



Co-Optimization of Fuels and Engines

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



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Fuel and Engine Co-Optimization

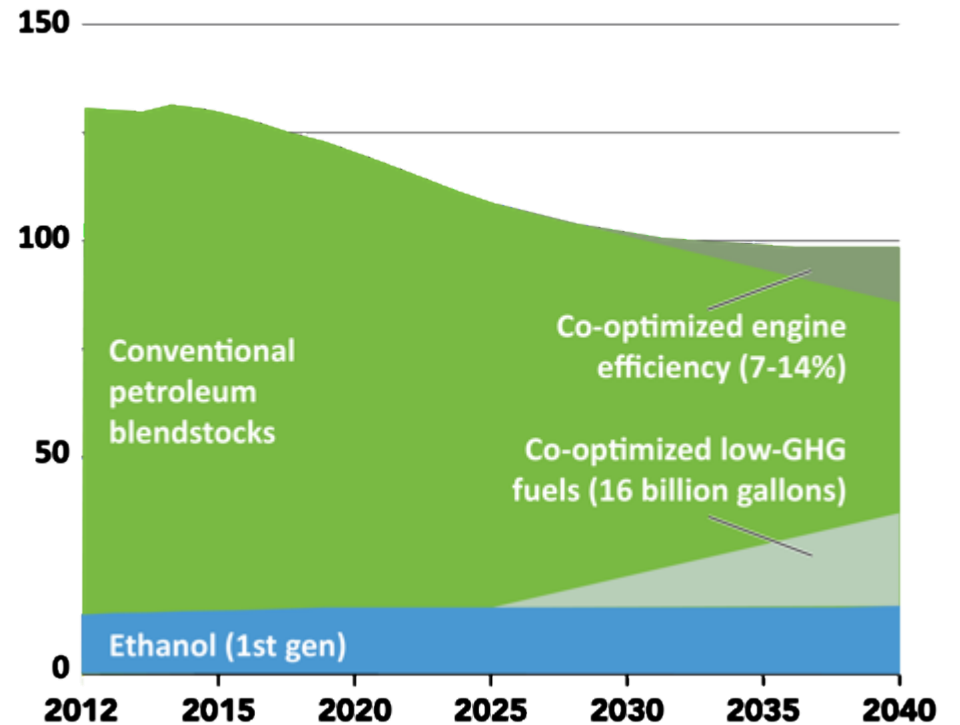
- What fuel properties maximize engine performance?
- How do engine parameters affect efficiency?
- What fuel and engine combinations are sustainable, affordable, and scalable?

**30% per vehicle
petroleum
reduction via
efficiency and
displacement**



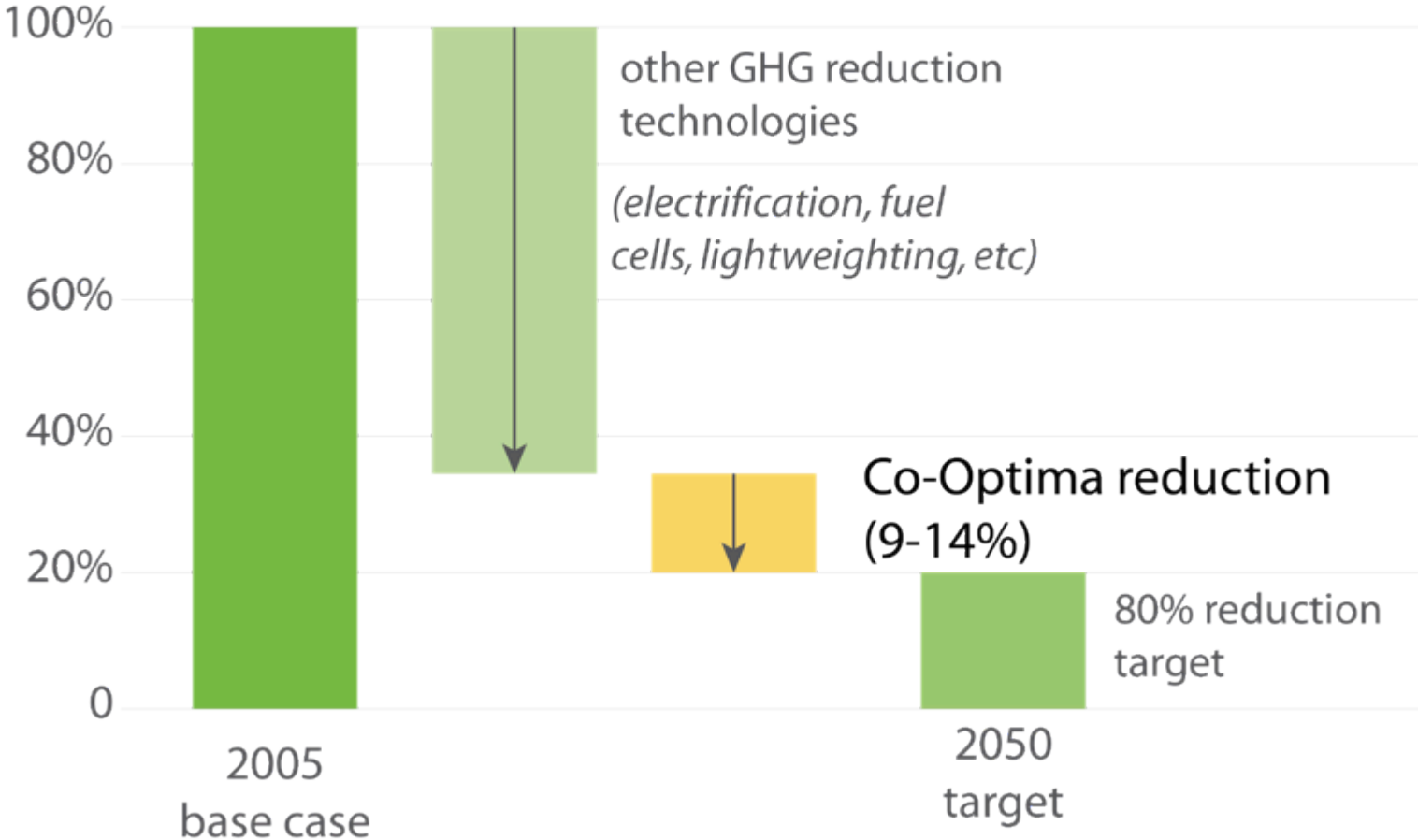
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Light duty fuel consumption (billion gallons/year)



source: EIA 2014 reference case

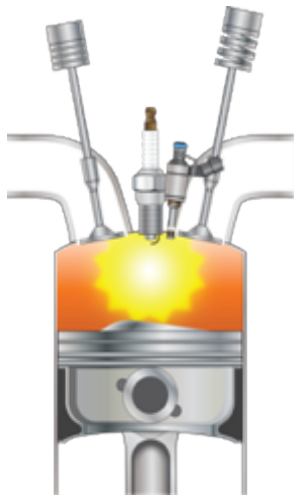
National goal: 80% reduction in transportation GHG by 2050



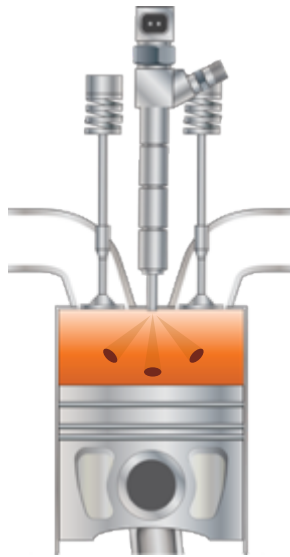
Parallel efforts are underway

Thrust I: Spark Ignition (SI)

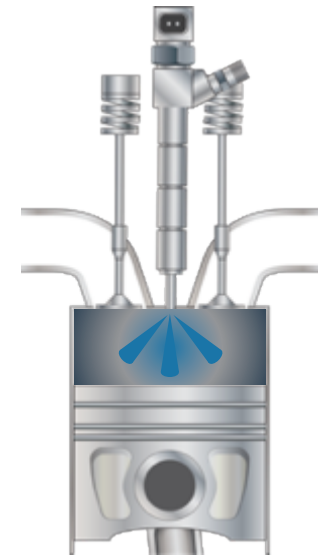
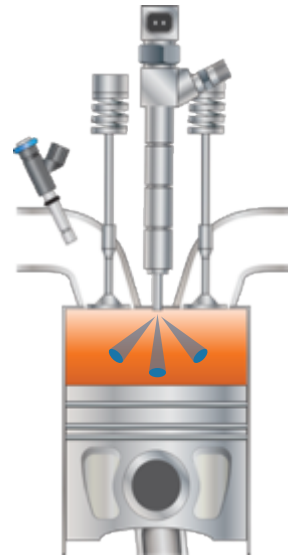
Thrust II: Advanced Compression Ignition (ACI)
kinetically-controlled and compression-ignition combustion



Low reactivity fuel



Range of fuel properties TBD



High reactivity fuel

Applicable to
light, medium, and heavy-duty engines
hybridized and non-hybridized powertrains

6



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

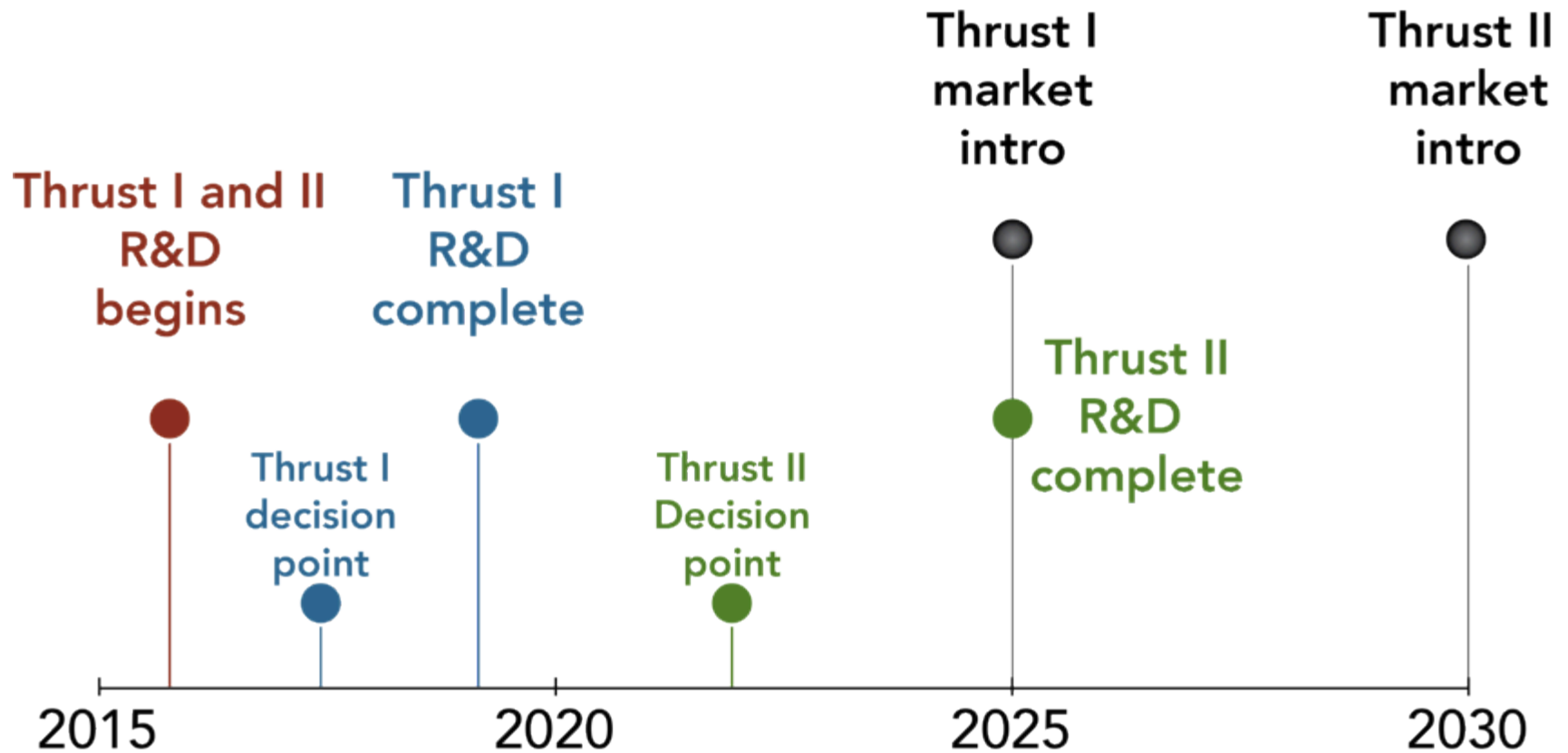
Regulatory
agencies



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End consumer
organizations

R&D and commercialization targets



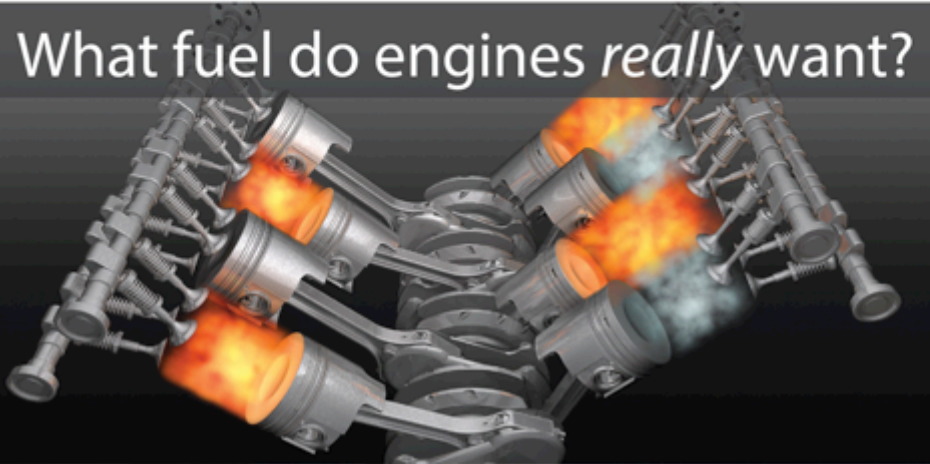
Major Co-Optima Challenges



Co-Optima Technical Challenges



What fuel do engines *really* want?



What fuels can we make?



What will work in the real world?



How do we "co-optimize"?





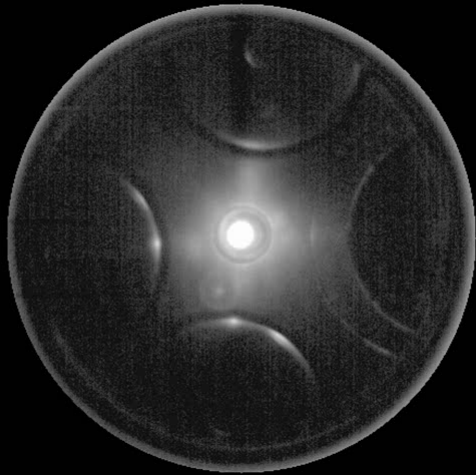
What fuels do engines want?



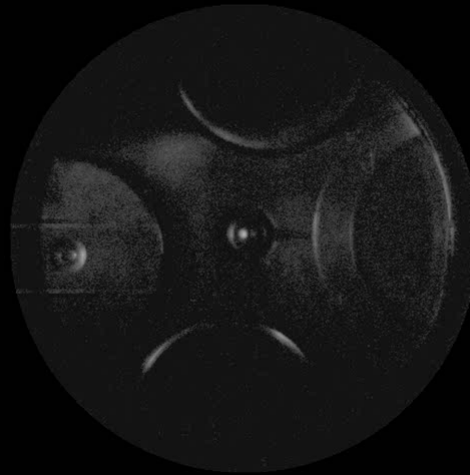
Fundamentally different **combustion dynamics**
require **different fuel properties**



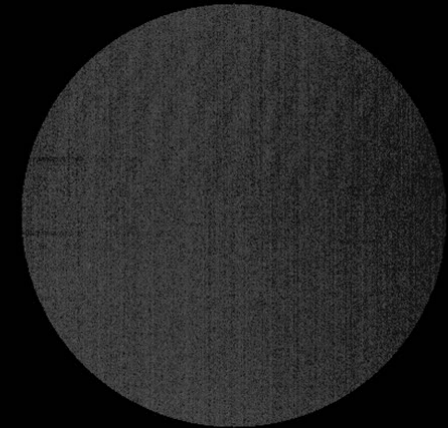
Spark ignition
(gasoline) – Thrust I



Advanced Compression
Ignition (ACI) – Thrust II



Compression ignition
(diesel) – Thrust II



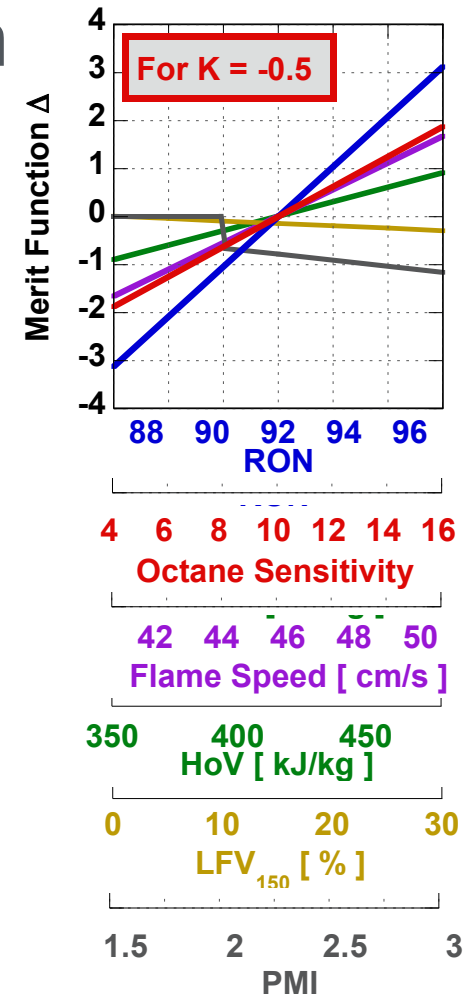
Engine performance merit function

$$\text{Merit} = \alpha \cdot [\text{RON} - 92] - \beta \cdot K \cdot [S - 10] + \gamma \cdot \text{ON} \cdot [\text{HOV} - 415] + \delta \cdot [\text{HOV} - 415] + \varepsilon \cdot [S_L - 46] - \text{LFV}_{150} - H(\text{PMI} - 2.0)[\zeta + 0.5(\text{PMI} - 2.0)]$$

RON
Octane Sensitivity
Heat of Vaporization

Flame Speed
Distillation
Particulate Emissions

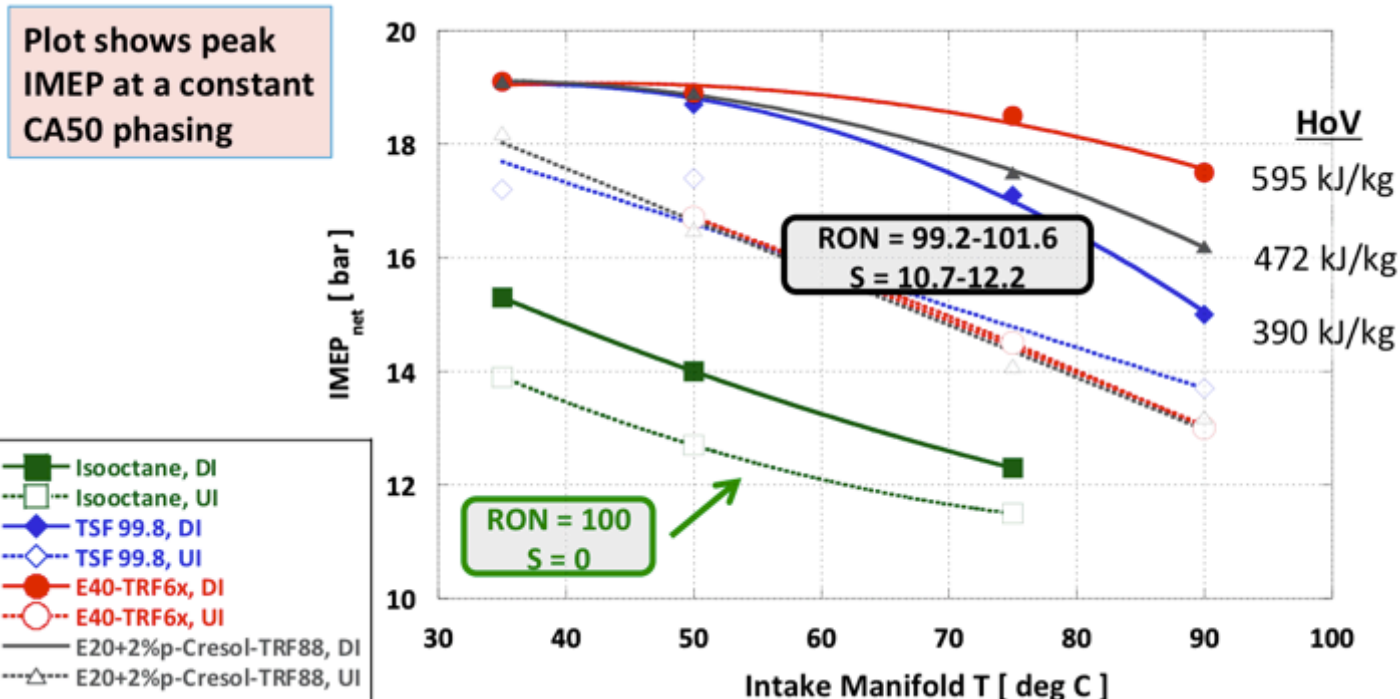
- Merit function being developed and refined
 - Are these the right fuel properties?
 - Are their effects properly quantified?
- We'll test the central fuel hypothesis using biofuels with different structures / functional groups than petroleum fuels



HoV can be important for DI at high intake temperatures

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

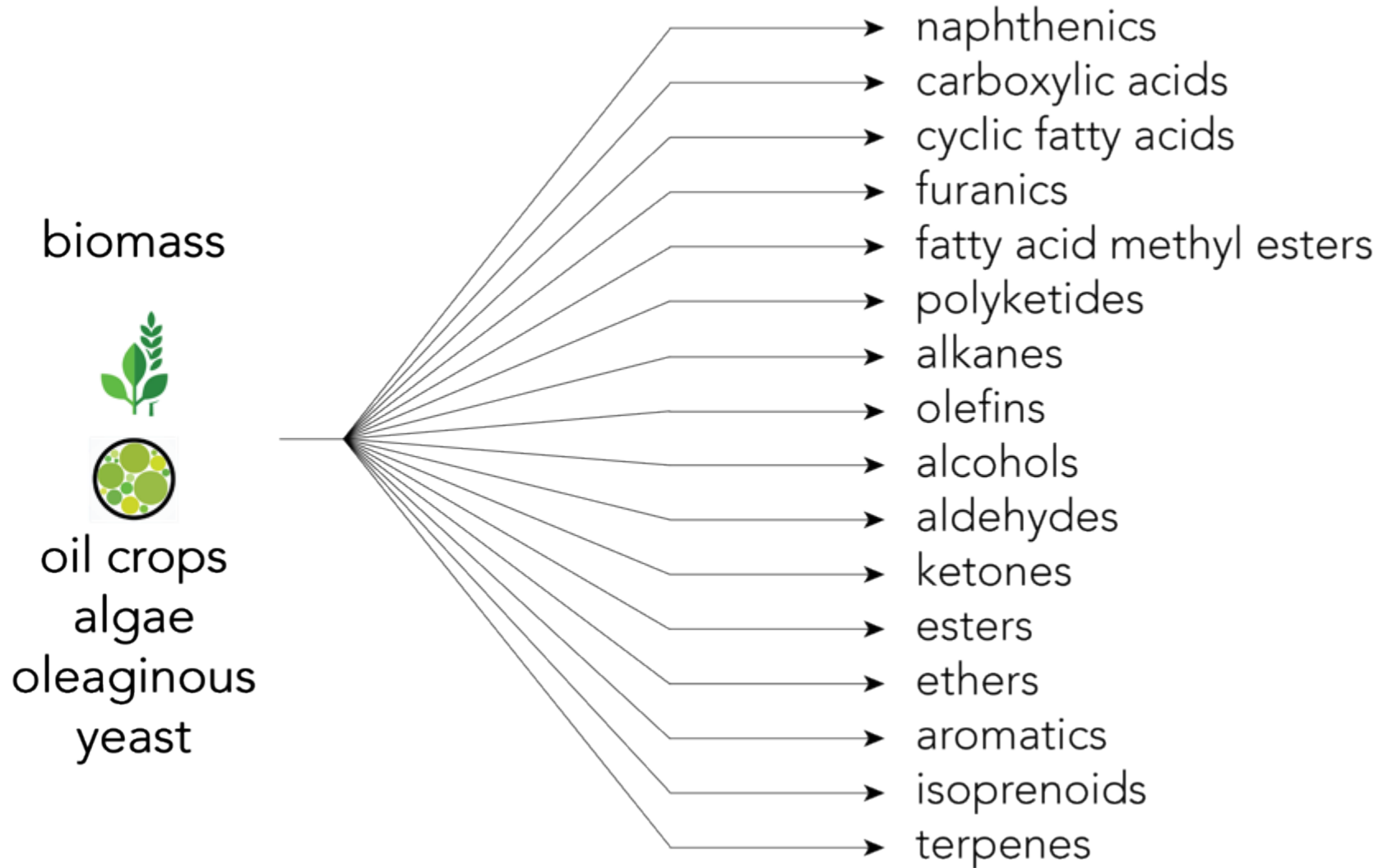
- Direct injection (DI) of iso-octane has HoV benefit, but less than $S \approx 11$ effect
- DI of $S \approx 11$ fuels also has HoV benefit, which increases with manifold temp.



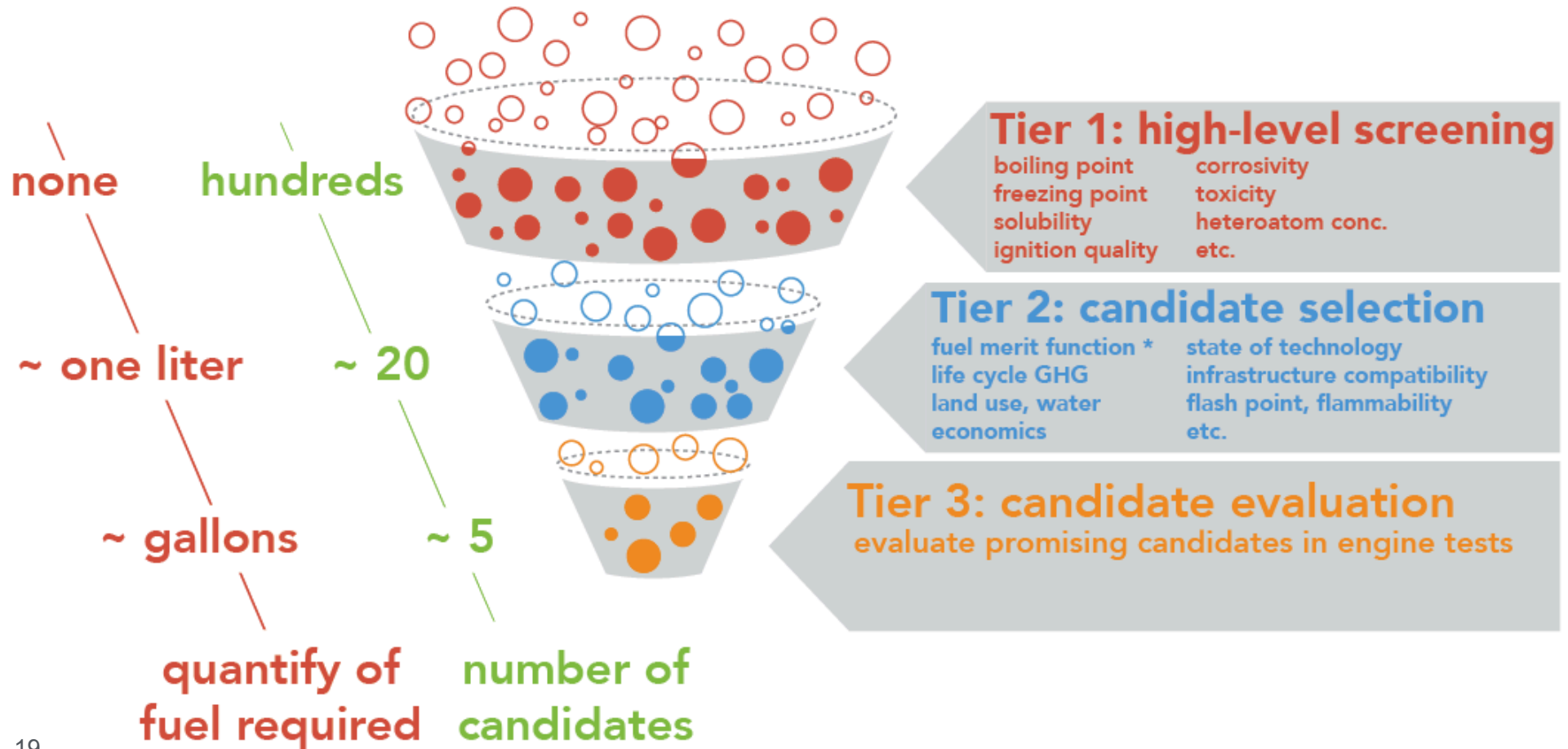


What fuels can we make?





Fuel selection criteria (“decision funnel”)

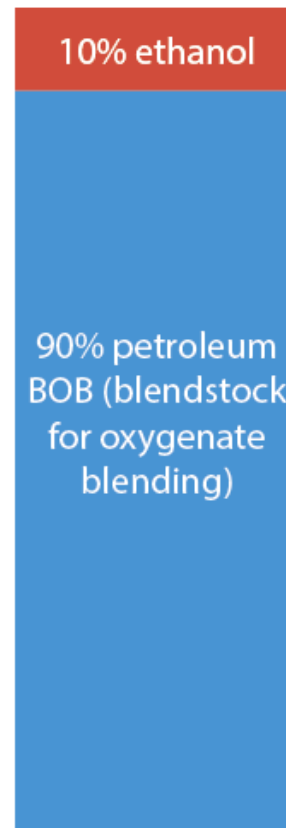


Fuel candidate blendstock evaluation

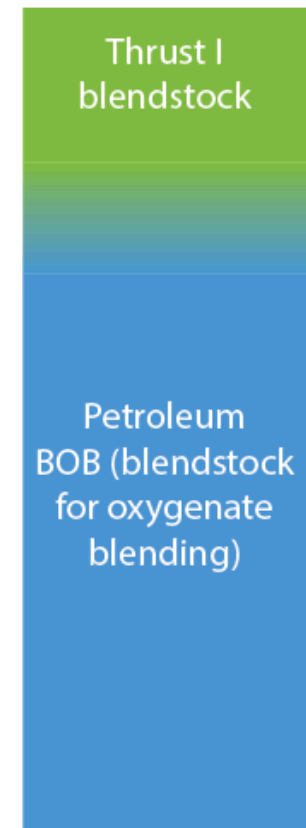


Fuel candidates will be evaluated as blendstocks in petroleum-based blendstocks

Today's Gasoline



Thrust I Fuel





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

Found Pure Compound Correct or Update this record

IUPAC name required

Molecular Weight

Molecular Formula

CAS#

Functional Group

Drop an image of the Structure here

SEARCH PROPERTIES

Both "pure" (IUPAC name) and "blend" (IUPAC name) records will be searched. If the name AND a boiling point range between 0 and 14 will be searched.

Molecular Weight

Molecular Formula

CAS#

Safety

LFL LEL (%)

UFL LEL (%)

Flash Point (°C)

Autoignition Temp (°C)

Peroxide Former

Health

Rat Oral LD50 (mg/kg)

Properties

Melting Point (°C) <input type="text"/>	Boiling Point (°C) <input type="text"/>	Peroxide Value <input type="text"/>	T80 (°C) <input type="text"/>
Cloud Point (°C) <input type="text"/>	Heat of Vaporization (kJ/mol) <input type="text"/>	BP (°C) <input type="text"/>	T90 (°C) <input type="text"/>
Density (g/cm³) <input type="text"/>	Viscosity (cSt) <input type="text"/>	FBP (°C) <input type="text"/>	Surface Tension (dyne/cm) <input type="text"/>
Viscosity (cSt) <input type="text"/>	Vapor Pressure (kPa) <input type="text"/>	Corrosion <input type="text"/>	Plat <input type="text"/>
MON <input type="text"/>	RON <input type="text"/>	Lubricity <input type="text"/>	
LVV <input type="text"/>	DCN <input type="text"/>	Stability <input type="text"/>	Functional Group <input type="text"/>
Critical Pressure (kPa) <input type="text"/>	Critical Temperature (K) <input type="text"/>	Oxidation Stability <input type="text"/>	Thermal Stability <input type="text"/>
Aromatic Factor <input type="text"/>	Acid Value <input type="text"/>	Water Solubility (mg/L) <input type="text"/>	Dispersion <input type="text"/>



Identification of Thrust I candidates

Tier I criteria

Melting point/cloud point below -10°C

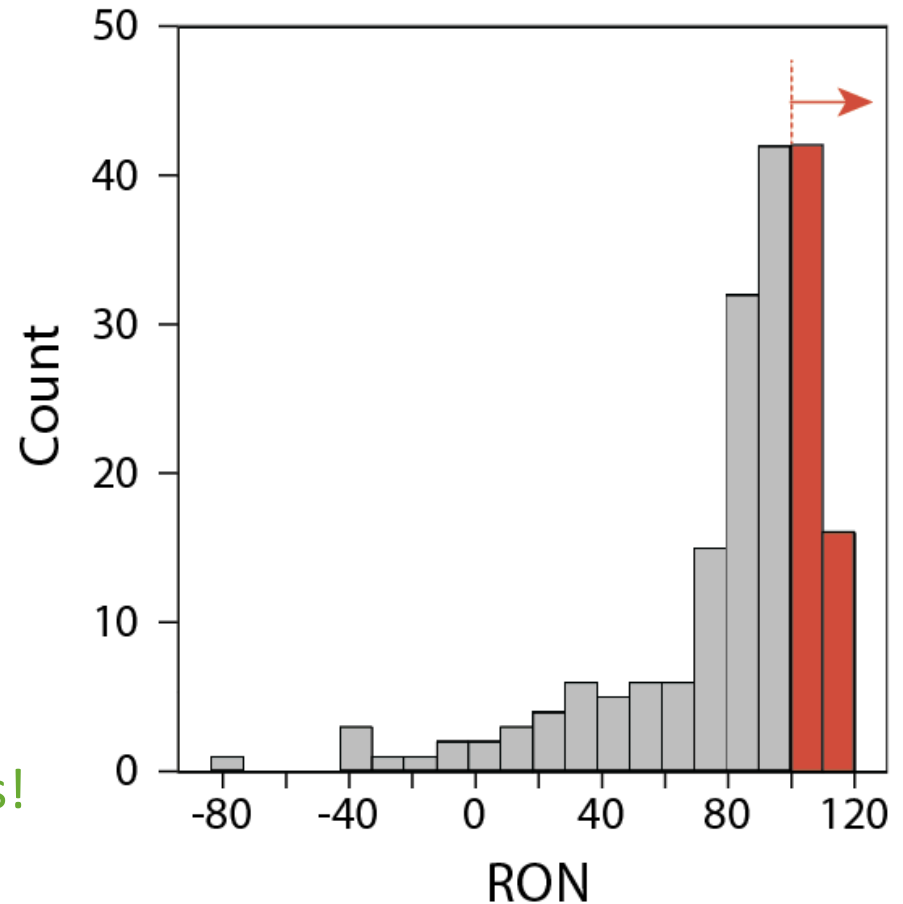
Boiling point between 20°C and 165°C

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	Aromatics	Ethers
Ethanol (reference only)	1,3,5-trimethylbenzene (mesitylene)	Methoxybenzene (anisole)
Methanol	Vertifuel (60%+ aromatics)	
n-Propanol	Fractional condensation of sugars + upgrading	Furans
2-Propanol	Methanol-to-gasoline	2-Methylfuran
1-Butanol	Catalytic fast pyrolysis	2,5-Dimethylfuran
2-Butanol	Catalytic conversion of sugars	40/60 Mixture of 2-methylfuran/2,5-dimethylfuran
2-Methylpropan-1-ol (isobutanol)		
2-Methylbutanol	Esters	Ketones
2-Methyl-3-buten-2-ol	Acetic acid, methyl ester (methyl acetate)	2-Propane (acetone)
2-Pentanol	Butanoic acid, methyl ester (methyl butyrate)	2-Butane (methyl ethyl ketone; MEK)
Guerbet alcohols	Pentanoic acid, methyl ester (methyl pentanoate)	2-Pentanone
	2-Methylpropanoic acid, methyl ester	3-Pentanone
Alkanes	2-Methylbutanoic acid, methyl ester	Cyclopentanone
Isooctane	Acetic acid, ethyl ester (ethyl acetate)	3-Hexanone
2,2,3-trimethyl-butane (triptane)	Butanoic acid, ethyl ester (ethyl butanoate)	4-Methyl-2-pentanone (Methylisobutylketone)
	2-Methylpropanoic acid, ethyl ester	2,4-Dimethyl-3-pentanone
Alkenes	Acetic acid, 1-methylethyl ester	3-Methyl-2-butanone
Isooctene (2,4,4-trimethyl-1-pentene)	Acetic acid, butyl ester (butyl acetate)	
	Acetic acid, 2-methylpropyl ester	Multifunctional Mixtures
	Acetic acid, 3-methylbutyl ester	Methylated lignocellulosic bio-oil
	Anaerobic acid fermentation plus esterification mixture	



What will work in the real world?

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

Assessing Candidate Viability



Technology Readiness

SOT - fuel production
SOT - vehicle use
Conversion TRL level
Feedstock sensitivity
Process robustness
Feedstock quality
of viable pathways



Environmental

Carbon efficiency
Target yield
Life cycle GHG
Life cycle water
Life cycle FE use



Economics

Target Cost
Needed cost reduction
Co-product economics
Feedstock cost
Alternative high-value use



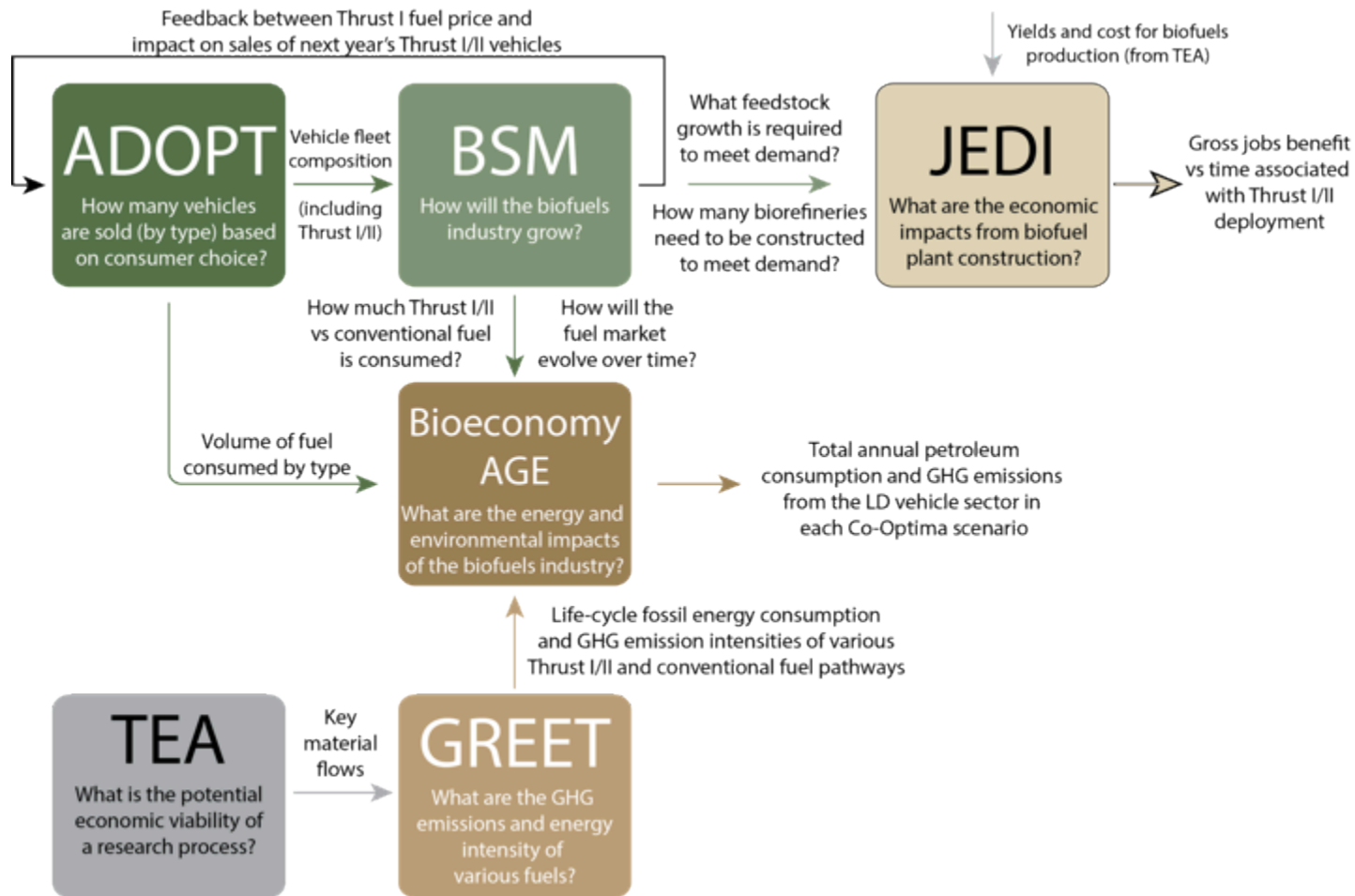
Market

Uncertainty
Regulatory requirements
Geographic factors
Political factors
Infrastructure compatibility

Analysis of 20 representative candidates

Alcohols		Esters		Ketones	
0	Ethanol (reference)	9	Acetic Acid, methyl ester (methyl acetate)	14	2-butanone
1	Methanol	10	Acetic Acid, ethyl ester (ethyl acetate)	15	2-pentanone (methyl ethyl ketone)
2	1-butanol	11	Acetic Acid, butyl ester (butyl acetate)	Aromatics	
3	2-methyl-butanol	12	Anaerobic acid fermentation and esterification mixture	16	Vertifuel (60% aromatics)
4	2-butanol			17	Fractional condensation of sugars + upgrading
5	2-methylpropan-1-ol			18	Methanol-to-gasoline
6	Guerbet alcohol mixture			19	Catalytic fast pyrolysis
Alkanes		Furans		20	Catalytic conversion of sugars
7	2,2,3-trimethylbutane	13	2,5-dimethylfuran/ 2-methylfuran mixture		
Alkenes					
8	Iso-octene				

Integrated analysis tools and approach



Assessing Candidate Viability

	SOT-fuel	SOT-vehicle	Conversion TRL	Feedstock quality	# viable routes	Feedstock sensitivity	Process robustness	Target cost	Cost reduction	Coproducts	Blendstock competition	Feedstock cost	Carbon efficiency	Yield	Life cycle GHG	Life cycle FE consumption	Life cycle water	Infrastructure compatibility	Regulatory requirements	Geographical factors	Political factors	Uncertainty
Candidate 1	Green	Yellow	Green	Green	Red	Yellow	Yellow	Green	Green	Yellow	Yellow	Green	Yellow	Green	Green	Yellow	White	White	White	White	White	White
Candidate 2	Yellow	Red	Yellow	Green	Yellow	Yellow	Yellow	Yellow	Green	Red	Yellow	Green	Red	Red	Yellow	Green	Yellow	White	White	White	White	White
Candidate 3	Yellow	Green	Red	Yellow	Green	Yellow	Yellow	Yellow	Green	Green	Green	Green	Red	Yellow	Red	Green	Yellow	White	White	White	White	White
Candidate 4	Yellow	Green	Red	Green	Green	Yellow	Yellow	Green	Green	Green	Yellow	Green	Red	Green	Green	Green	Yellow	White	White	White	White	White
Candidate 5	Yellow	Yellow	Red	Green	Yellow	Yellow	Yellow	Yellow	Green	Green	Green	Green	Red	Red	Green	Yellow	Green	White	White	White	White	White
Candidate 6	Yellow	Yellow	Red	Yellow	Yellow	Yellow	Yellow	Red	Green	Green	Yellow	Green	Red	Yellow	Yellow	Green	Yellow	White	White	White	White	White
Candidate 7	Yellow	Red	Yellow	Green	Yellow	Yellow	Yellow	Yellow	Green	Green	Green	Green	Red	Yellow	Yellow	Green	Yellow	White	White	White	White	White
Candidate 8	Yellow	Red	Red	Green	Yellow	Yellow	Yellow	Yellow	Green	Green	Yellow	Green	Red	Green	Green	Green	Yellow	White	White	White	White	White
Candidate 9	Yellow	Red	Red	Green	Yellow	Yellow	Yellow	Yellow	Green	Green	Green	Green	Red	Yellow	Yellow	Green	Yellow	White	White	White	White	White
Candidate 10	Green	Red	Yellow	Green	Red	Yellow	Yellow	Yellow	Green	Green	Yellow	Green	Green	Green	Green	Green	Yellow	White	White	White	White	White
Candidate 11	Yellow	Red	Red	Green	Yellow	Yellow	Yellow	Red	Red	Green	Green	Green	Red	Red	Red	Green	Yellow	White	White	White	White	White
Candidate 12	Red	Red	Red	Green	Yellow	Yellow	Yellow	Yellow	Red	Green	Green	Green	Red	Red	Yellow	Green	Yellow	White	White	White	White	White
Candidate 13	Yellow	Green	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Green	Green	Green	Green	Red	Red	Yellow	Green	Yellow	White	White	White	White	White
Candidate 14	Yellow	Red	Yellow	Green	Yellow	Yellow	Yellow	Yellow	Green	Green	Green	Green	Red	Green	Green	Green	Yellow	White	White	White	White	White
Candidate 15	Red	Red	Red	Green	Yellow	Yellow	Yellow	Red	Green	Green	Yellow	Green	Red	Yellow	Green	Green	Green	White	White	White	White	White
Candidate 16	Red	Red	Yellow	Green	Yellow	Yellow	Yellow	Yellow	Yellow	Green	Yellow	Green	Red	Red	Red	Green	Yellow	White	White	White	White	White
Candidate 17	Yellow	Red	Red	Green	Yellow	Yellow	Yellow	Red	Green	Green	Yellow	Green	Red	Yellow	Yellow	Green	Yellow	White	White	White	White	White
Candidate 18	Yellow	Green	Yellow	Green	Red	Green	Yellow	Yellow	Green	Red	Yellow	Green	Red	Red	Green	Green	Yellow	White	White	White	White	White
Candidate 19	Yellow	Red	Red	Green	Red	Red	Red	Green	Green	Green	Green	Green	Red	Green	Green	Green	Green	White	White	White	White	White
Candidate 20	Yellow	Yellow	Red	Green	Green	Yellow	Yellow	Yellow	Green	Green	Green	Green	Yellow	Green	Green	Green	Green	White	White	White	White	White



How do we co-optimize?

Identifying the best options, subject to many constraints



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
\vdots	\vdots	\vdots

Scenario constraints

"Optimizer"

Engine/vehicle merit function

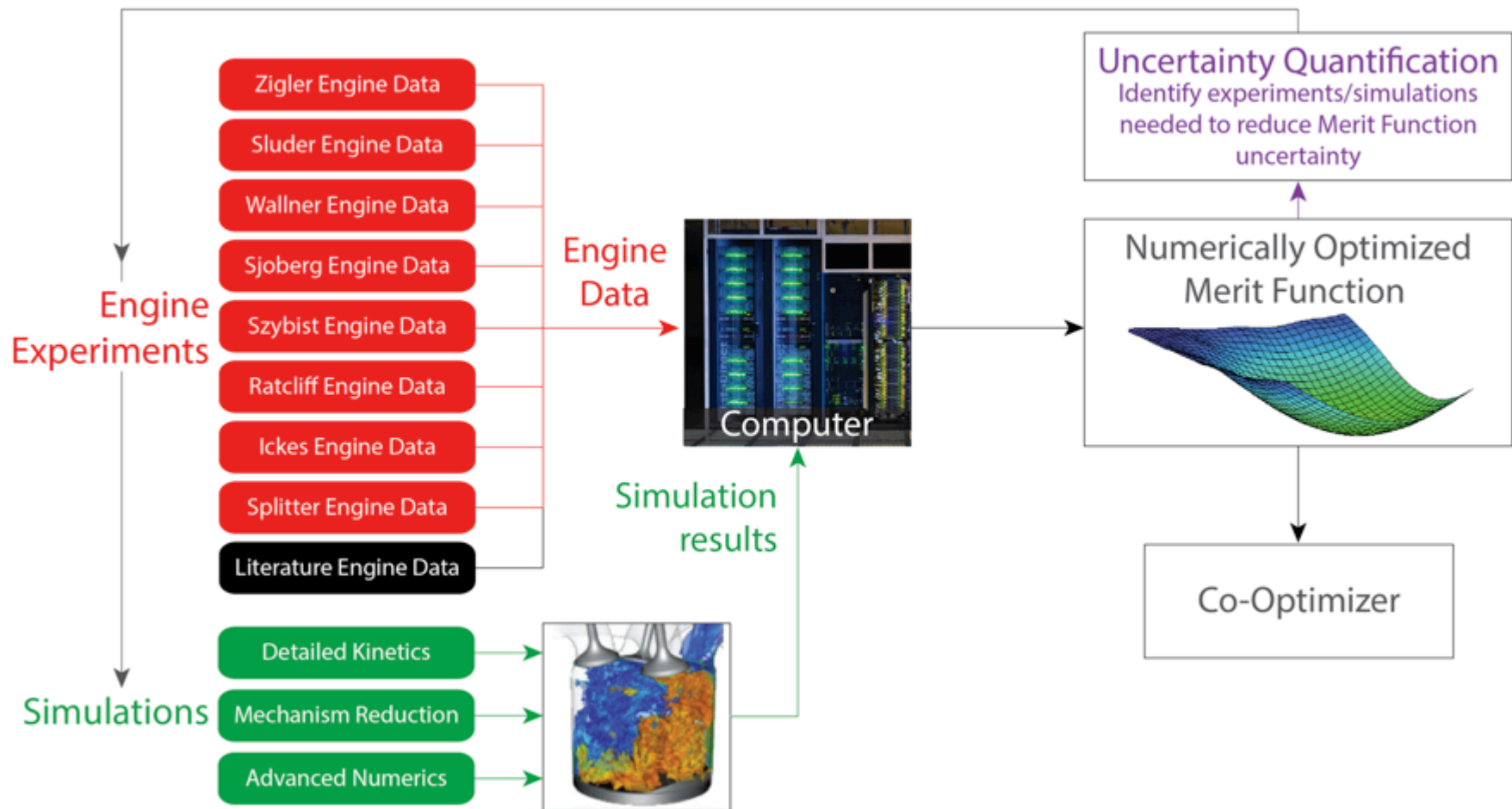
$$\sum \left[\frac{\text{RON}_{90} - 92}{1.6} + \text{Oc Sens} - K(S) - \text{Distillation} - \text{LFV}_{150} \right]$$



Optimal fuel blend formulations

Need to explicitly account for uncertainty

Numerically optimized merit function





Thank You