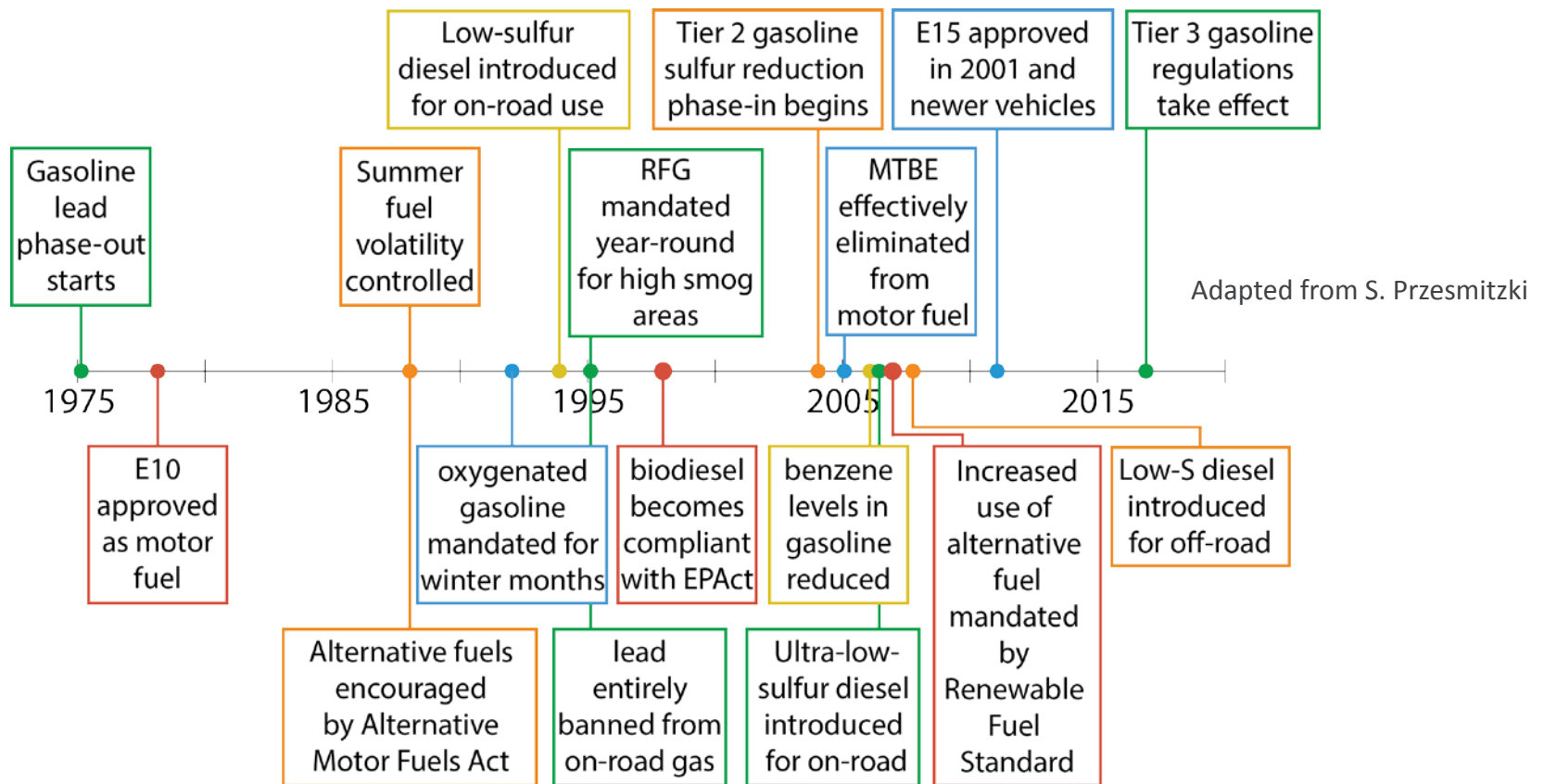
Evaluation of 20 Thrust I

blendstocks underway

* LCA = Life cycle analysis; TEA = techno-economic analysis;
   TRL = technology readiness level

Tornado chart — Change to $/gge vs Base Case

Parameter	Low	High
Plant Size (metric tons/day)	-$0.50	$0.60
Pyrolyzer Installed Cost	-$0.30	$0.30
FP + HT Yield	-$0.29	$0.21
HDO Reactor Capital	-$0.14	$0.14
2nd Stage HDO Rxtr LHSV	-$0.04	$0.12
Fast Pyrolysis Yield	-$0.12	$0.07
Stabilizer Rxtr LHSV	-$0.05	$0.7
Hydrocracker Size	-$0.07	$0.04

Identifying/mitigating market barriers

Adapted from S. Przesmitzki

Identify and mitigate challenges of moving new fuels/ engines to markets

Historical analysis of new fuel and vehicle introduction

Engage stakeholders across value chain

18 Month Decision Point

- Marks completion of Thrust I (advanced spark ignition) fuel discovery efforts (i.e., candidate identification)

- Will conduct rigorous assessment of fuel/engine options and identify promising* low-GHG fuel/engine combinations

- Will identify whether new low-GHG fuel candidates have been identified that require additional development work

- Outcome will dictate balance between Thrust I vs Thrust II work after 18 months
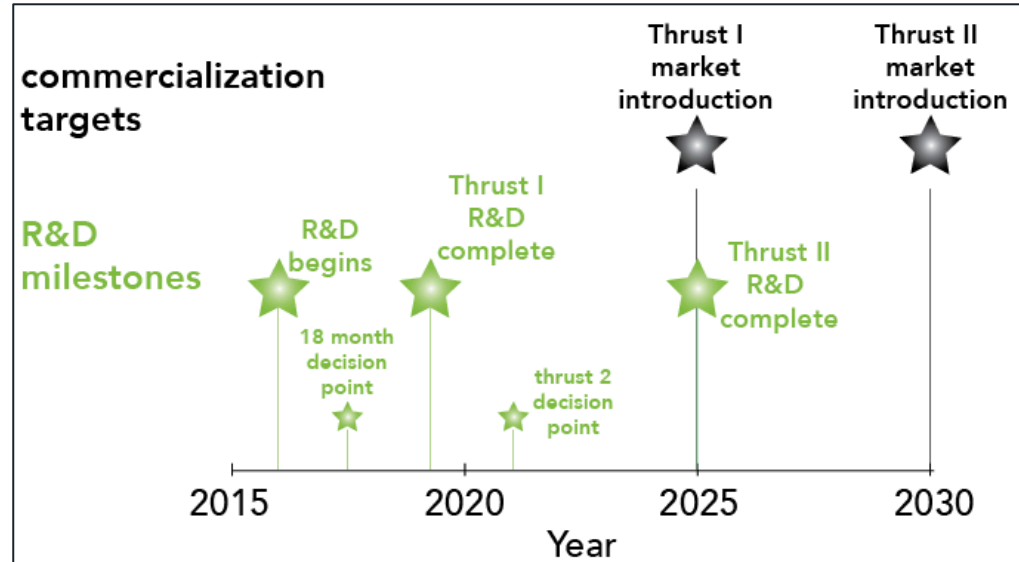
* Sustainable, affordable, scalable

Collaborations and Coordination

- Nine national labs funded in FY16

Collaborations and Coordination: Stakeholder Listening Days

- Stakeholder Listening Day held in June 2015 to obtain input into FY16 R&D plan

  – Report available on-line*

- Two Listening Days planned in FY16

  – Week of July 11 Washington DC (coincident with BioEnergy 2016) focused on ASSERT/MT metrics

  – ~ September focused on engine merit function

* http://energy.gov/eere/bioenergy/downloads/co-optima-stakeholder-listening-day-summary-report

Collaborations and Coordination: Stakeholder Engagement

- $5M university FOA in FY16 jointly funded by BETO and VTO

  – Intent – leverage national lab capabilities, with focus on Thrust II

- Monthly stakeholder telecons held to provide technical updates

- Over two dozen one-on-one stakeholder visits held to date

- Coordination with related activities

  – U.S. DRIVE: Fuels Working Group and ACEC Tech Team

  – CRC

  – AEC MOU

  – Tailor-Made Fuels From Biomass (European initiative)

- Additional project-level collaborations with industry and academia (highlighted in following presentations)

Status and Future Work

- Initiative started October 1 2016

- FY16 budget: $26M; FY17 budget request: $30M

- Stakeholder input actively solicited for maximizing impact of Co-Optima R&D efforts

  - ASSERT and Market Transformation metrics

  - Engine merit function

  - Fuel property data

  - Scenario development and optimizer tool for 18 month decision point

  - Multi-year Project Plan