Co-Optimization of Fuels and Engines

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SAE High Efficiency Internal Combustion Engine Symposium

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Goal: better fuels and better vehicles sooner

Fuel and Engine Co-Optimization

- What fuel properties maximize engine performance?
- How do engine parameters affect efficiency?
- What fuel and engine combinations are sustainable, affordable, and scalable?
30% per vehicle petroleum reduction via efficiency and displacement

source: EIA 2014 reference case
Fuel selection overview

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.

Governing Co-Optima hypotheses:

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

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.
Current fuels 

**constrain** engine design

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**Brake Thermal Efficiency (%)**

- **RON 100.9**
- **RON 90.7**

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**Brake Mean Effective Pressure (kPa)**

- 0
- 400
- 800
- 1200
- 1600
- 2000
- 2400

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*Engine: Ford Ecoboost 1.6L 4-cylinder, turbocharged, direct-injection, 10.1 CR source: C.S. Sluder, ORNL*
Fuel is more than just octane.
Leveraging expertise and facilities from 10 national labs
Integrated multi-lab teams with significant external stakeholder engagement

- Light and heavy duty vehicle manufacturers: 13
- Oil companies/refiners: 10
- Biofuel companies: 8
- Regulatory agencies: 4
- End consumer organizations: 2
Parallel efforts are underway

Thrust I: Spark Ignition (SI)

- Low reactivity fuel

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

- Range of fuel properties TBD
- High reactivity fuel
Applicable to light, medium, and heavy-duty engines hybridized and non-hybridized powertrains.
Identify and mitigate barriers to wide-scale deployment
National goal:
80% reduction in transportation GHG by 2050

Co-Optimization:
9-14% GHG reduction (beyond “business as usual”)
Six integrated teams

- Low Greenhouse Gas Fuels
- Advanced Engine Development
- Fuel Properties
- Modeling and Simulation Toolkit
- Analysis of Sustainability, Scale, Economics, Risk, and Trade
- Market Transformation
FY16 Activities
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
  - corruption
  - toxicity
  - heteroatom conc.

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

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

- none
- hundreds
- ~ one liter
- ~ 20
- ~ gallons
- ~ 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

**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
Fuel property database

Database of critical fuel properties of bio-derived and petroleum blendstocks
366 molecules, 12 mixtures (at present)
25 database fields for fuel properties
Will add capability for fully blended fuels
Data from experiment and literature or calculated/estimated (where needed)
Shared resource for team and public

Fioroni et al., NREL
Identification of Thrust I candidates

Tier I criteria
Melting point/cloud point below -10°C
Boiling point between 20°C and 165°C
Measured or estimated RON ≥ 98
Meet toxicity, corrosion, solubility, and biodegradation requirements

34 promising bio-blendstocks from many functional group classes

Not final – this is an iterative process!
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
Identifying/mitigating market barriers

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

Historical analysis of new fuel and vehicle introduction

Engage stakeholders across value chain

Adapted from S. Przesmitzki
# Fuel-related tasks

<table>
<thead>
<tr>
<th>Topic</th>
<th>Lead PI (Lab)</th>
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<tbody>
<tr>
<td><strong>Fuel Component and Blendstock Studies</strong></td>
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<tr>
<td>Development of Fuel Screening Criteria</td>
<td>McCormick (NREL), Gaspar (PNNL)</td>
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<td>Szybist (ORNL), Miles (SNL)</td>
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<tr>
<td>High-level TEA, LCA, feedstock implication analyses for 20 candidate blendstocks</td>
<td>Biddy (NREL), Jones (PNNL)</td>
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<td>Dunn (ANL)</td>
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<tr>
<td>Development of Fuel Property Database</td>
<td>McCormick/Fioroni (NREL)</td>
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<tr>
<td>Heat of Vaporization Measurement</td>
<td>Fioroni (NREL)</td>
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<tr>
<td><strong>Fuel Property Blending Model and Structure-Property Correlations</strong></td>
<td>McCormick (NREL), Mueller (SNL)</td>
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<td>Bays (PNNL)</td>
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<tr>
<td>Measurement of Autoignition Properties with Small Volumes (experiment and modeling)</td>
<td>Fioroni/McCormick (NREL)</td>
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<td>McNenly (LLNL)</td>
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<td>Goldsborough (ANL)</td>
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<tr>
<td>Chemical Kinetic Mechanism Development</td>
<td>Pitz (LLNL)</td>
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<tr>
<td>Chemical Kinetic Measurements</td>
<td>Goldsborough (ANL) - RCM</td>
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<td>Zigler (NREL) - IQT</td>
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## Fuel-related tasks (continued)

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<tr>
<td><strong>Fuel Component and Blendstock Studies</strong></td>
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<tr>
<td>Development of Fuel Blending Model for Calculating Simulation Inputs</td>
<td>Grout (NREL)</td>
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<tr>
<td>Input Parameters for Numerical Simulation</td>
<td>Grout (NREL)</td>
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<tr>
<td>Extreme Mechanism Reduction for SIDI based on Uncertainty Quantification</td>
<td>Lacaze (SNL)</td>
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<td>Fuel Surrogate Optimizer</td>
<td>Whitesides (LLNL)</td>
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<tr>
<td>Enhanced Models for Modeling Kinetic Laboratory Experiments</td>
<td>McNenly (LLNL)</td>
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<tr>
<td>Develop downselect metrics, definitions, guidance related to sustainability, economics, scale, and feedstocks</td>
<td>Dunn (ANL)</td>
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<tr>
<td>Combined feedstock supply system analysis and risk and trade/opportunity analysis</td>
<td>Searcy (INL)</td>
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<tr>
<td>Guidance document on fuel infrastructure barriers</td>
<td>Moriarty (NREL)</td>
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<tr>
<td>Guidance document on feedstock market evolution</td>
<td>Shirk (INL)</td>
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</table>
Heat of vaporization (HOV): complex mixtures

Pure compound approach not applicable to gasoline
True HOV underestimated

Approach: directly measure HOV by DSC/TGA* and calculate via detailed hydrocarbon analysis

Very similar HOV for wide range of gasolines and ethanol blends

* DSC = differential scanning calorimetry; TGA = thermogravimetric analysis

Fioroni et al., NREL
Kinetics and SI autoignition behavior

Rapid compression machine study of CRC FACE-F / ethanol blends (E0–E30, E100)
Data to validate LLNL gasoline surrogate kinetic mechanism

Bench-scale autoignition studies combined with engine experiments
Data from customized IQT to validate LLNL kinetic mechanisms Zigler (NREL)

Goldsborough, ANL
Kinetic mechanism development
Develop archival mechanisms for representative bio-blendstocks and surrogates

Validate against high-fidelity experimental data

Anisole - surrogate for methylated phenolics from biomass (Pitz et al., LLNL)

![Graph showing mole fraction vs temperature for JSR expt - Nancy and Model - LLNL. The graph includes a molecule structure of anisole and oxygen.](image1)

![Graph showing mole fraction vs temperature for JSR expt - CNRS and Model - LLNL. The graph includes a molecule structure of benzaldehyde and methane.](image2)
## Thrust I tasks

<table>
<thead>
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<td><strong>Thrust I</strong></td>
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<tr>
<td>Merit Function Definition</td>
<td>Miles (SNL) et al.</td>
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<tr>
<td>Efficiency Benefits of High Octane Fuels</td>
<td>Sluder (ORNL)</td>
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<tr>
<td>Effects of RON, HoV, and Octane Sensitivity</td>
<td>Ratcliff (NREL)</td>
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<td>Kolodziej/Ickes (ANL)</td>
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<tr>
<td>Dilution Limits on SI Combustion</td>
<td>Szybist (ORNL)</td>
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<tr>
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<td>Kolodziej/Wallner (ANL)</td>
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<tr>
<td>Fuel Effects on LSPI</td>
<td>Splitter (ORNL)</td>
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<tr>
<td>Advanced LD SI Engine Fuels Research</td>
<td>Sjöberg (SNL)</td>
</tr>
<tr>
<td>CFD of Thrust I Experiments</td>
<td>Som (ANL)</td>
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</tbody>
</table>
Engine performance merit function

Provides systematic ranking of blendstock candidates on engine efficiency when multiple fuel properties are varying simultaneously.

Allows fuel economy gains to be estimated based on fuel properties.

\[
\text{Merit} = \frac{(RON_{\text{mix}} - 92)}{1.6} - K \frac{(S_{\text{mix}} - 10)}{1.6} + \frac{0.01[ON / kJ/kg](HoV_{\text{mix}} - 415[kJ/kg])}{1.6} \\
+ \frac{(HoV_{\text{mix}} - 415[kJ/kg])}{130} + \frac{(S_{L_{\text{mix}}} - 46[cm/s])}{3} \\
- LFV_{150} - H \left( PMI - 2.0 \right) \left[ 0.67 + 0.5 \left( PMI - 2.0 \right) \right]
\]

RON = research octane number
K = engine-dependent constant
S = sensitivity (RON-MON)
ON = effective octane number
HoV = heat of vaporization
SL = flame speed
LFV = liquid fuel volume at 150°C
H = Heaviside function
PMI = particle mass index
Inconsistencies in literature regarding HOV impact on knock

HOV effect only been observed when covariant with octane sensitivity

Main conclusion: HOV is a thermal contributor to sensitivity

Consistent with vaporization effects in RON and MON tests

HOV appears to improve performance at elevated intake air temperatures

Sluder, Szybist (ORNL) McCormick, Ratcliff, Zigler (NREL)
Fuel effects on EGR and lean dilution limits

Quantify relative fuel impact on dilution tolerance and compare vs engine parameters
Fuel properties: flame speed, HOV
Engine: tumble, ignition energy, etc.

Hypothesis: laminar flame speed predicts dilution tolerance (lean and EGR) of an SI fuel
Preliminary results confirm positive correlation
Fuel effects on EGR and lean dilution limits

Single cylinder version of GM Ecotec 2.0L, 9.2: CR

Dilution tolerance correlates to laminar flame speed

Flame speed at ignition provides good indication of spark-to-CA5, combustion stability
# Thrust II tasks

<table>
<thead>
<tr>
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<tr>
<td><strong>Thrust II</strong></td>
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<tr>
<td>Evaluate Thrust I Fuel Compatibility with ACI Strategies</td>
<td>Dec (SNL) - LTGC</td>
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<td>Ciatti (ANL) - GCI</td>
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<td>Curran (ORNL) - GCI</td>
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<tr>
<td>Accelerate ACI Combustion System Development</td>
<td>Curran (ORNL) - RCCI</td>
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<td>Musculus (SNL) - RCCI</td>
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<td>Mueller (SNL) - LLFC</td>
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<td>High-throughput spray chamber</td>
<td>Pickett (SNL)</td>
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<td>X-ray imaging of GDI sprays with alcohol blends</td>
<td>Powell (ANL)</td>
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<tr>
<td>PMI refinement - extension to bio-blendstocks</td>
<td>Ratcliff (NREL)</td>
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<tr>
<td>PM formation fundamentals</td>
<td>Storey (ORNL)</td>
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<tr>
<td>Fuel effects on gaseous emission control</td>
<td>Toops/Pihl (ORNL)</td>
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Thrust I Fuel Behavior in GCI

Evaluate Thrust I fuel performance in GCI engine,
Particular focus: challenging low load operation

Identify relationships of fuel HoV, sensitivity with GCI combustion, emissions, and performance
Multi-cylinder RCCI experiments

1.9L GM diesel engine platform with production viable hardware
Modified for both single- and dual-fuel LTC operation

Identify performance trends in CI/LTC strategies spanning RCCI + GCI
Vary reactivity differential between premixed and DI fuels

Matched experiments to optical work at SNL

ORNL RCCI Multi-Cylinder 1.9L GM (Curran)
Optical diagnostics of RCCI

Measure in-cylinder mixing/kinetics to optimize dual-fuel heat-release
Noise, efficiency, and load range

Understand mixing/ignition interaction for different reactivity combinations

Provides in-cylinder diagnostic for measuring reactivity stratification
Adds new insights for CFD as well
18 month decision point
First major milestone: 18 month decision point

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

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
The 18 months decision point

FP
Impact of fuel properties on engine performance

AED
Experimental assessment of impacts of engine parameters on efficiency and emissions

ASSERT
Environmental impacts, cost, scalability, feed logistics

MT
Infrastructure and legacy fleet compatibility

TK
Simulation of fuel and engine parameter impacts on efficiency and emissions

Database

Data for defining co-optimized technology options

LGGF
Low-GHG blendstock properties and pathway attributes
Approach

Need to explicitly account for uncertainty
Identifying options: a multi-objective optimization problem

Maximize:
- Engine Efficiency [x]
- Vehicle Fuel Economy [ ]

Minimize:
- Number of blendstocks [x]
- Other parameter [ ]

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<tr>
<th>Constraints:</th>
<th>Base scenario</th>
<th>Alt scenario 1</th>
<th>Alt scenario 2</th>
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<tbody>
<tr>
<td>High</td>
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<td>Med</td>
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<td>Low</td>
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<td>\Delta GHG</td>
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<tr>
<td>H\textsubscript{2}O consumption</td>
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<td>Viable routes</td>
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<td>Feedstock cost</td>
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<td>Pipeline compatibility</td>
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<td>Tech Readiness Level</td>
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<td>Energy density</td>
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Solution set A
Solution set B
Solution set C
Status and next steps

Initiative started October 1 2016

FY16 budget: $27M; FY17 budget request: $30M

External advisory board formed

Active stakeholder engagement efforts underway (sign up!)
Acknowledgements

DOE Sponsors:
Alicia Lindauer (BETO)
Kevin Stork and Gurpreet Singh (VTO)

Co-Optima Technical Team Leads:
Dan Gaspar (PNNL), Paul Miles (SNL), Jim Szybist (ORNL), Jennifer Dunn (ANL), Matt McNenly (LLNL), Doug Longman (ANL)

Other Co-Optima Leadership Team Members:
John Holladay (PNNL), Art Pontau (SNL), Robert Wagner (ORNL)
Thank You