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

# Big-Picture Issues Confronting Co-Optima

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Sustainable Transportation Summit

Washington, D.C.

July 12, 2016

**NREL/PR-5400-66904**
NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

# Major Co-Optima Challenges



# What fuels do engines want?

# Fundamentally different **combustion dynamics** require **different fuel properties**

| Spark ignition (gasoline) – Thrust I | Advanced Compression Ignition (ACI) – Thrust II | Compression ignition (diesel) – Thrust II |
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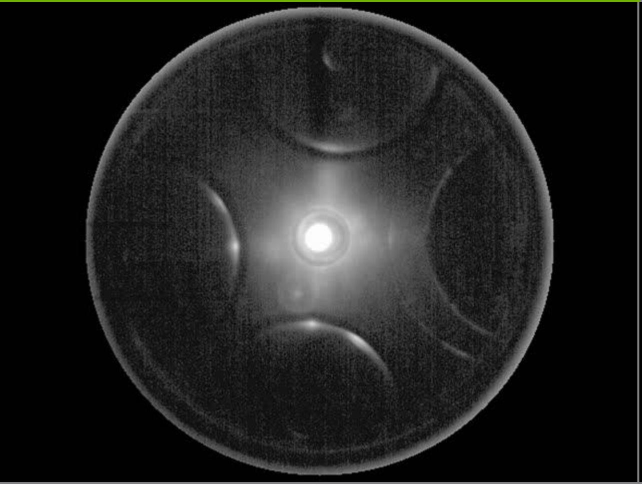
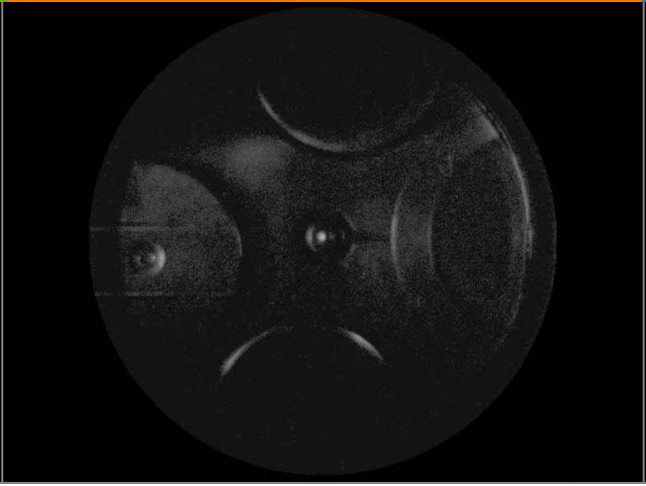
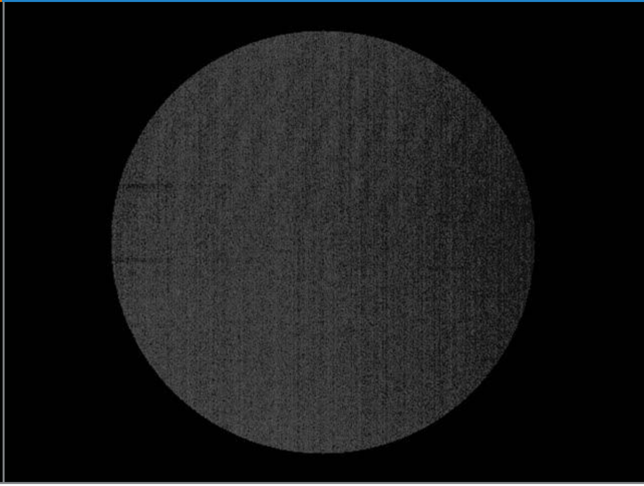
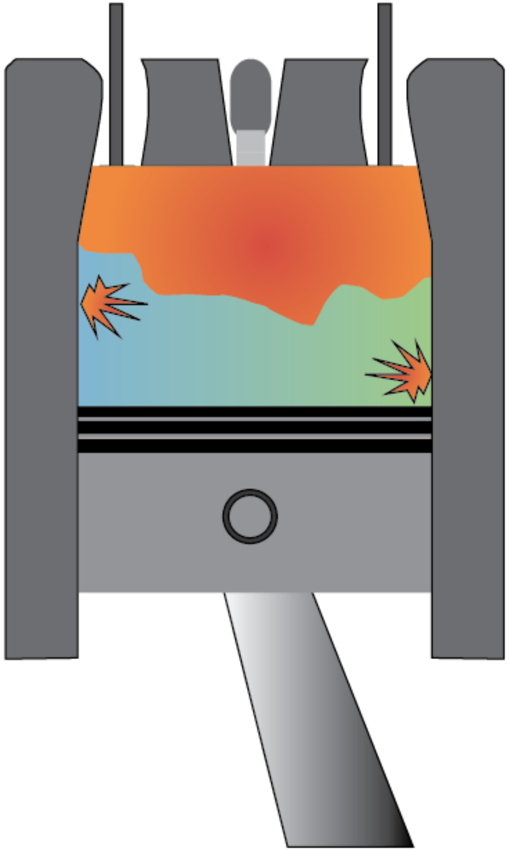
|  |  |  |

# Spark ignition (Thrust I) engines

## Central challenge: avoiding knock

## Important fuel properties:

- Octane number (RON and MON)
- Heat of vaporization
- Flame speed
- Particulate matter index
- Distillation



# 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

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

RON = research octane number
K = engine-dependent constant
S = sensitivity (RON-MON)
ON = effective octane number
HoV = heat of vaporization
$S_L$ = flame speed
LFV = liquid fuel volume at 150° C
H = Heaviside function
PMI = particle mass index

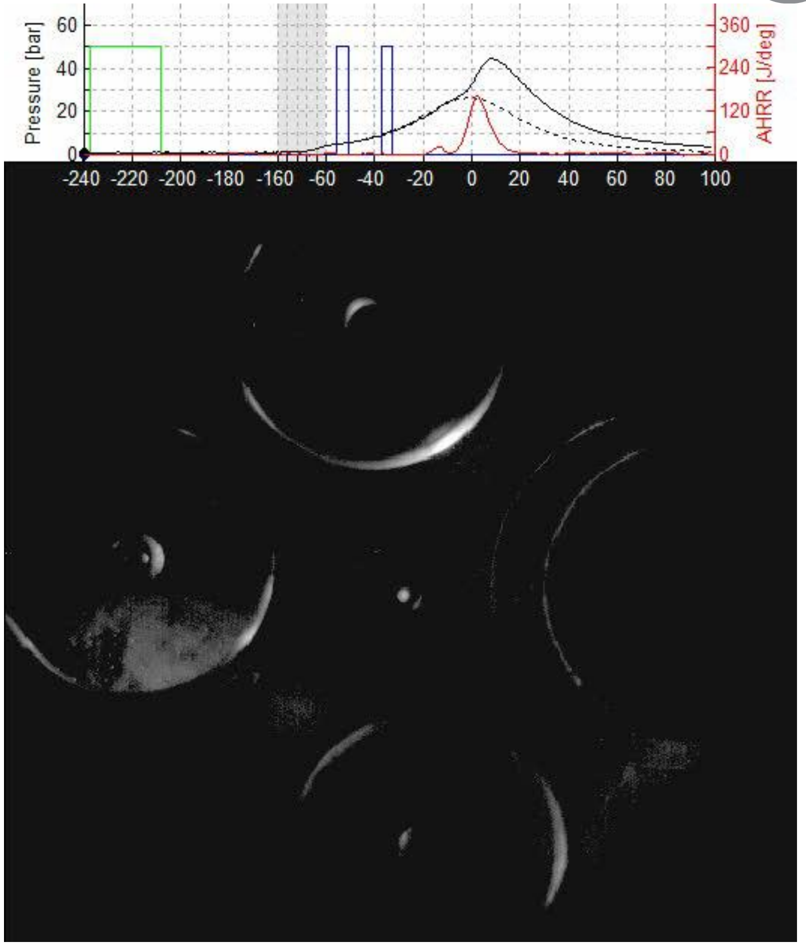
# Thrust II engines: the Wild West

In-cylinder mixing/ kinetics needs to be optimized to control ignition timing

Requirements vary as speed/load changes

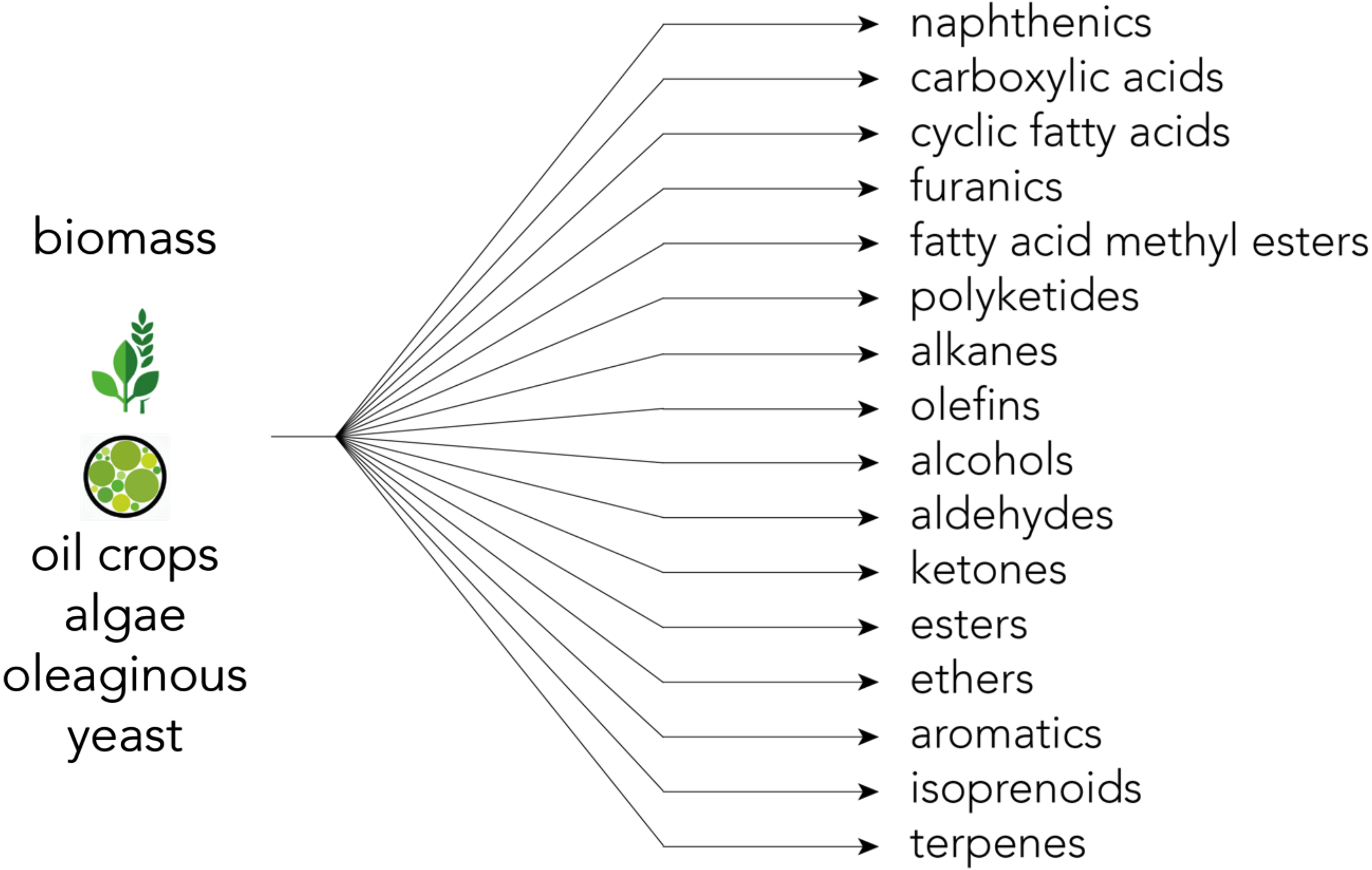
Significant engineering innovations required

Much progress already achieved with air handling, fuel injection, novel strategies




Source: Mark Musculus SNL

# 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

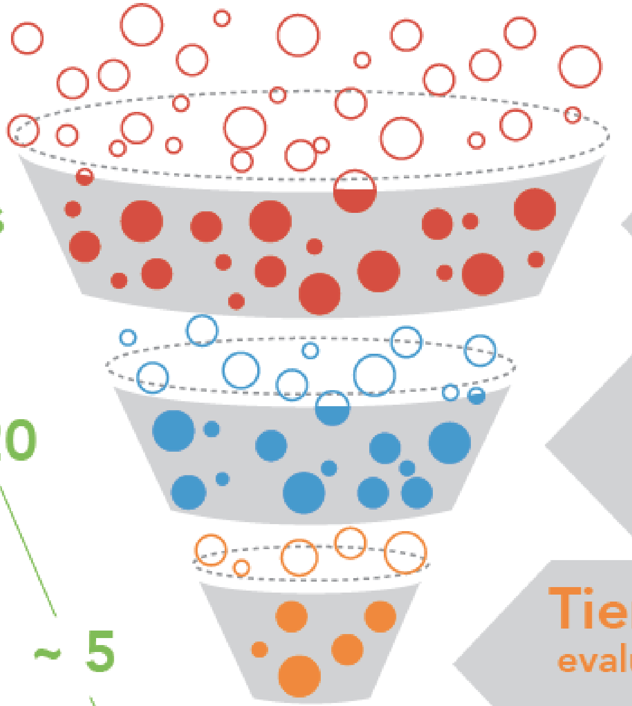
# Fuel selection criteria ("decision tree")

none | hundreds

~ one liter | ~ 20

~ gallons | ~ 5

quantify of fuel required | number of candidates



## 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

# 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

# What will work in the real world?

New fuels must be sustainable, affordable, and scalable

# Cost and environmental impact analyses

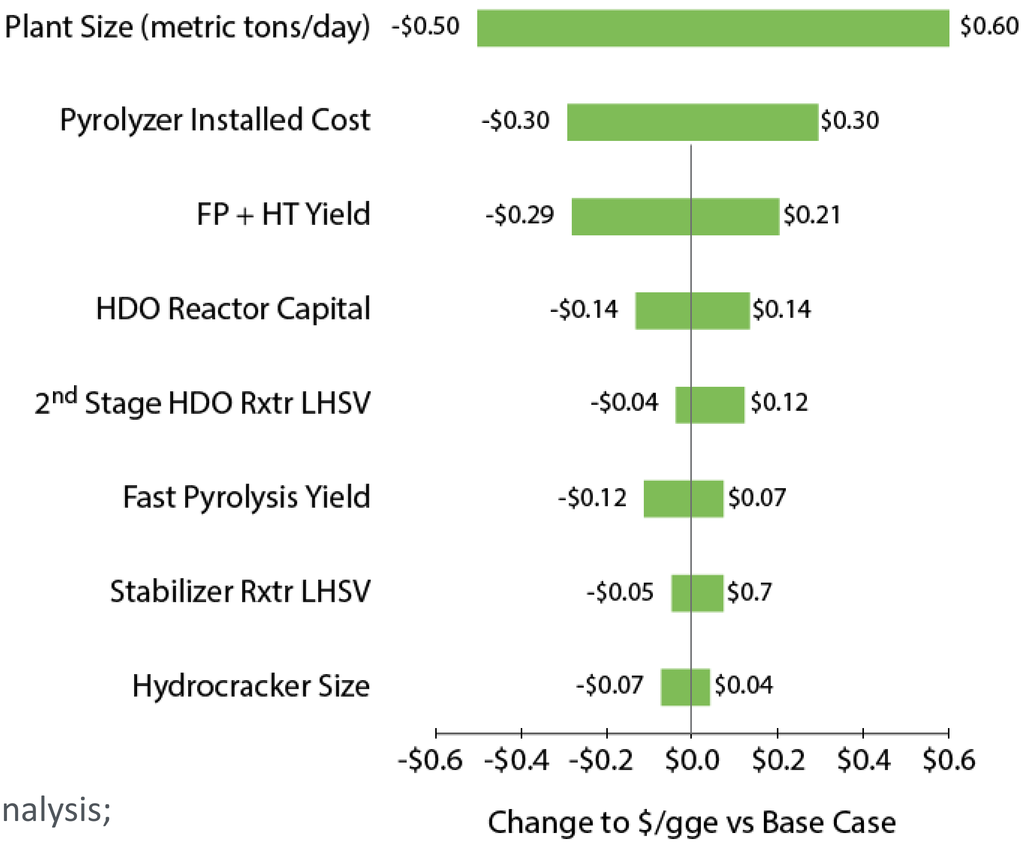
## High-level LCA, TEA,* feedstock availability analyses

Identify cost/environmental/scale attributes

## Fifteen key metrics identified

GHG, water, economics, TRL

## Evaluation of 20 Thrust I blendstocks underway



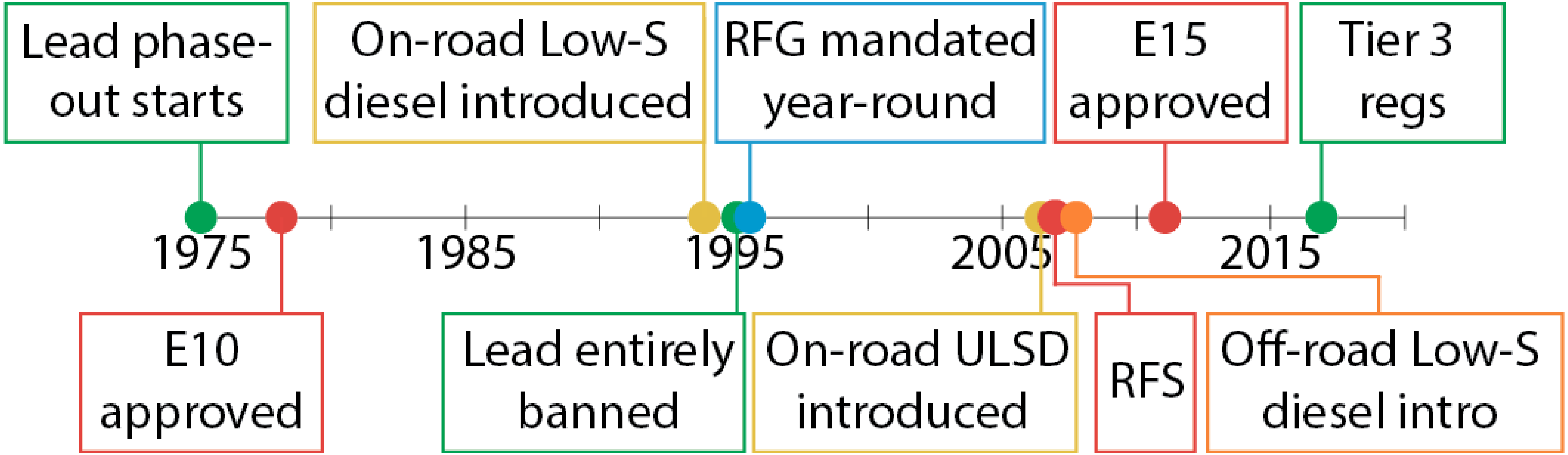

* LCA = Life cycle analysis; TEA = techno-economic analysis; TRL = technology readiness level

# Identifying/mitigating market barriers

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

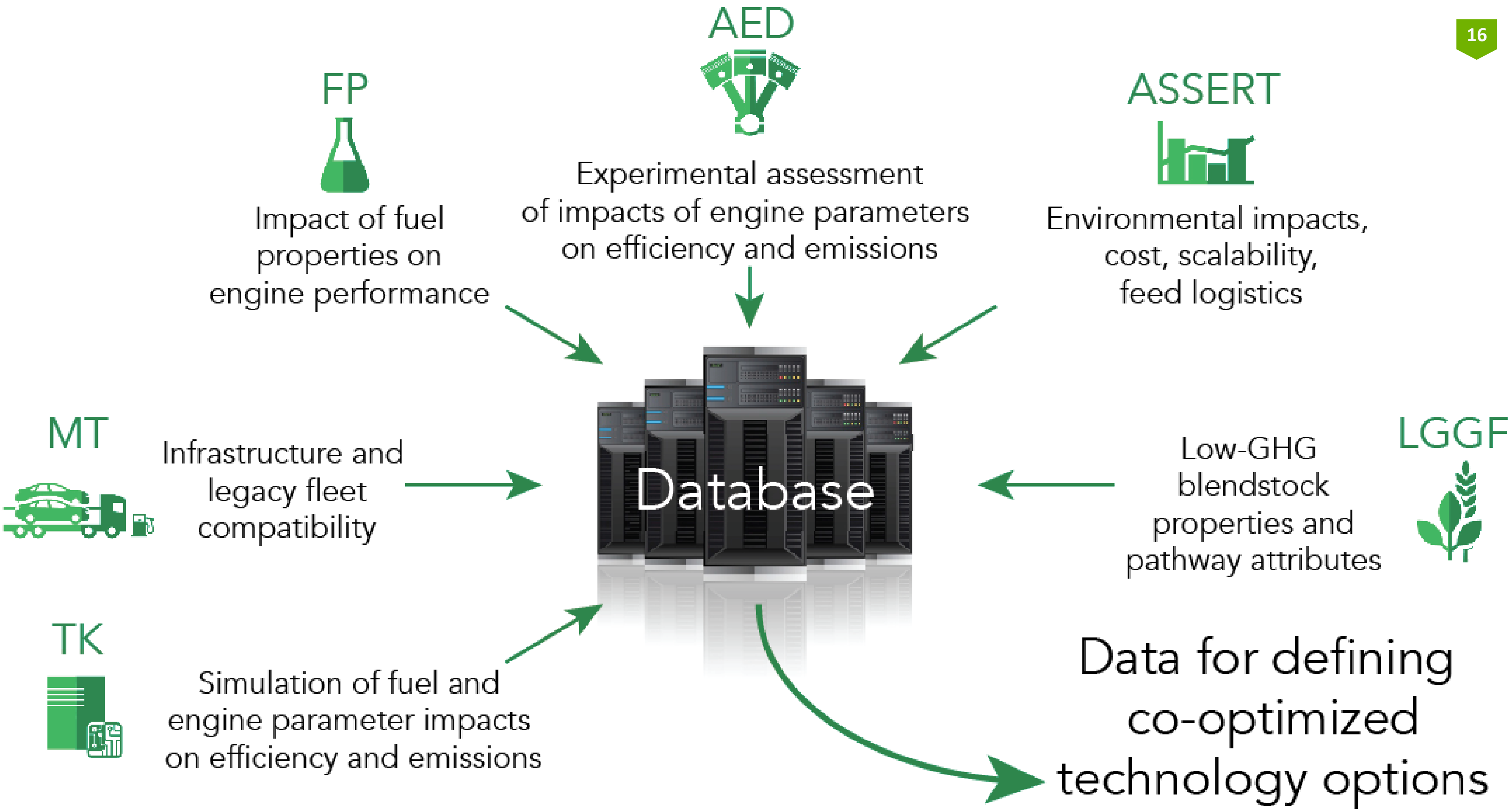
Analysis of new fuel and vehicle introduction

Engage stakeholders across value chain



# How do we co-optimize?

Identifying the best options, subject to many constraints


AED
Experimental assessment of impacts of engine parameters on efficiency and emissions
FP
Impact of fuel properties on engine performance
ASSERT
Environmental impacts, cost, scalability, feed logistics
MT
Infrastructure and legacy fleet compatibility
Database
LGGF
Low-GHG blendstock properties and pathway attributes
TK
Simulation of fuel and engine parameter impacts on efficiency and emissions
Data for defining co-optimized technology options

# Approach

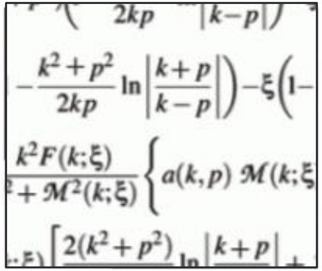
Database: fuel properties, sustainability, affordability, scalability, infrastructure, and retail attributes

$\Delta$GHG = *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

"Optimizer"

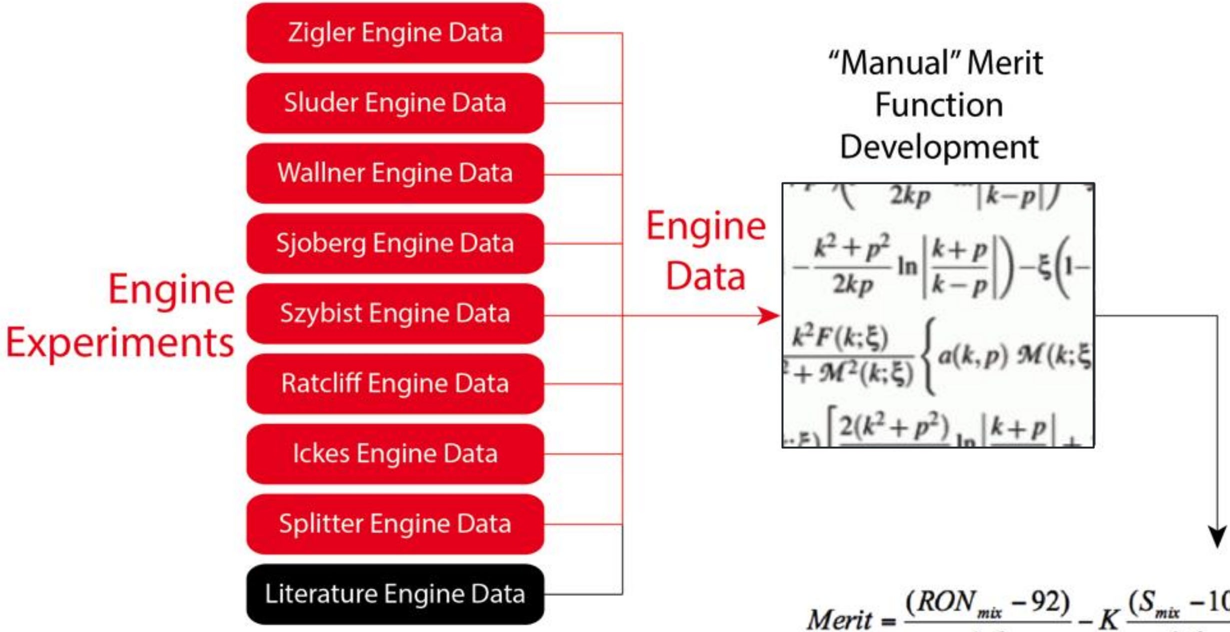
Engine/vehicle merit function



Optimal fuel blend formulations

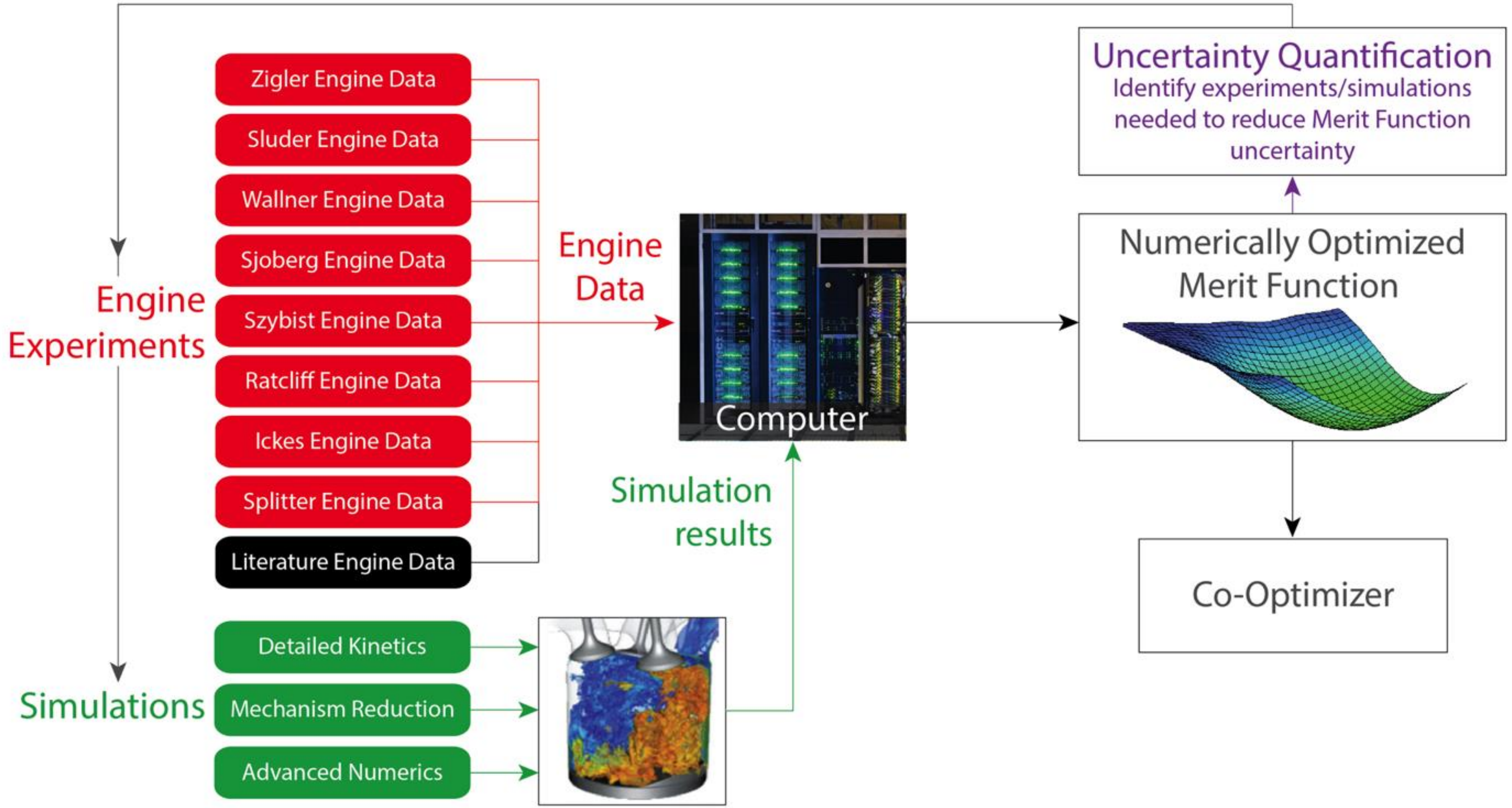
Need to explicitly account for uncertainty

# Current merit function development approach




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

# Numerically optimized merit function



# Identifying options: a multi-objective optimization problem

| | | | | |
|---|---|---|---|---|
| Maximize: | Engine Efficiency | X | Vehicle Fuel Economy | ☐ |
| Minimize: | Number of blendstocks | X | Other parameter | ☐ |

| | Base scenario | | | Alt scenario 1 | | | Alt scenario 2 | | |
|---|---|---|---|---|---|---|---|---|---|
| Constraints: | High | Med | Low | High | Med | Low | High | Med | Low |
| ΔGHG | X | | | X | | | | X | |
| $H_2O$ consumption | | X | | | | X | | | X |
| Viable routes | | X | | X | | | X | | |
| Feedstock cost | | | X | | | | | | |
| Pipeline compatibility | X | | | | X | | | | X |
| Tech Readiness Level | | X | | | X | | | X | |
| Energy density | | X | | | | X | | | X |
| | Solution set A | | | Solution set B | | | Solution set C | | |

# Acknowledgements


## DOE Sponsors:

Alicia Lindauer and Borka Kostova (BETO)

Kevin Stork, Gurpreet Singh, and Leo Breton (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