Co-Optimization of Fuels and Engines

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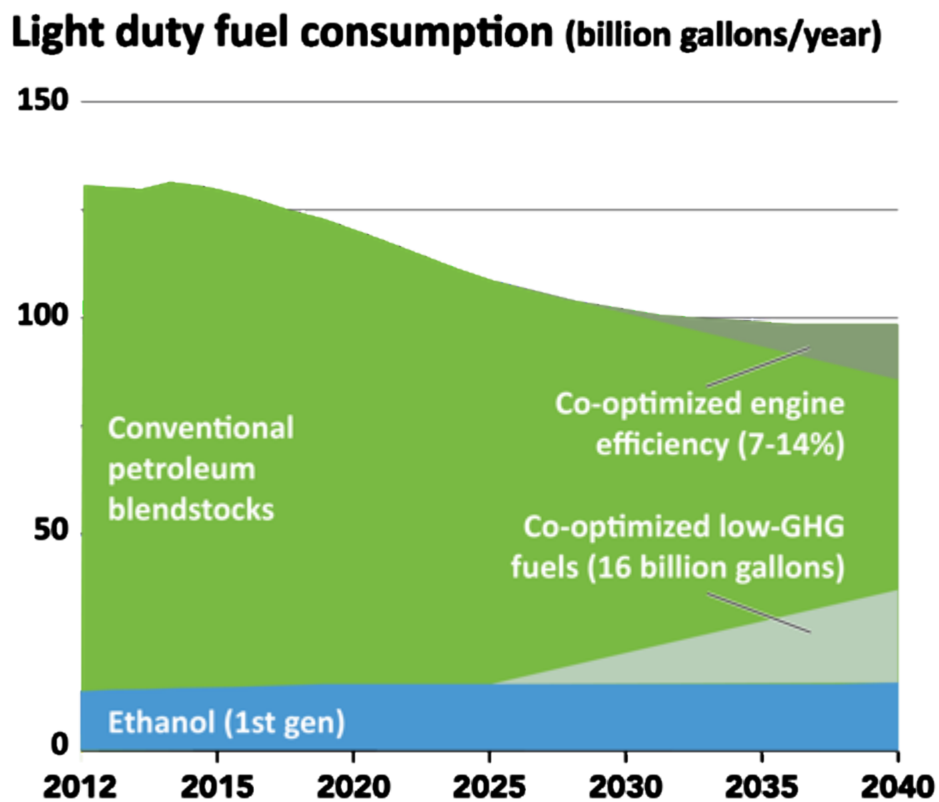
Goal: better fuels and better vehicles **sooner**

Fuel and Engine Co-Optimization

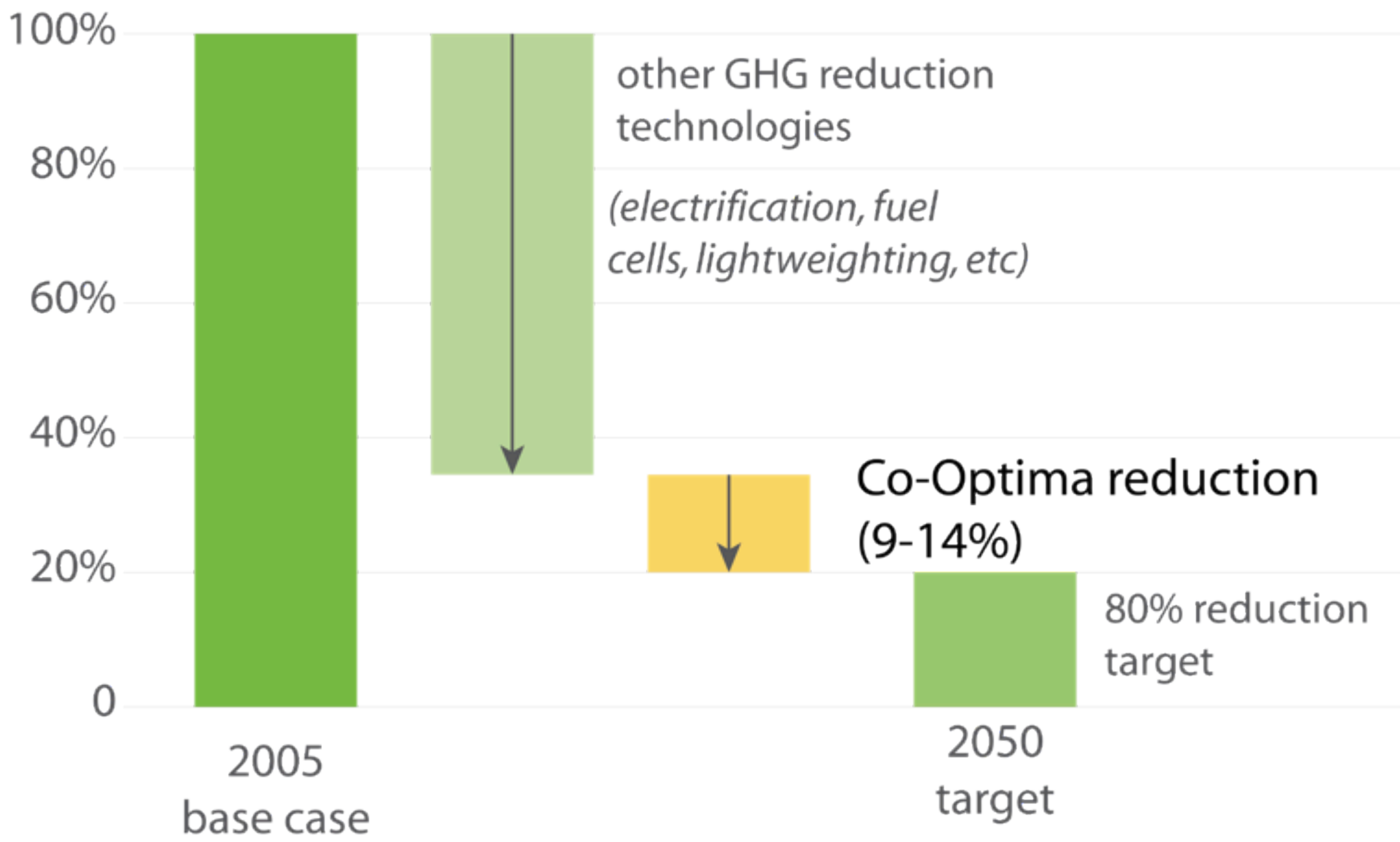
- What fuel properties maximize engine performance?
- How do engine parameters affect efficiency?
- What fuel and engine combinations are sustainable, affordable, and scalable?

30% per vehicle petroleum reduction via efficiency and displacement



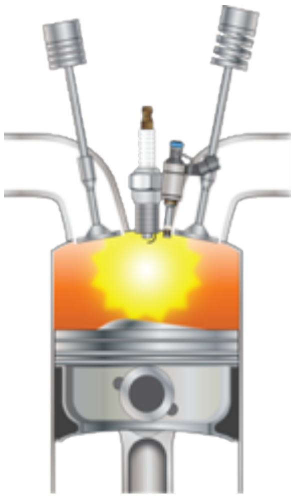
source: EIA 2014 reference case

National goal: 80% reduction in transportation GHG by 2050

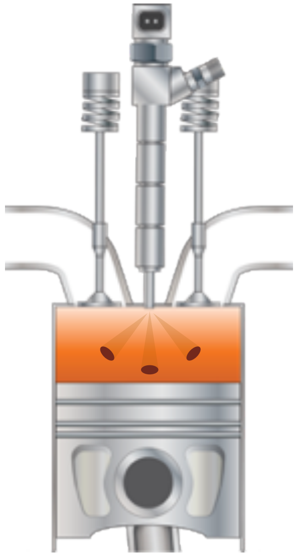


Parallel efforts are underway

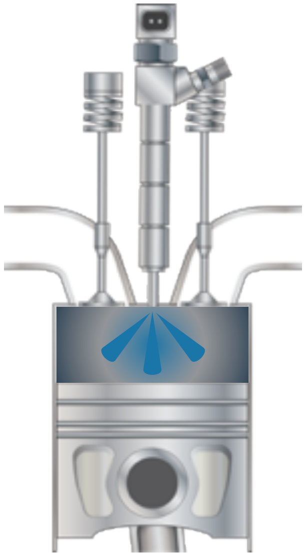
Thrust I: Spark Ignition (SI)	Thrust II: Advanced Compression Ignition (ACI) kinetically-controlled and compression-ignition combustion



Low reactivity fuel



Range of fuel properties TBD



High reactivity fuel

Applicable to

light, medium, and heavy-duty engines

hybridized and non-hybridized powertrains

Six integrated and coordinated teams

Low Greenhouse Gas Fuel Production

Advanced Engine Development

Fuel Properties

Modeling and Simulation Tools

Life-cycle, techno-economic, and feedstock analyses

Market Transformation

Leveraging expertise and facilities from 9 U.S. National Labs

and (starting in 2017) leading universities

Integrated multi-lab teams with significant external stakeholder engagement

13 Light and heavy duty vehicle manufacturers

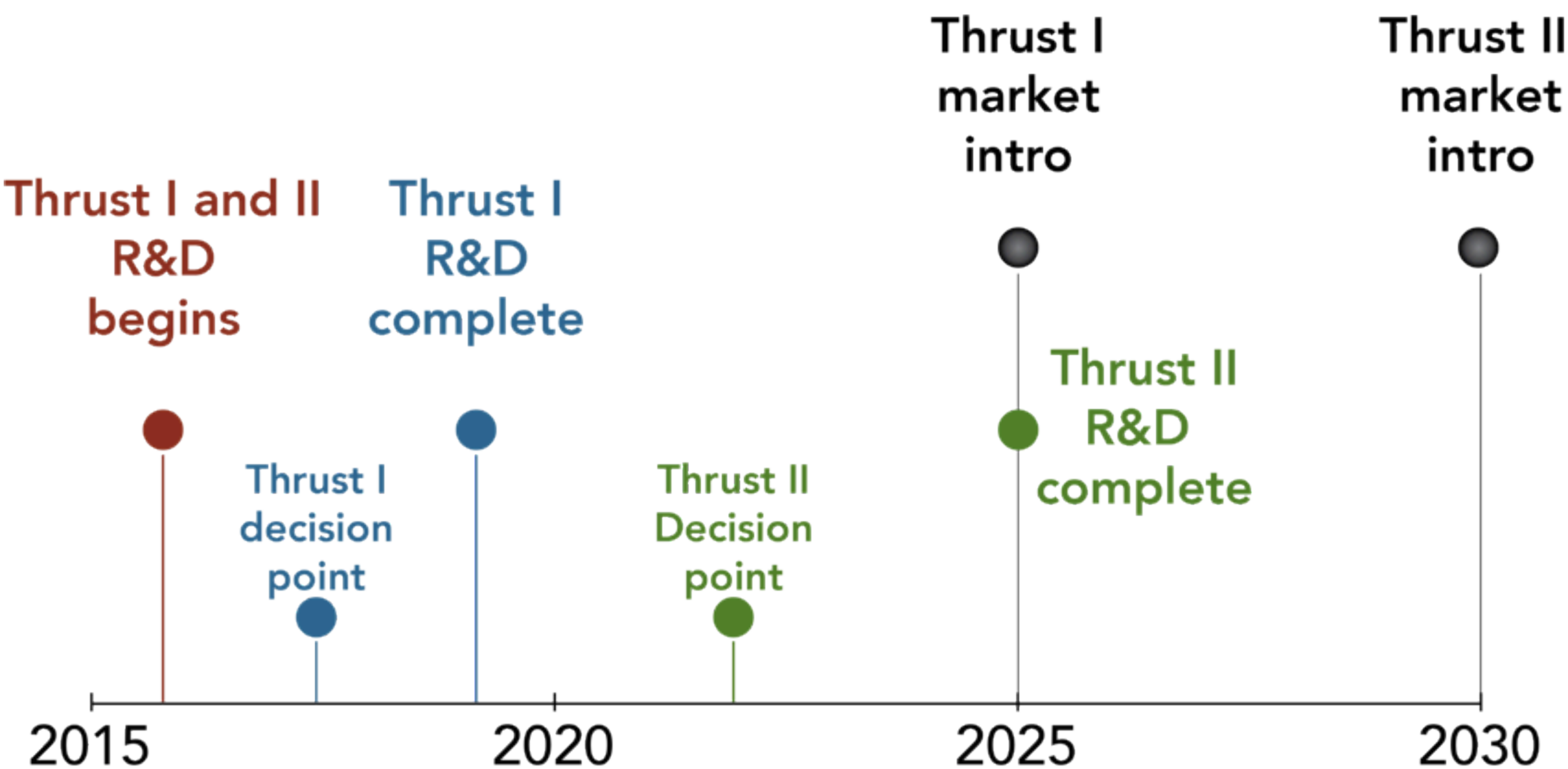
10 Oil companies/ refiners

8 Biofuel companies

4 Regulatory agencies

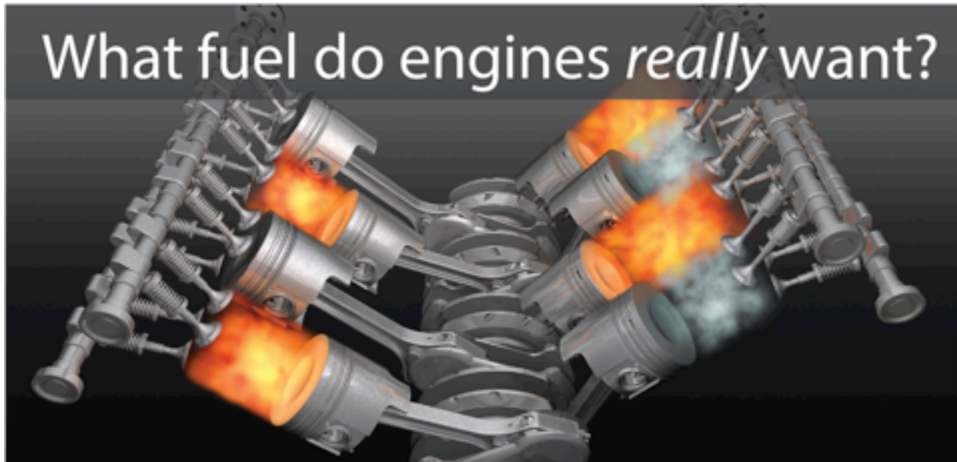
2 End consumer organizations

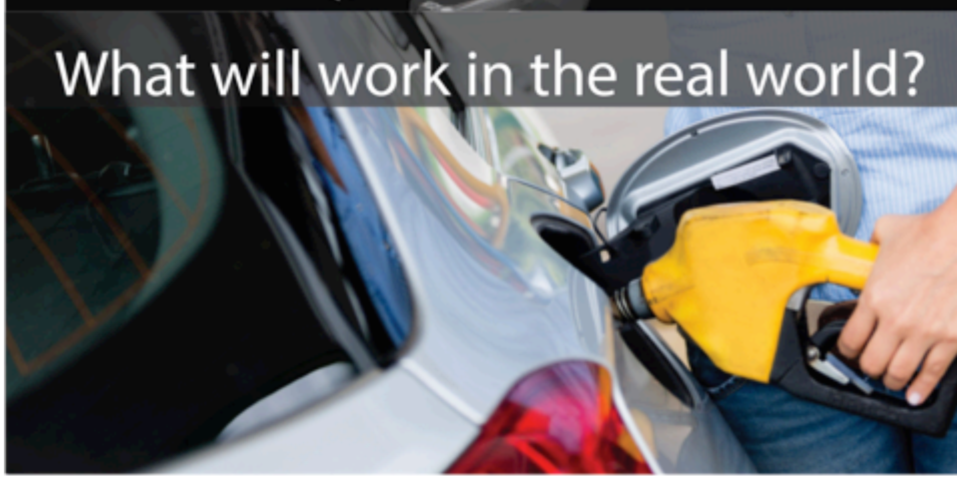
R&D and commercialization targets



Major Co-Optima Challenges

Co-Optima Technical Challenges



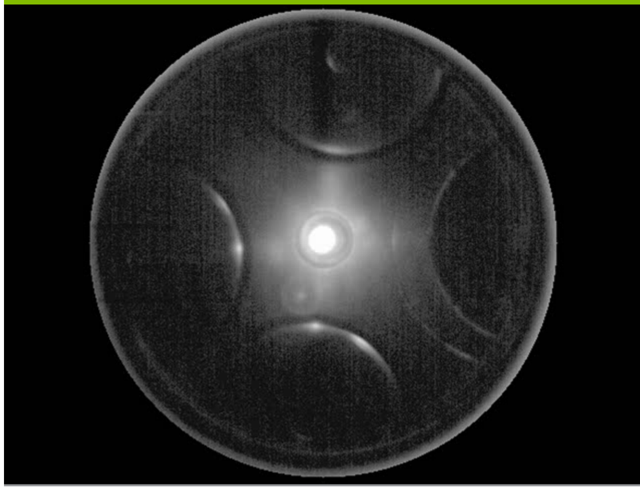


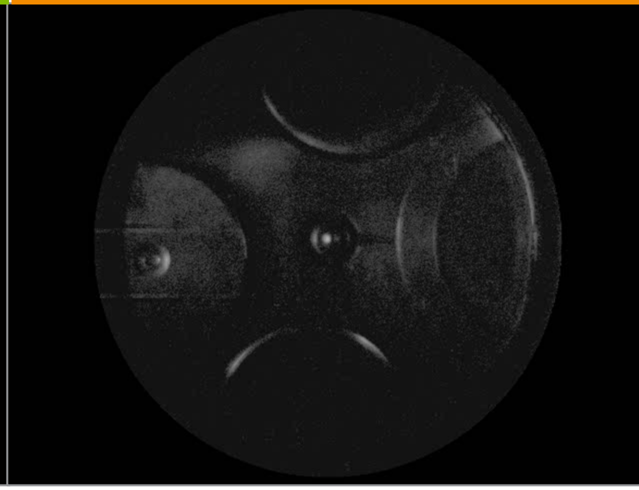
How do we “co-optimize”?

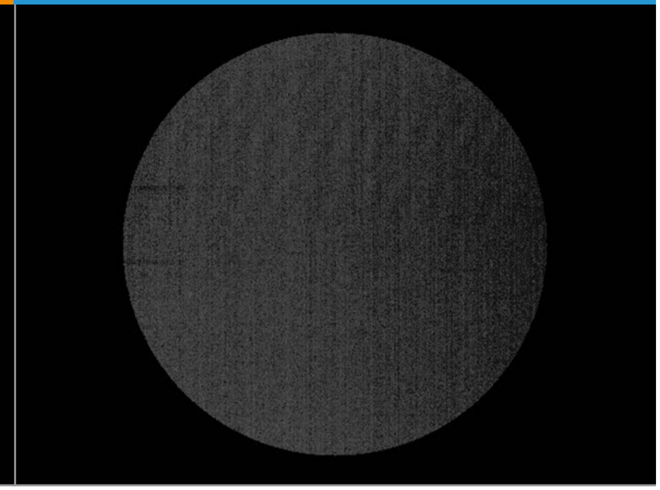
What fuels do engines want?

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

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







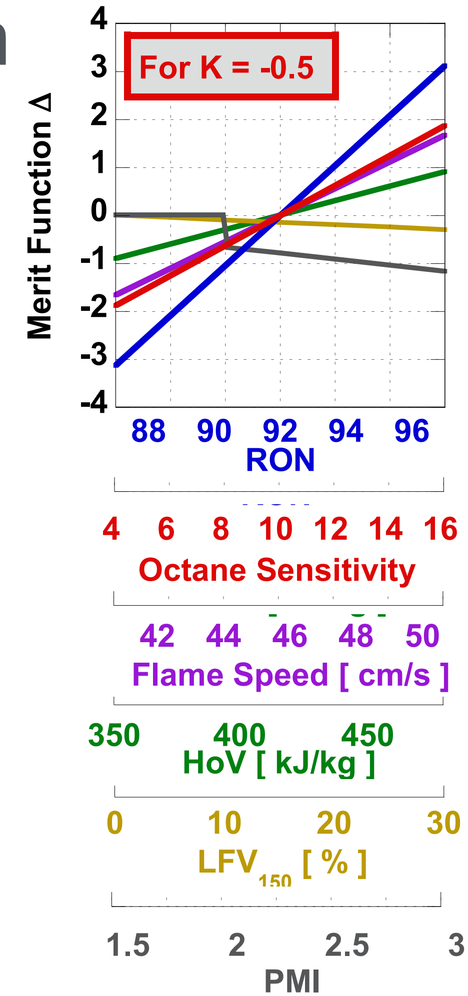
Engine performance merit function

RON | Octane Sensitivity | Heat of Vaporization

$$\text{Merit} = \alpha \bullet [RON - 92] - \beta \bullet K \bullet [S - 10] + \gamma \bullet ON \bullet [HOV - 415] + \delta \bullet [HOV - 415]$$

$$+ \varepsilon \bullet [S_L - 46] - LFV150 - H(PMI - 2.0)[\zeta + 0.5(PMI - 2.0)]$$

Flame Speed | Distillation | Particulate Emissions



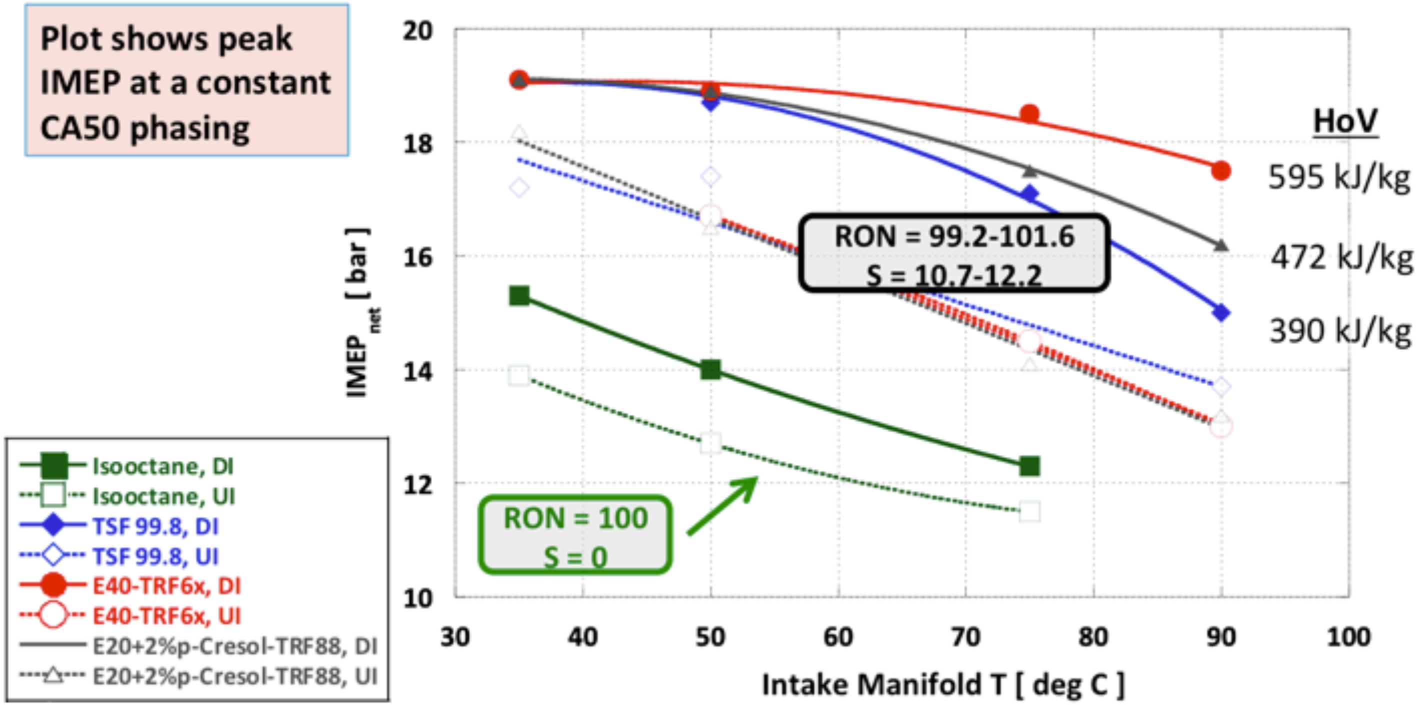
- Merit function being developed and refined
  - Are these the right fuel properties?
  - Are their effects properly quantified?
- We'll test the central fuel hypothesis using biofuels with different structures / functional groups than petroleum fuels

HoV can be important for DI at high intake temperatures

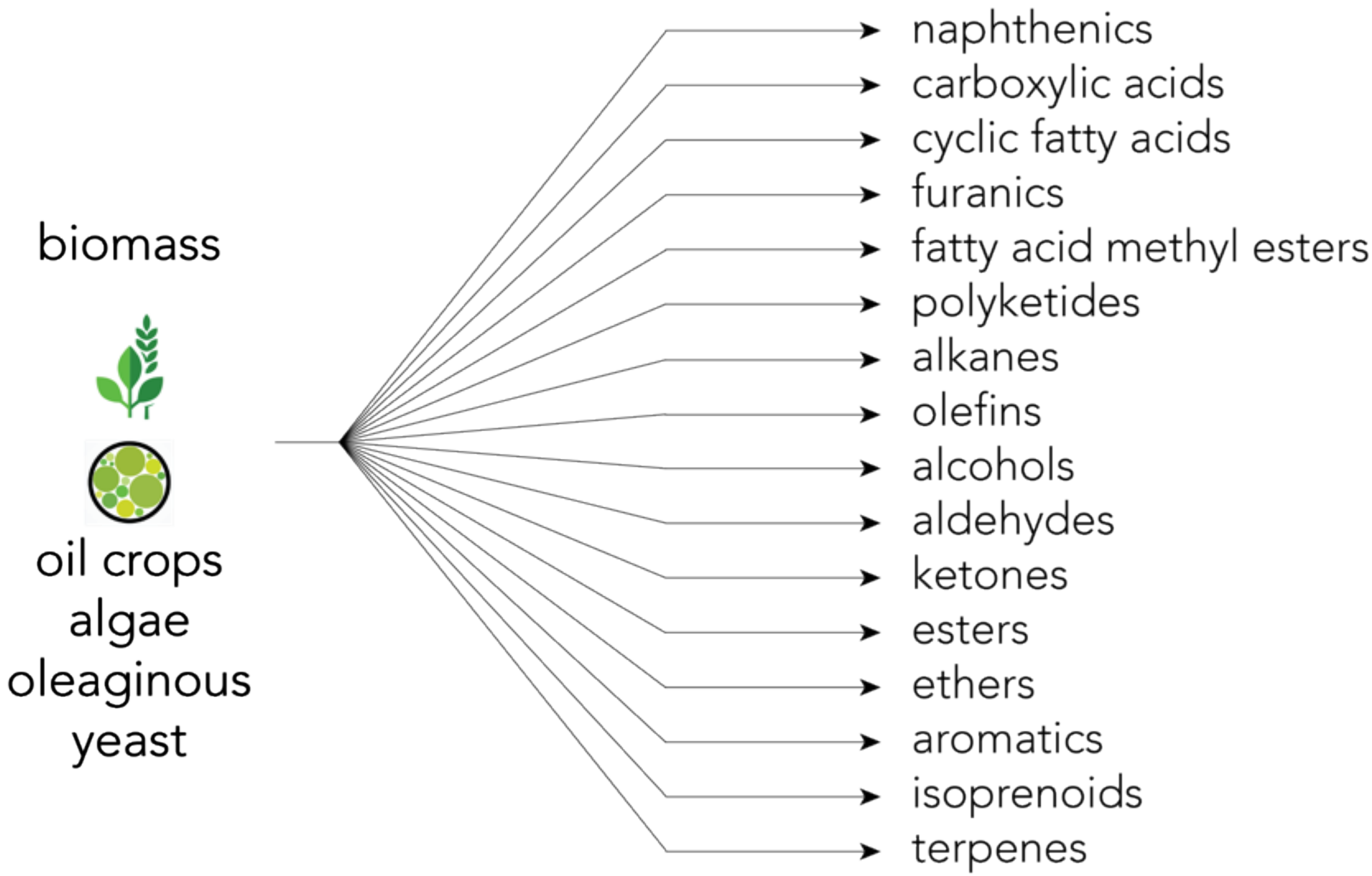
Upstream injected (UI) 100 RON, S ≈ 11 fuels have higher peak IMEP at constant CA50 than iso-octane (RON 100, S =0), and HoV has little effect (S is dominant)

- Direct injection (DI) of iso-octane has HoV benefit, but less than S ≈ 11 effect
- DI of S ≈ 11 fuels also has HoV benefit, which increases with manifold temp.

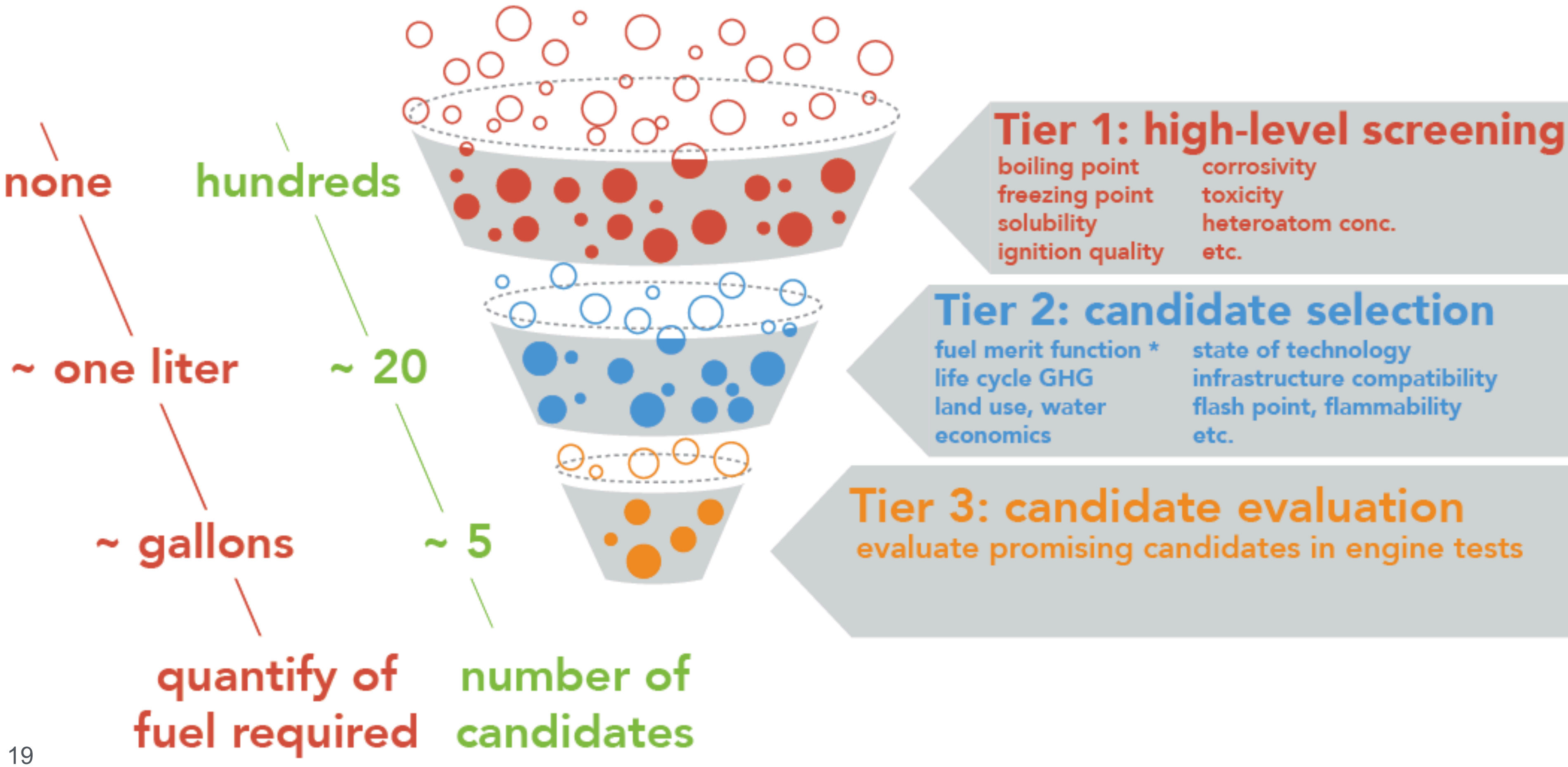
Plot shows peak IMEP at a constant CA50 phasing



What fuels can we make?

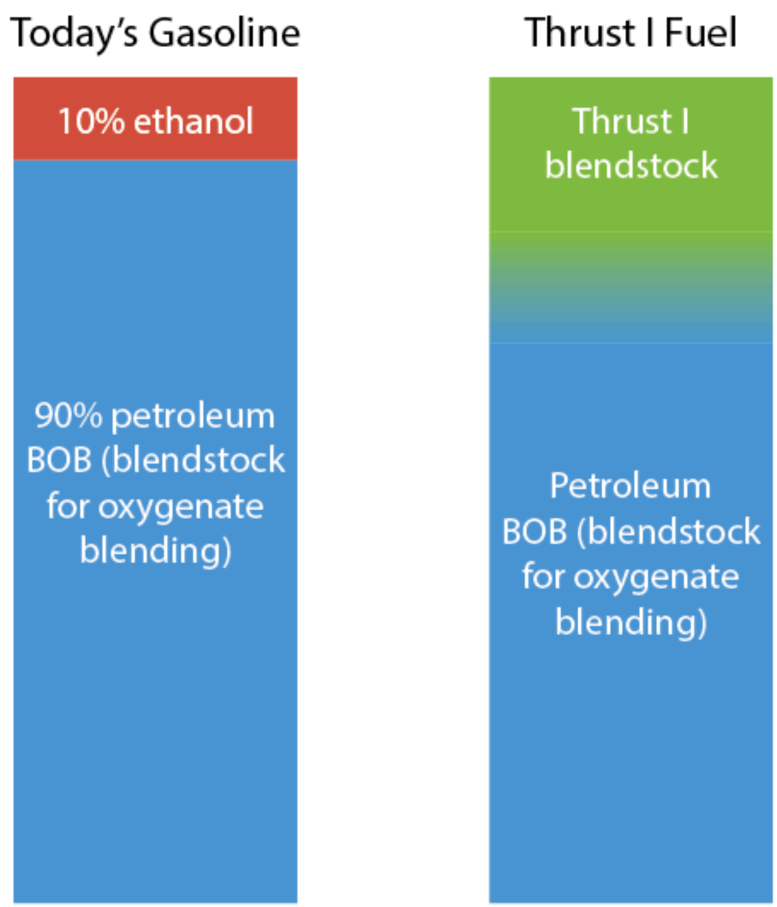

biomass
oil crops
algae
oleaginous
yeast
naphthenics
carboxylic acids
cyclic fatty acids
furanics
fatty acid methyl esters
polyketides
alkanes
olefins
alcohols
aldehydes
ketones
esters
ethers
aromatics
isoprenoids
terpenes

Fuel selection criteria ("decision funnel")



Fuel candidate blendstock evaluation

Fuel candidates will be evaluated as blendstocks in petroleum-based blendstocks



Fuel property database

Database of critical fuel properties of bio-derived and petroleum blendstocks

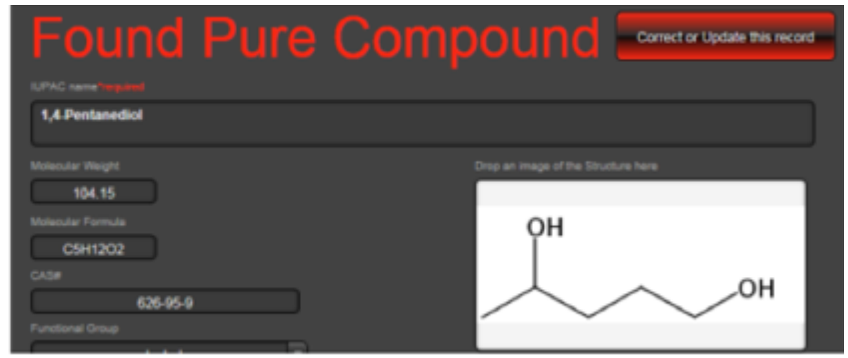
> 400 molecules/mixtures (at present)

25 database fields for fuel properties

Includes capability for fully blended fuels

Data from experiment and literature or calculated/estimated (where needed)

Shared resource for team and public



Identification of Thrust I candidates

Tier I criteria

Melting point/cloud point below -10°C

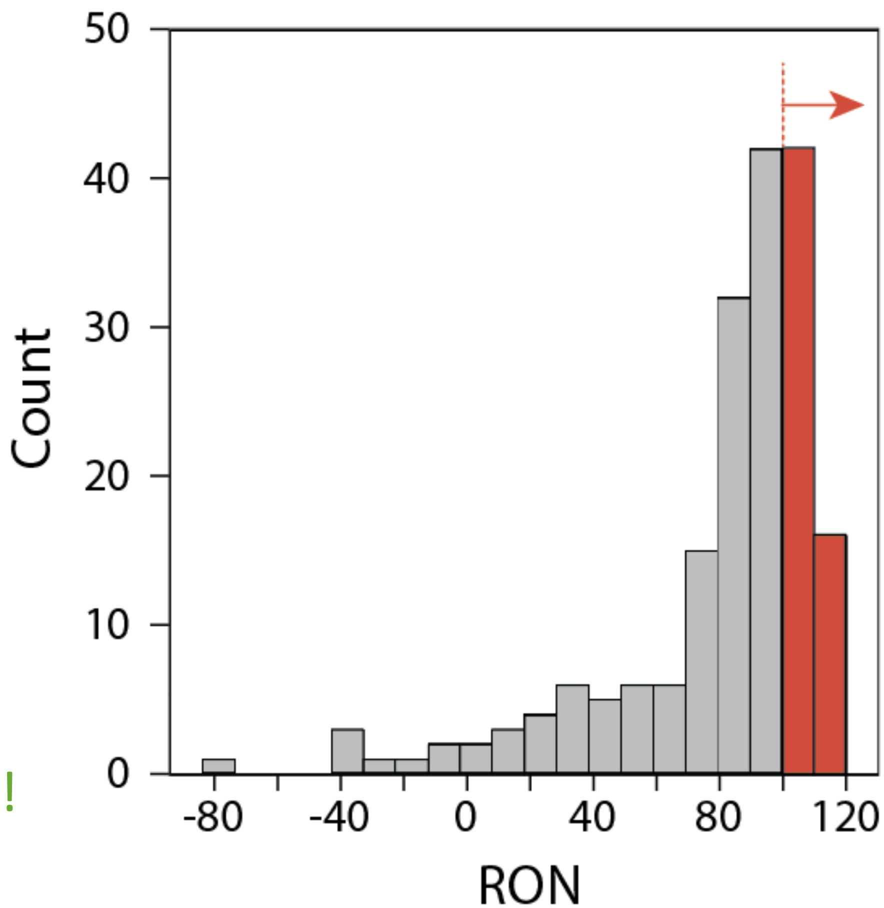
Boiling point between 20°C and 165°C

Measured or estimated RON ≥ 98

Meet toxicity, corrosion, solubility, and biodegradation requirements

> 40 promising bio-blendstocks from many functional group classes

Not final – this is an iterative process!



Current Thrust I blendstock candidates

Alcohols
Ethanol (reference only)
Methanol
n-Propanol
2-Propanol
1-Butanol
2-Butanol
2-Methylpropan-1-ol (isobutanol)
2-Methylbutanol
2-Methyl-3-buten-2-ol
2-Pentanol
Guerbet alcohols

Alkanes
Isooctane
2,2,3-trimethyl-butane (triptane)

Alkenes
Isooctene (2,4,4-trimethyl-1-pentene)

Aromatics
1,3,5-trimethylbenzene (mesitylene)
Vertifuel (60%+ aromatics)
Fractional condensation of sugars + upgrading
Methanol-to-gasoline
Catalytic fast pyrolysis
Catalytic conversion of sugars

Esters
Acetic acid, methyl ester (methyl acetate)
Butanoic acid, methyl ester (methyl butyrate)
Pentanoic acid, methyl ester (methyl pentanoate)
2-Methylpropanoic acid, methyl ester
2-Methlybutanoic acid, methyl ester
Acetic acid, ethyl ester (ethyl acetate)
Butanoic acid, ethyl ester (ethyl butanoate)
2-Methylpropanoic acid, ethyl ester
Acetic acid, 1-methylethyl ester
Acetic acid, butyl ester (butyl acetate)
Acetic acid, 2-methylpropyl ester
Acetic acid, 3-methylbutyl ester
Anaerobic acid fermentation plus esterification mixture

Ethers
Methoxybenzene (anisole)

Furans
2-Methylfuran
2,5-Dimethylfuran
40/60 Mixture of 2-methylfuran/2,5-dimethylfuran

Ketones
2-Propane (acetone)
2-Butane (methylethylketone; MEK)
2-Pentanone
3-Pentanone
Cyclopentanone
3-Hexanone
4-Methyl-2-pentanone (Methylisobutylketone)
2,4-Dimethyl-3-pentanone
3-Methyl-2-butanone

Multifunctional Mixtures
Methylated lignocellulosic bio-oil

What will work in the real world?

Which options are economical, scalable, sustainable, and compatible?

Assessing Candidate Viability

Technology Readiness	Environmental	Economics	Market
SOT - fuel production	Carbon efficiency	Target Cost	Uncertainty
SOT - vehicle use	Target yield	Needed cost reduction	Regulatory requirements
Conversion TRL level	Life cycle GHG	Co-product economics	Geographic factors
Feedstock sensitivity	Life cycle water	Feedstock cost	Political factors
Process robustness	Life cycle FE use	Alternative high-value use	Infrastructure compatibility
Feedstock quality			
# of viable pathways			

Analysis of 20 representative candidates

Alcohols	
0	Ethanol (reference)
1	Methanol
2	1-butanol
3	2-methyl-butanol
4	2-butanol
5	2-methylpropan-1-ol
6	Guerbet alcohol mixture

Alkanes	
7	2,2,3-trimethylbutane

Alkenes	
8	Iso-octene

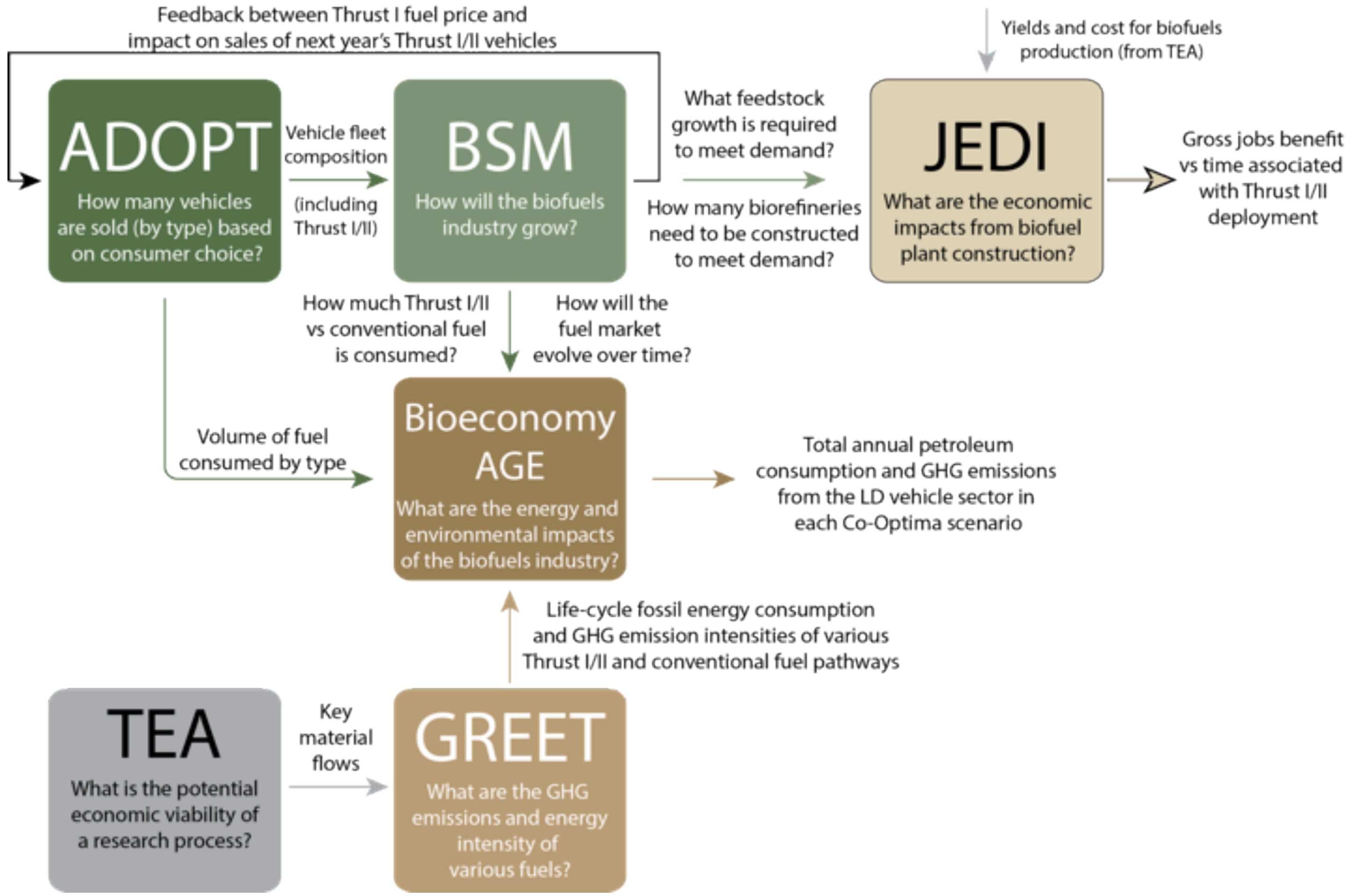
Esters	
9	Acetic Acid, methyl ester (methyl acetate)
10	Acetic Acid, ethyl ester (ethyl acetate)
11	Acetic Acid, butyl ester (butyl acetate)
12	Anaerobic acid fermentation and esterification mixture

Furans	
13	2,5-dimethylfuran/ 2-methylfuran mixture

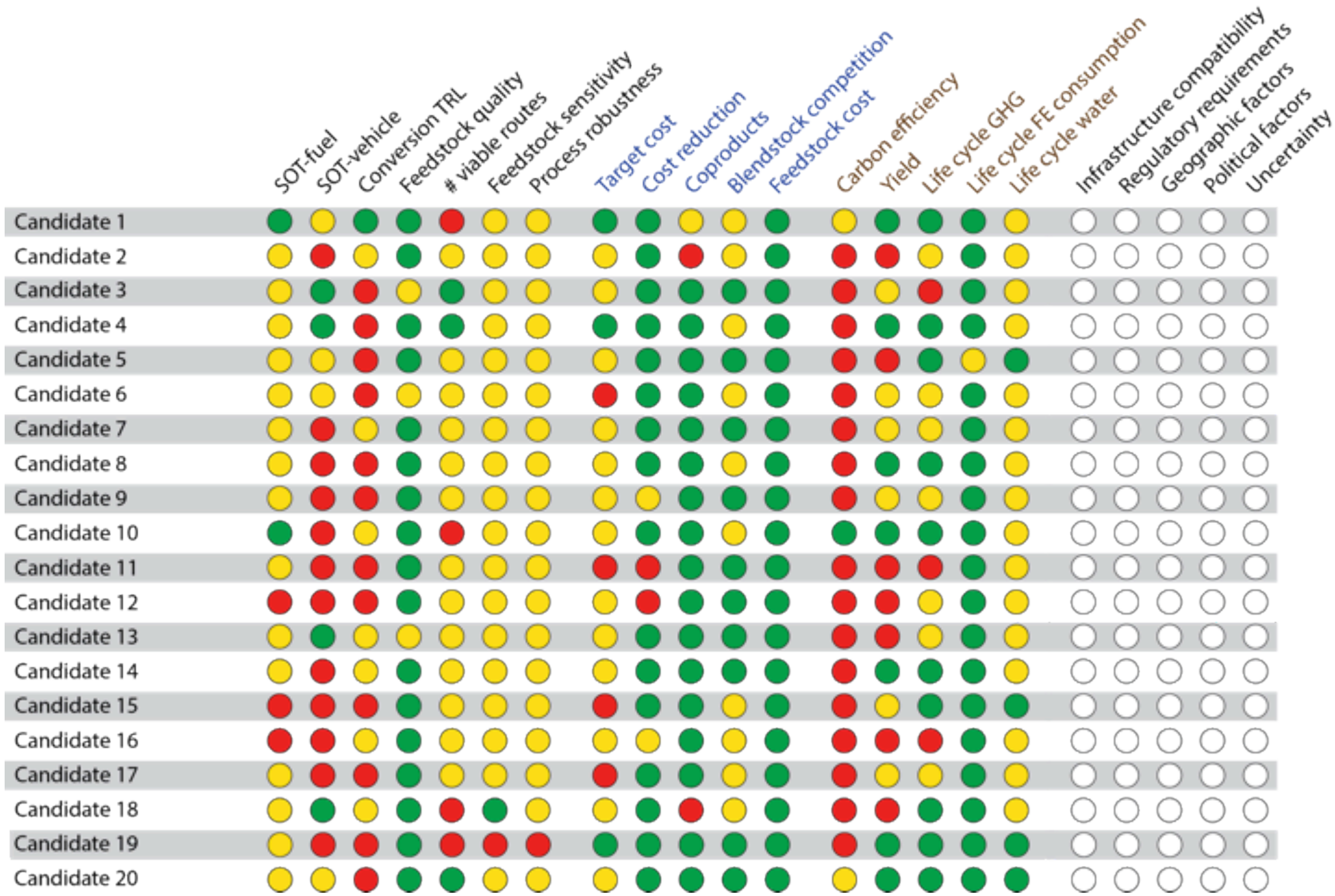
Ketones	
14	2-butanone
15	2-pentanone (methyl ethyl ketone)

Aromatics	
16	Vertifuel (60% aromatics)
17	Fractional condensation of sugars + upgrading
18	Methanol-to-gasoline
19	Catalytic fast pyrolysis
20	Catalytic conversion of sugars

Integrated analysis tools and approach



Assessing Candidate Viability



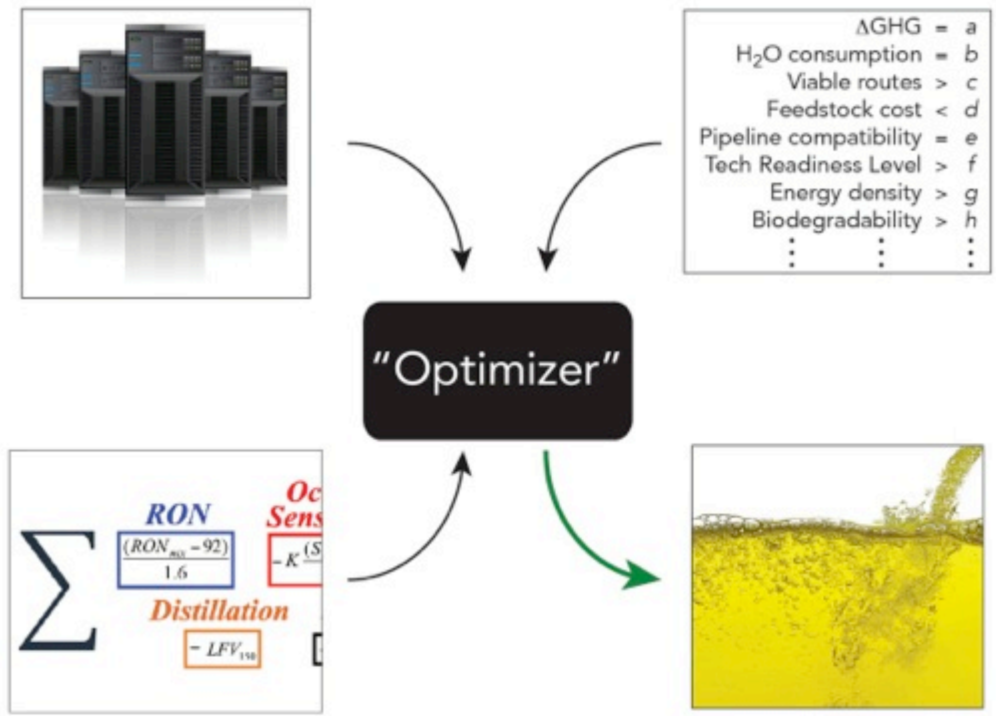
How do we co-optimize?

Identifying the best options, subject to many constraints

Approach

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

Scenario constraints

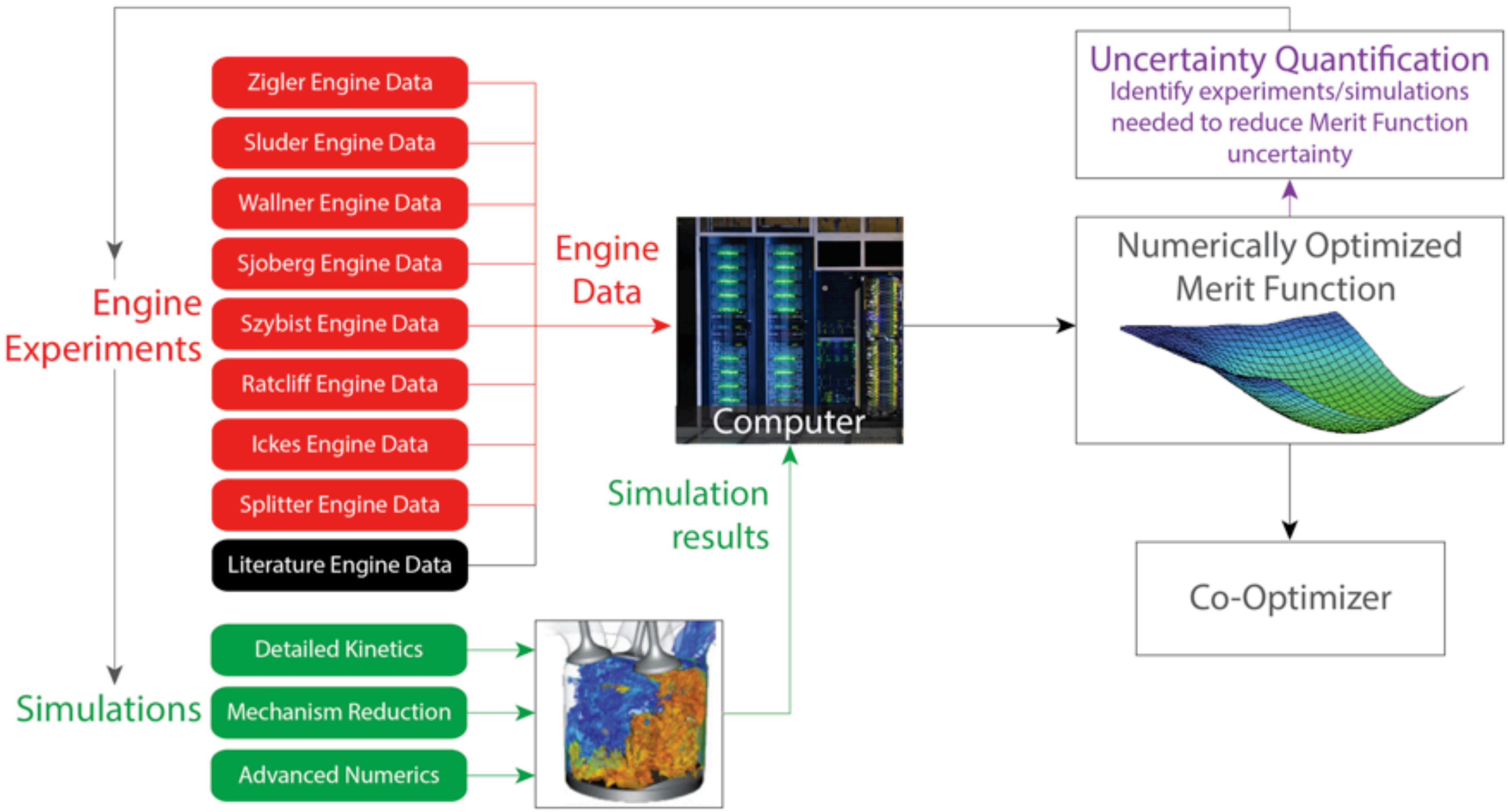


Engine/vehicle merit function

Optimal fuel blend formulations

Need to explicitly account for uncertainty

Numerically optimized merit function



Thank You