Co-Optimization of Fuels & Engines

FOR TOMORROW’S ENERGY-EFFICIENT VEHICLES

Co-Optima Overview
June 9, 2016
Co-Optimization of Fuels and Engines (Co-Optima) Overview

June 9th, 2016

John Farrell,1 John Holladay,2 Art Pontau,3 Robert Wagner 4

1. National Renewable Energy Laboratory
2. Pacific Northwest National Laboratory
3. Sandia National Laboratories
4. Oak Ridge National Laboratory

Co-Optima DOE VTO Management Team:
Kevin Stork and Gurpreet Singh (VTO)
Alicia Lindauer (BETO)
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

<table>
<thead>
<tr>
<th>Item</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Project start date</td>
<td>FY16</td>
</tr>
<tr>
<td>Project end date</td>
<td>FY19*</td>
</tr>
<tr>
<td>Percent complete</td>
<td>20%</td>
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</tbody>
</table>

## Budget

<table>
<thead>
<tr>
<th>Item</th>
<th>Details</th>
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</thead>
<tbody>
<tr>
<td>Funding for FY16</td>
<td>$26M</td>
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<tr>
<td>VTO funding</td>
<td>$12M</td>
</tr>
<tr>
<td>BETO funding**</td>
<td>$14M</td>
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</tbody>
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## 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

## 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

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*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)

Low reactivity fuel

Range of fuel properties TBD

Thrust II: Advanced Compression Ignition (ACI)
kinetically-controlled and compression-ignition combustion

High reactivity fuel
Applicable to **light, medium, and heavy-duty** engines and **hybridized and non-hybridized** powertrains
R&D timeline / commercialization targets

Commercialization targets:

- **R&D milestones**
  - R&D begins
  - 18 month decision point
  - Thrust I R&D complete
  - Thrust I market introduction
  - Thrust II R&D complete
  - Thrust II market introduction

Year:
- 2015
- 2020
- 2025
- 2030
Approach/Strategy: Organizational Structure

Board of Directors
R. Sarkar, J. Male, C. Cooper, DOE EERE
B. Goodman, NREL, G. Jacobs, ORNL, J. Virdun, PNNL, M. Walck, SNL,

Leadership Team
G. Singh and K. Stork, DOE VTO
A. Lindauer, DOE BETO
J. Farrell, NREL, J. Holladay, PNNL, A. Pontau, SNL, R. Wagner, ORNL

Steering Committee
D. Longman (ANL)
B. Marrone (LANL)
B. Pitz (LLNL)
R. Wagner (ORNL)
A. Pontau (SNL)
R. Hess (INL)
V. Battaglia (LBNL)
J. Farrell (NREL)
J. Holladay (PNNL)

Technical Coordinator
M. Musculus, SNL

External Advisory Board
USCAR
EPA
EMA
Dave Foster (U. Wisc)
API
Fuels Institute
CARB
UL
Joe Norbert (U.C Riverside)

Technical Teams
Low Greenhouse Gas Fuels
D. Gaspar, PNNL
Advanced Engine Development
P. Miles, SNL
Fuel Properties
J. Szybist, ORNL
Toolkit Development
M. McNenly, LLNL
ASSERT
J. Dunn, ANL
Market Transformation
D. Longman, ANL
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**
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

VTO-led tasks and deliverables will be discussed in following presentations
BETO-led tasks are performed in close collaboration with VTO-led tasks to ensure critical knowledge discovery for “end-to-end” decision making.

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
# Low Greenhouse Gas Fuels Tasks

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

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

* Task Complete
# Market Transformation Tasks

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<tr>
<td><strong>Market Transformation</strong></td>
<td></td>
</tr>
<tr>
<td>Guidance document on previous fuel/vehicle introductions (4Q)</td>
<td>West (ORNL)</td>
</tr>
<tr>
<td>Guidance document on fuel/vehicle distribution (4Q)</td>
<td>Mintz (ANL)</td>
</tr>
<tr>
<td>Guidance document on laws and incentives for biofuel and new vehicle market introduction (4Q)</td>
<td>Alleman (NREL)</td>
</tr>
<tr>
<td>Mitigate market acceptance barriers with SAE, focus on misfueling (4Q)</td>
<td>Sluder (ORNL)</td>
</tr>
<tr>
<td>Guidance document on fuel infrastructure barriers (4Q)</td>
<td>Moriarty (NREL)</td>
</tr>
<tr>
<td>Guidance document on feedstock market evolution (4Q)</td>
<td>Shirk (INL)</td>
</tr>
<tr>
<td>Develop MT evaluation metrics related to infrastructure compatibility, market acceptance, etc. (3Q)</td>
<td>Longman (ANL)</td>
</tr>
<tr>
<td>Stakeholder Engagement - monthly teleconferences, individual visits, Listening Days, etc</td>
<td>Longman (ANL)</td>
</tr>
</tbody>
</table>
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
Fuel selection criteria ("decision tree")

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

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

- Tier 3: candidate evaluation
  - evaluate promising candidates in engine tests

- none
- hundreds
- ~ one liter
- ~ gallons
- ~ 20
- ~ 5
- quantify of fuel required
- number of candidates
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

Normal paraffins
  - Iso-paraffins
  - Cycloparaffins
  - Olefins
  - Alcohols

Aromatics
  - Ketones
  - Simple/volatile fatty acid esters
  - Cyclic ethers/furanics
  - Linear ethers

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
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

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)
• 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