Big-picture issues confronting Co-Optima

John Farrell

Sustainable Transportation Summit

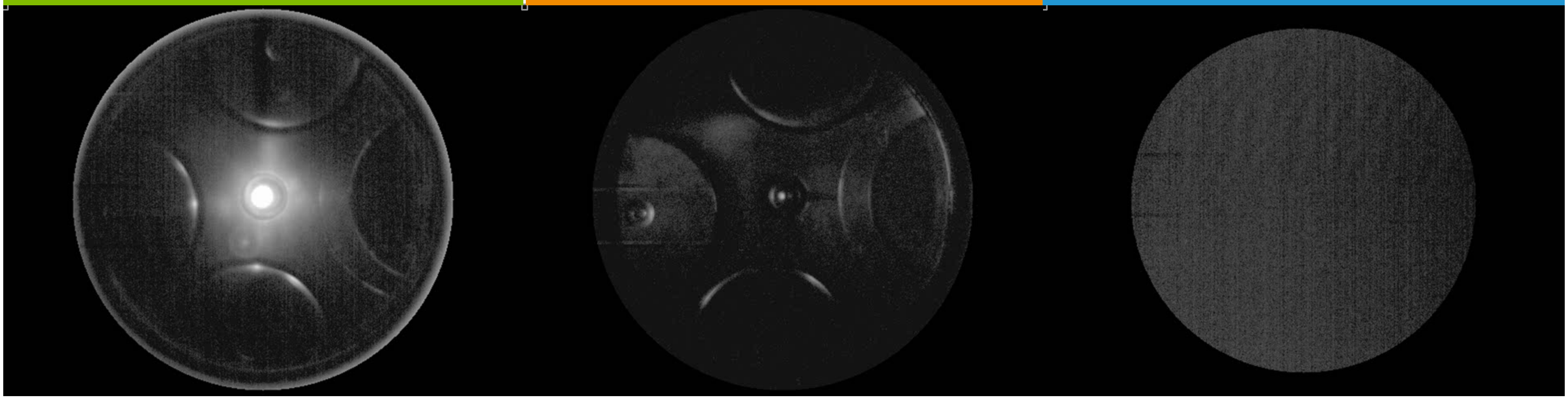
July 12, 2016

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



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

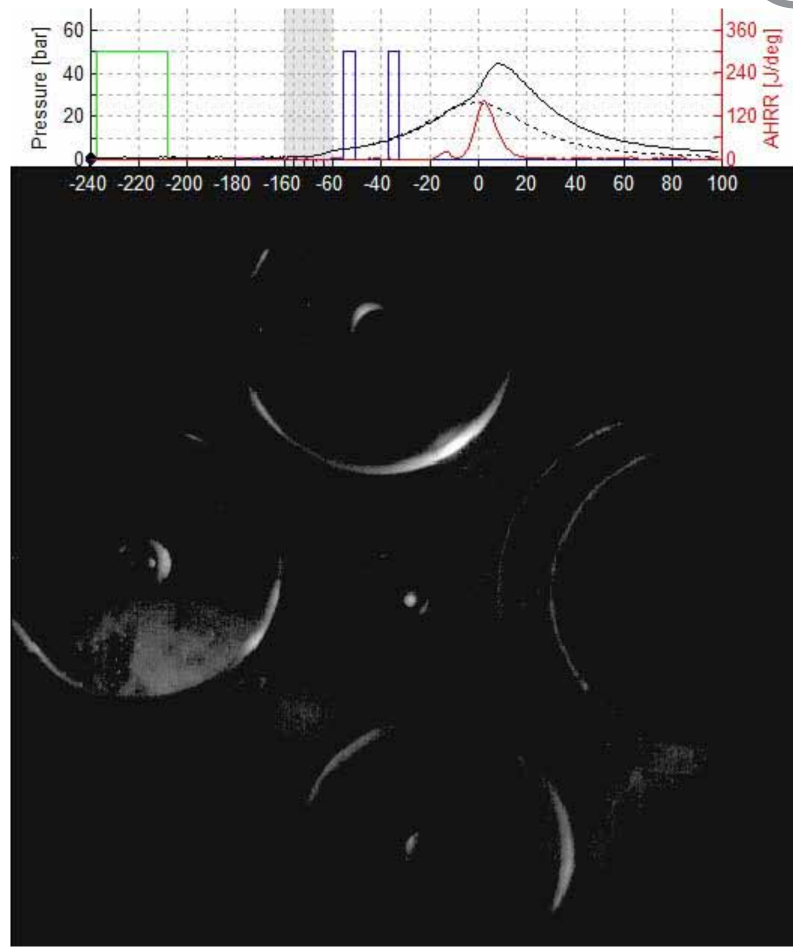
Thrust II engines: the Wild West

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

Requirements vary as speed/load changes

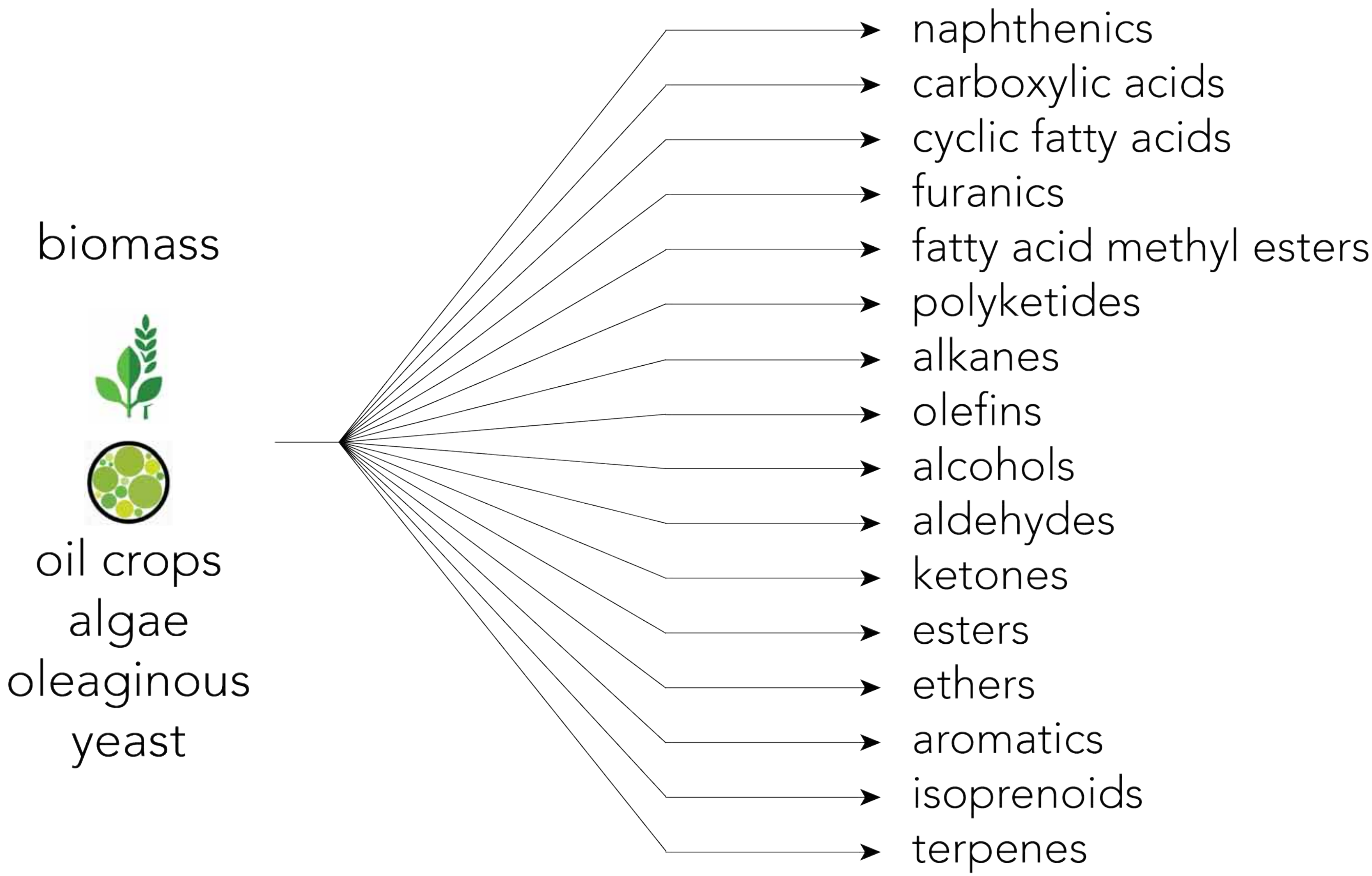
Significant engineering innovations required

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

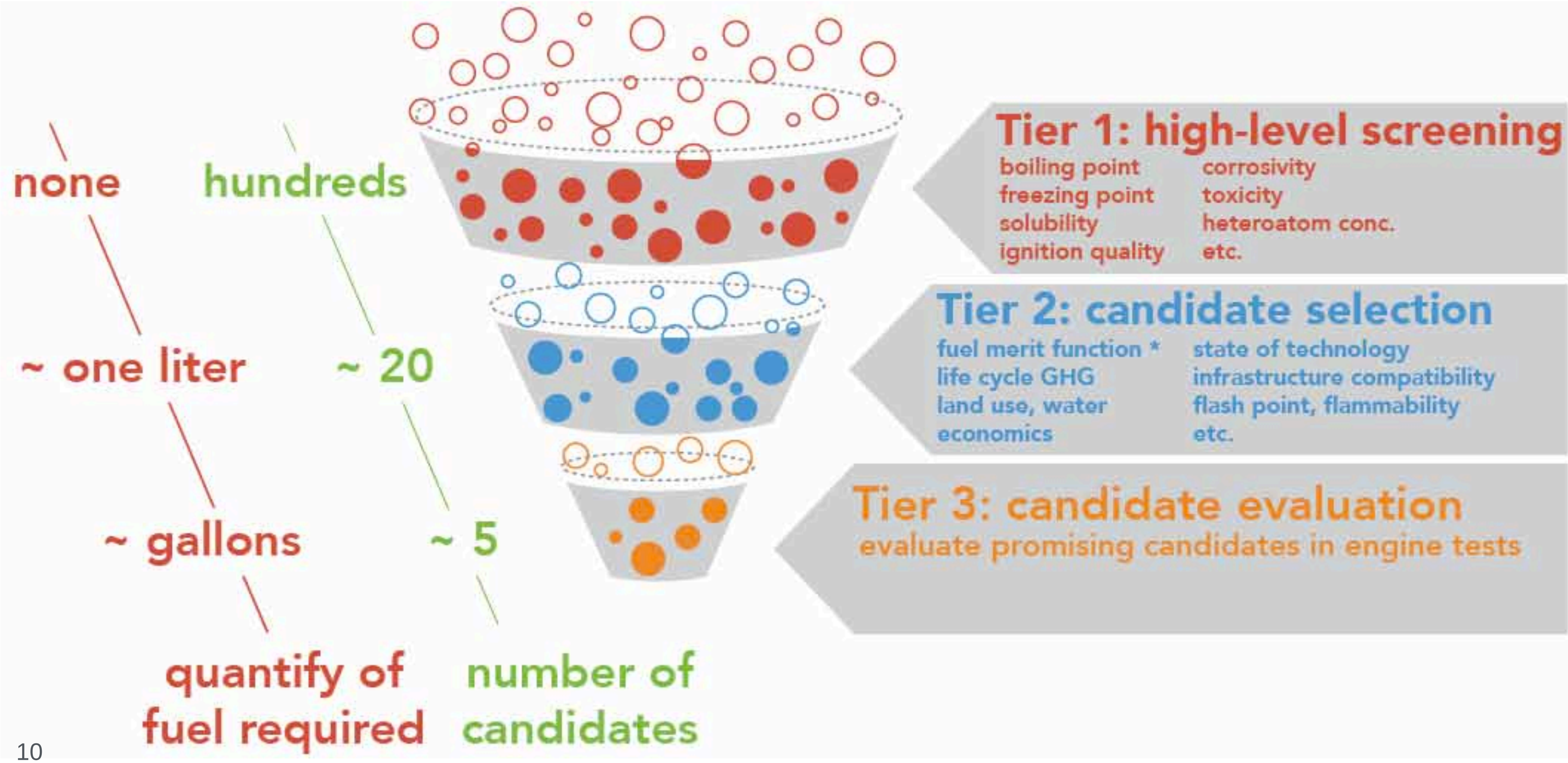


Source: Mark Musculus SNL

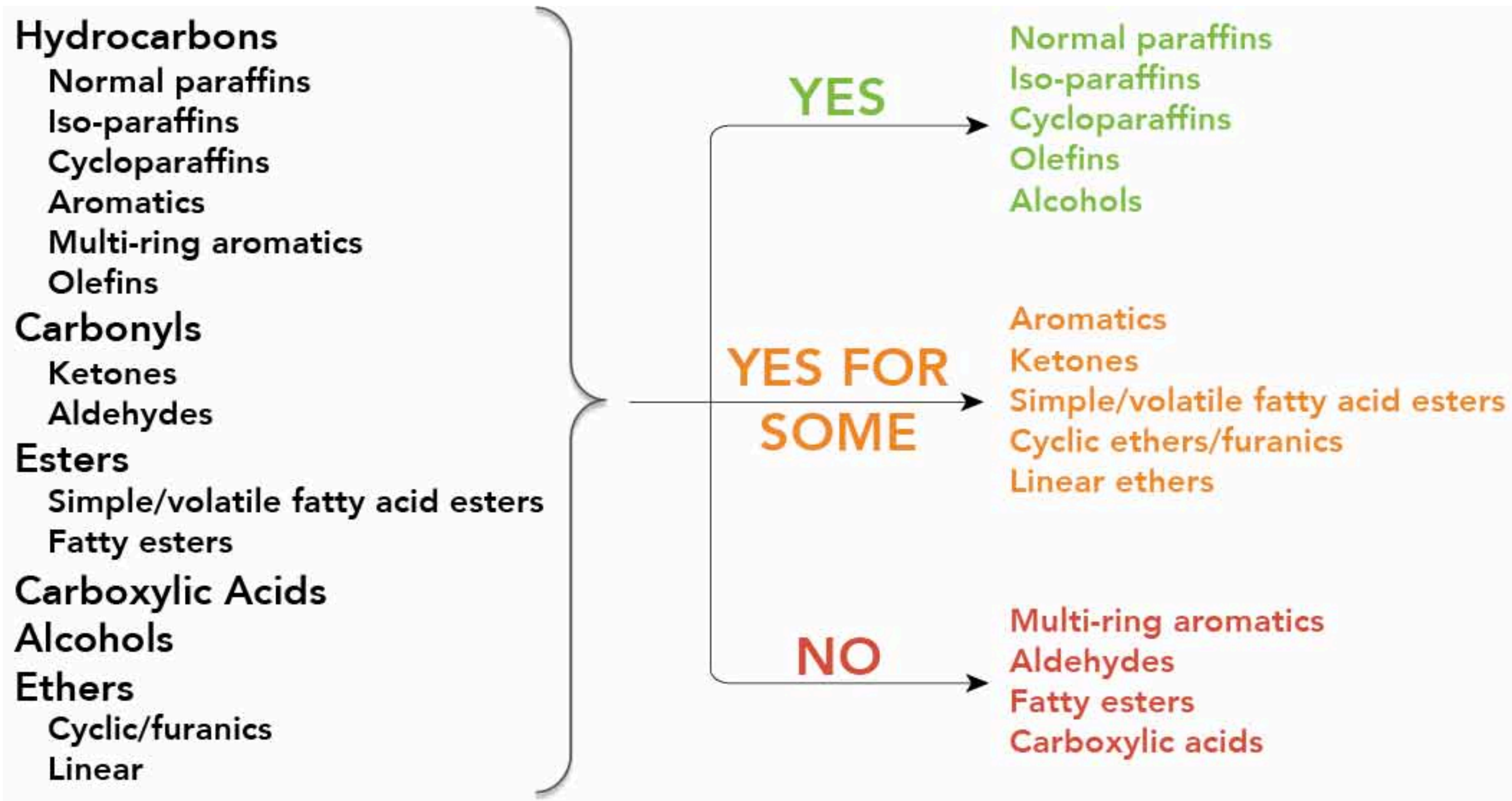
What fuels can we make?


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”)



Thrust I decision tree results



What will work in the real world?

New fuels must be sustainable, affordable, and scalable

Cost and environmental impact analyses

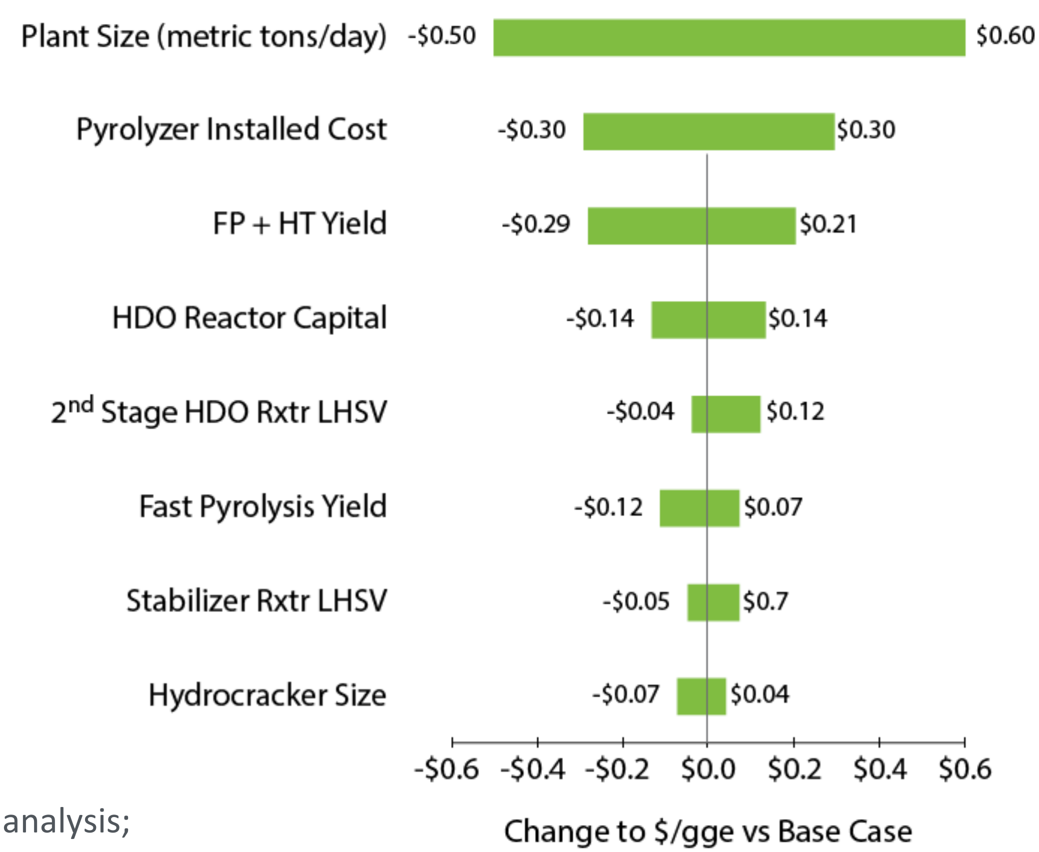
High-level LCA, TEA,*
feedstock availability analyses

Identify cost/environmental/
scale attributes

Fifteen key metrics identified

GHG, water, economics, TRL

Evaluation of 20 Thrust I
blendstocks underway



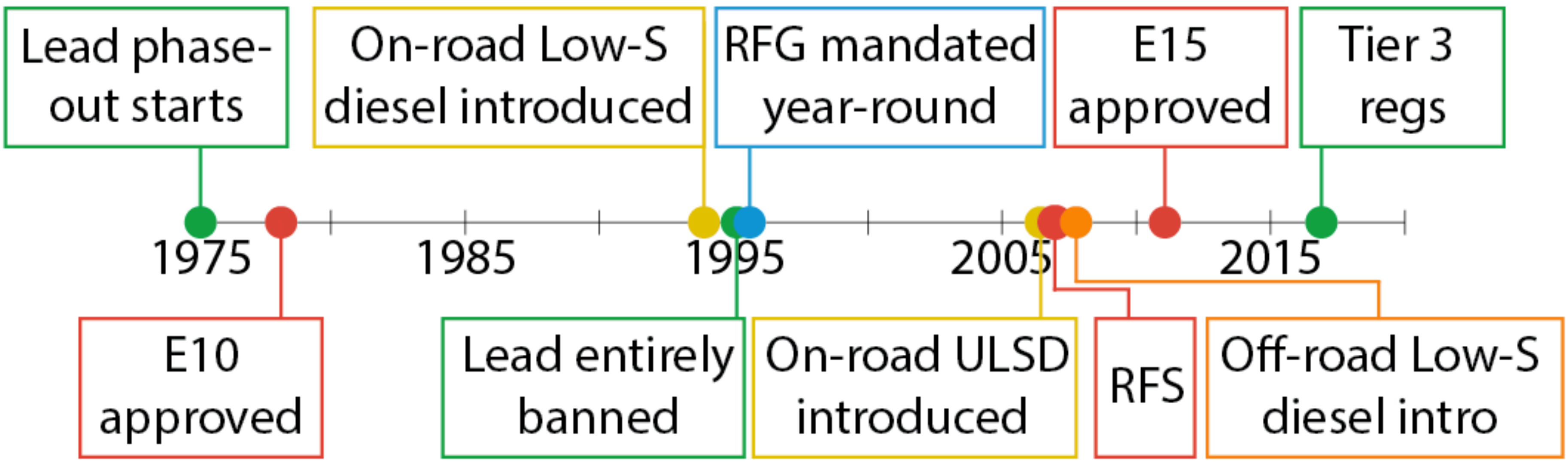
* LCA = Life cycle analysis; TEA = techno-economic analysis;
TRL = technology readiness level

Identifying/mitigating market barriers

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

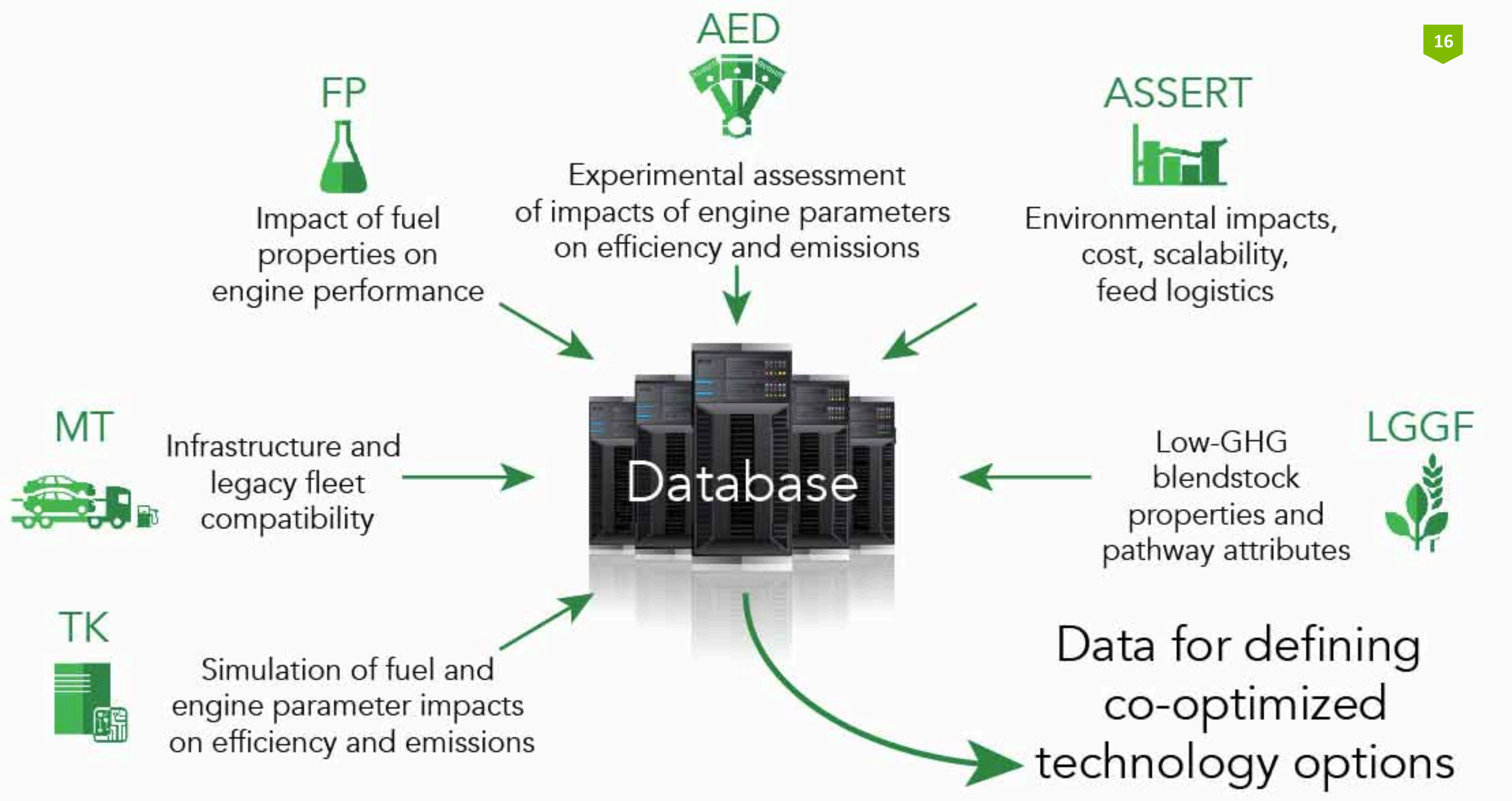
Analysis of new fuel and vehicle introduction

Engage stakeholders across value chain



How do we co-optimize?

Identifying the best options, subject to many constraints


AED
FP
ASSERT
Experimental assessment of impacts of engine parameters on efficiency and emissions
Impact of fuel properties on engine performance
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

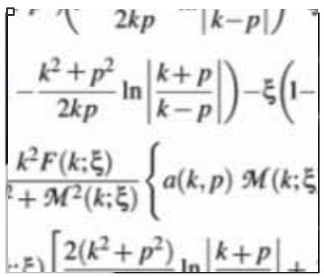
Database: fuel properties, sustainability, affordability, scalability, infrastructure, and retail attributes

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

"Optimizer"

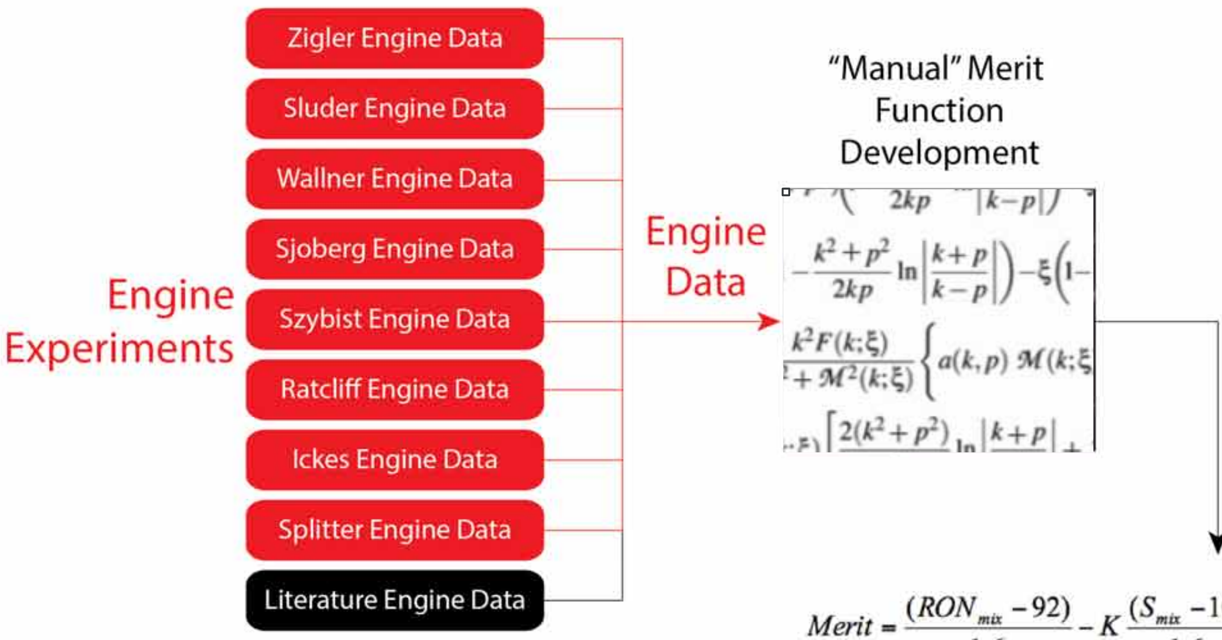
Engine/vehicle merit function



Optimal fuel blend formulations

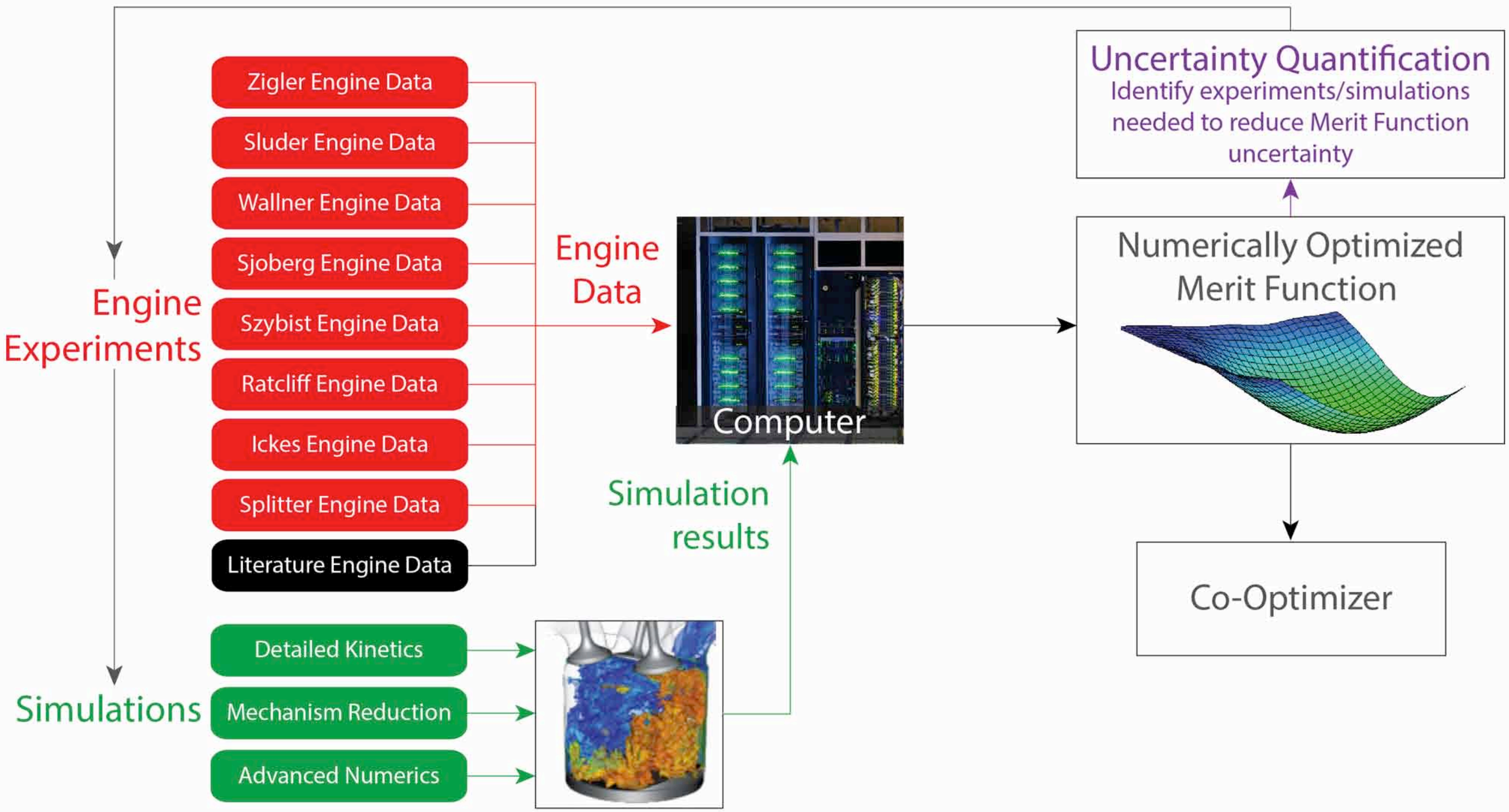
Need to explicitly account for uncertainty

Current merit function development aproach



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

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 [ ]

Constraints:	Base scenario High	Base scenario Med	Base scenario Low	Alt scenario 1 High	Alt scenario 1 Med	Alt scenario 1 Low	Alt scenario 2 High	Alt scenario 2 Med	Alt scenario 2 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