Co-Optimization of Fuels and Engines

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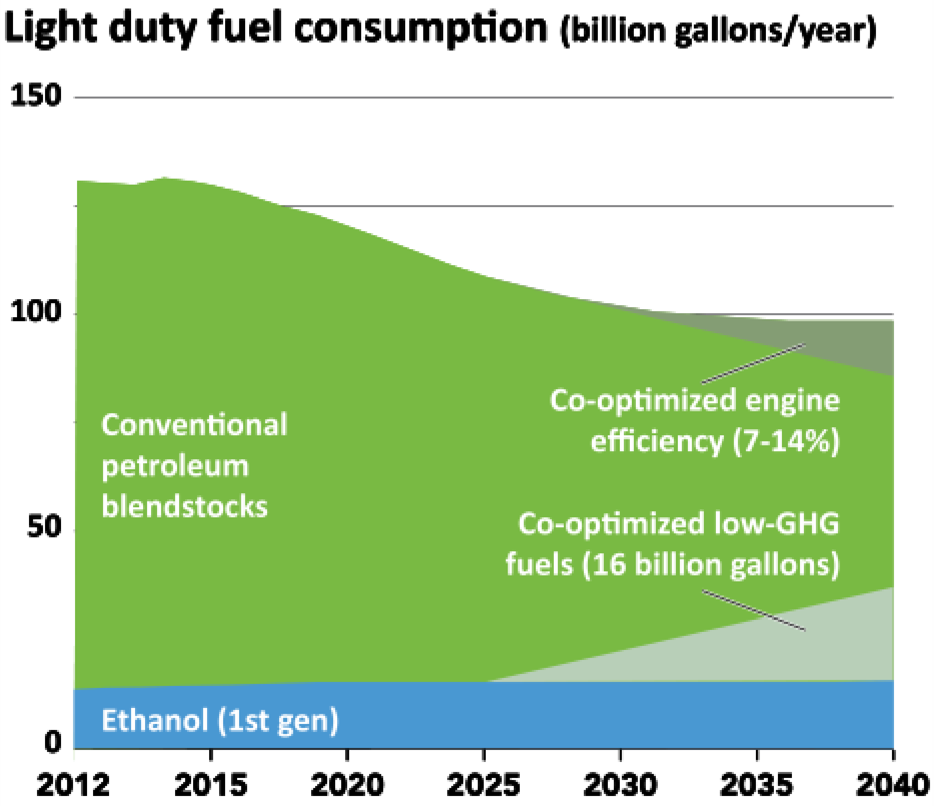
NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

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**



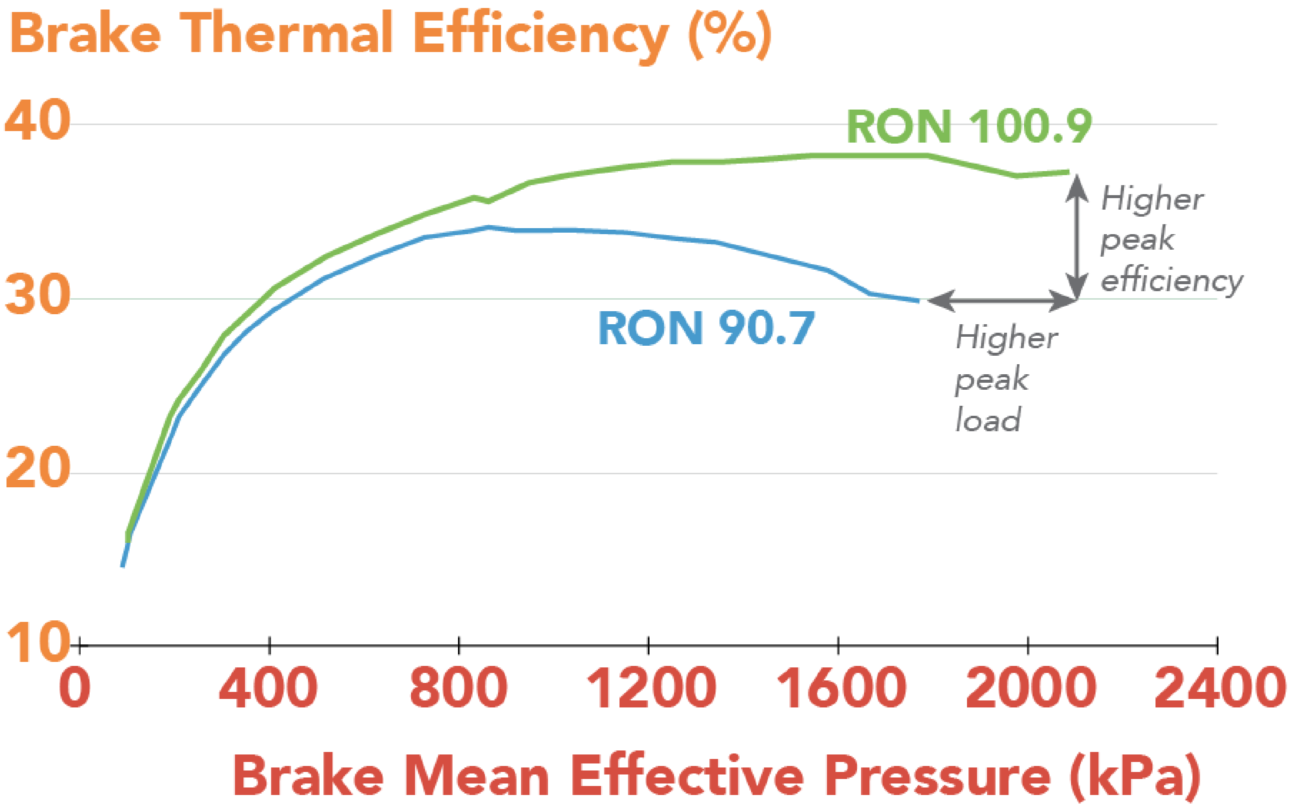
source: EIA 2014 reference case

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

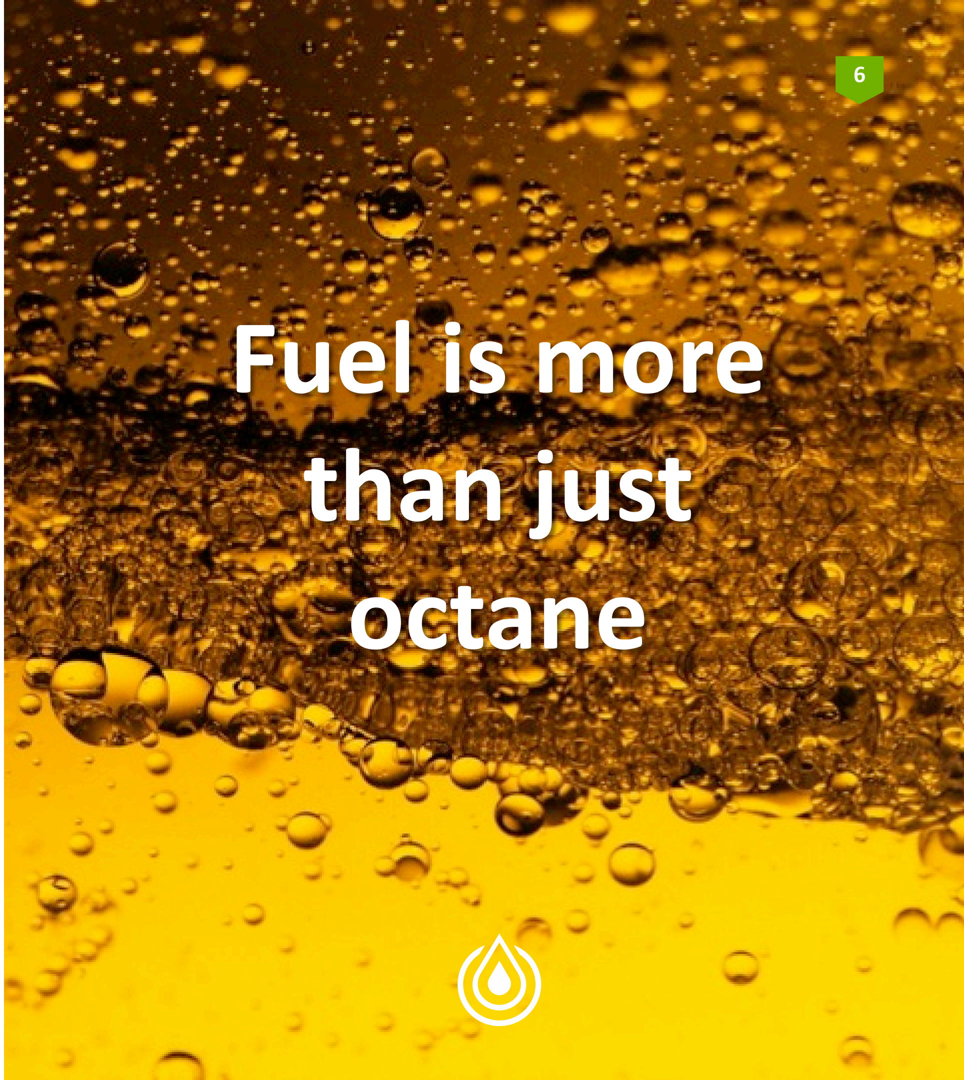
If we identify target values for the critical fuel properties that maximize efficiency and emissions performance for a given engine architecture, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance

Current fuels **constrain** engine design



Engine: Ford Ecoboost 1.6L 4-cylinder, turbocharged, direct-injection, 10.1 CR source: C.S. Sluder, ORNL

RON viscosity MON
volatility cloud point
bulk modulus of compressibility Wobbe index heating value
sensitivity heat of vaporization
soot precursor formation PMI flammability limits smoke point
cetane number T50
heat of combustion flame stretch ignition limits
C/H ratio strain sensitivity
density specific heat ratio
naphthene level Markstein length
T10 surface tension flash point T90
exergy destruction olefin level
energy density sulfur level
laminar burning velocity
diffusivity drivability index flame speed
aromatics level oxygenate level



Leveraging expertise and facilities from 10 national labs

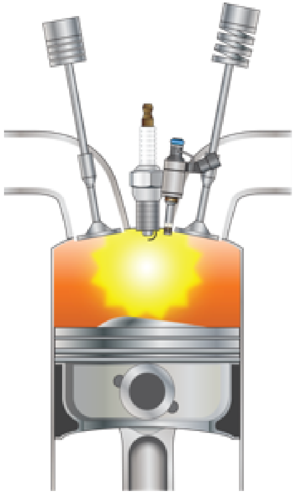
Integrated multi-lab teams with significant external stakeholder engagement

- **13** Light and heavy duty vehicle manufacturers
- **10** Oil companies/ refiners
- **8** Biofuel companies
- **4** Regulatory agencies
- **2** End consumer organizations

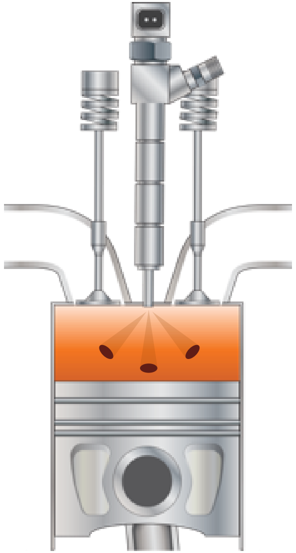
Parallel efforts are underway

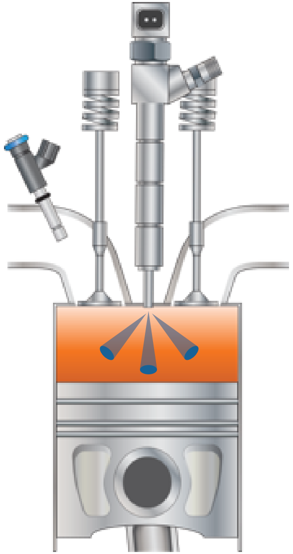
Thrust I: Spark Ignition (SI)

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

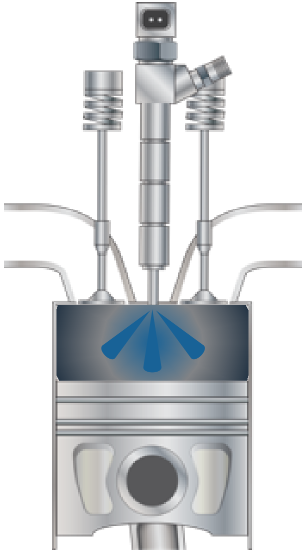


Low reactivity fuel





Range of fuel properties TBD



High reactivity fuel

Applicable to

light, medium, and heavy-duty engines

hybridized and non-hybridized powertrains

Identify and mitigate barriers to wide-scale deployment

National goal:

80%

reduction in transportation GHG by

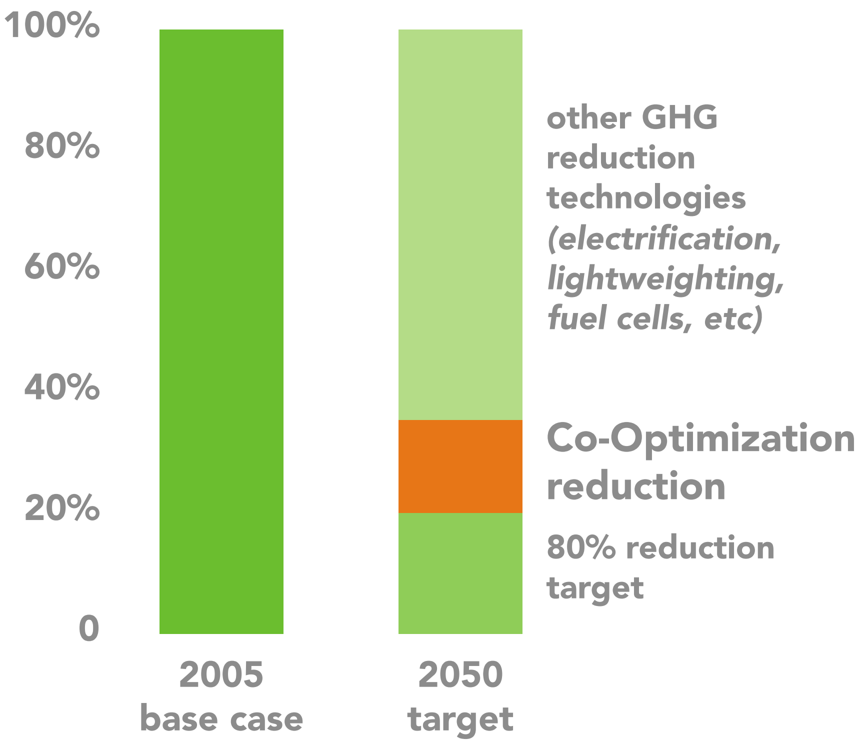
2050

Co-Optimization:

9-14%

GHG reduction

(beyond "business as usual")

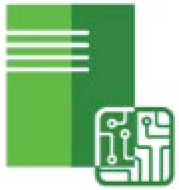


Six integrated teams

Low Greenhouse Gas Fuels

Advanced Engine Development

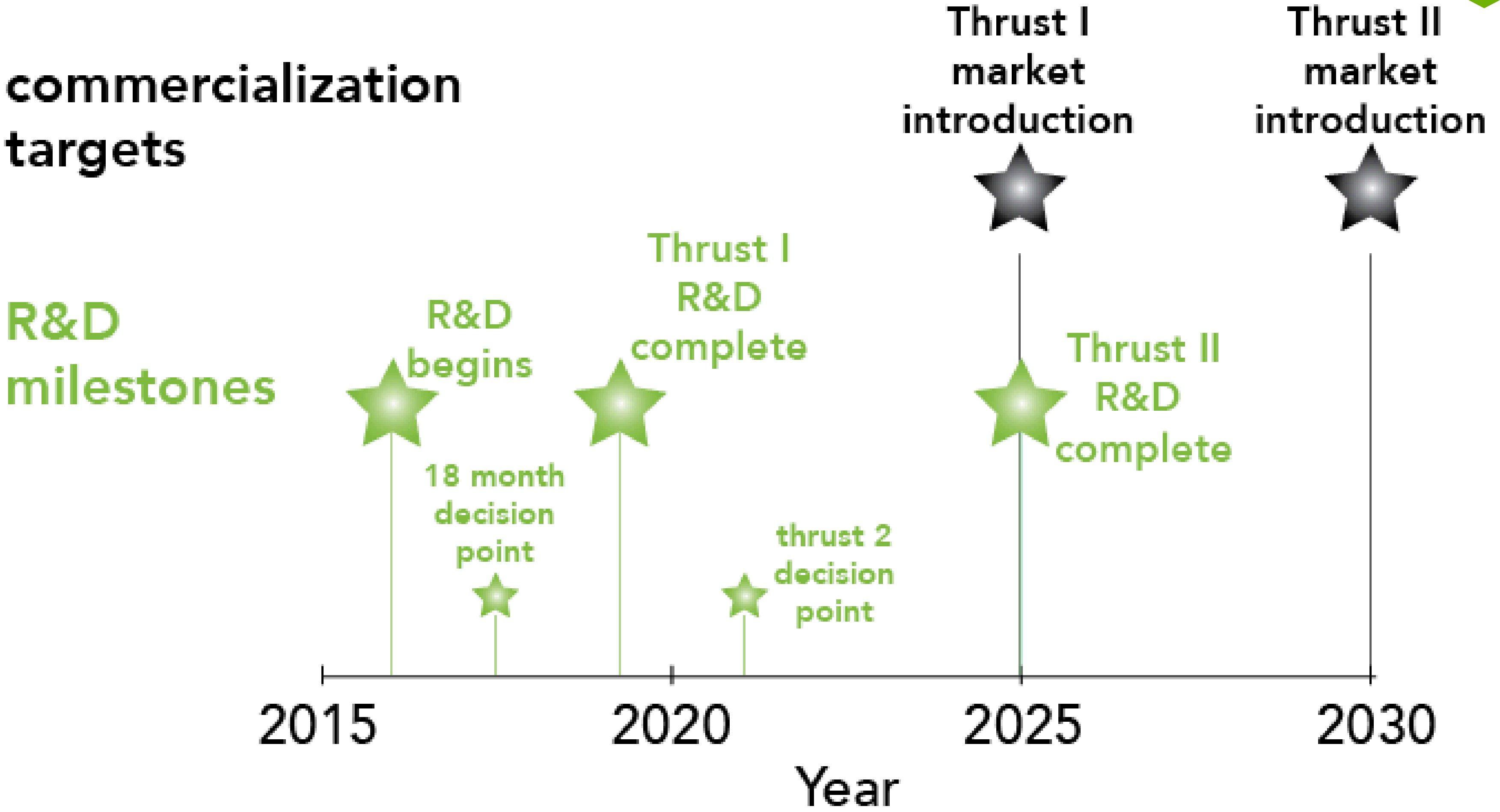
Fuel Properties



Modeling and Simulation Toolkit

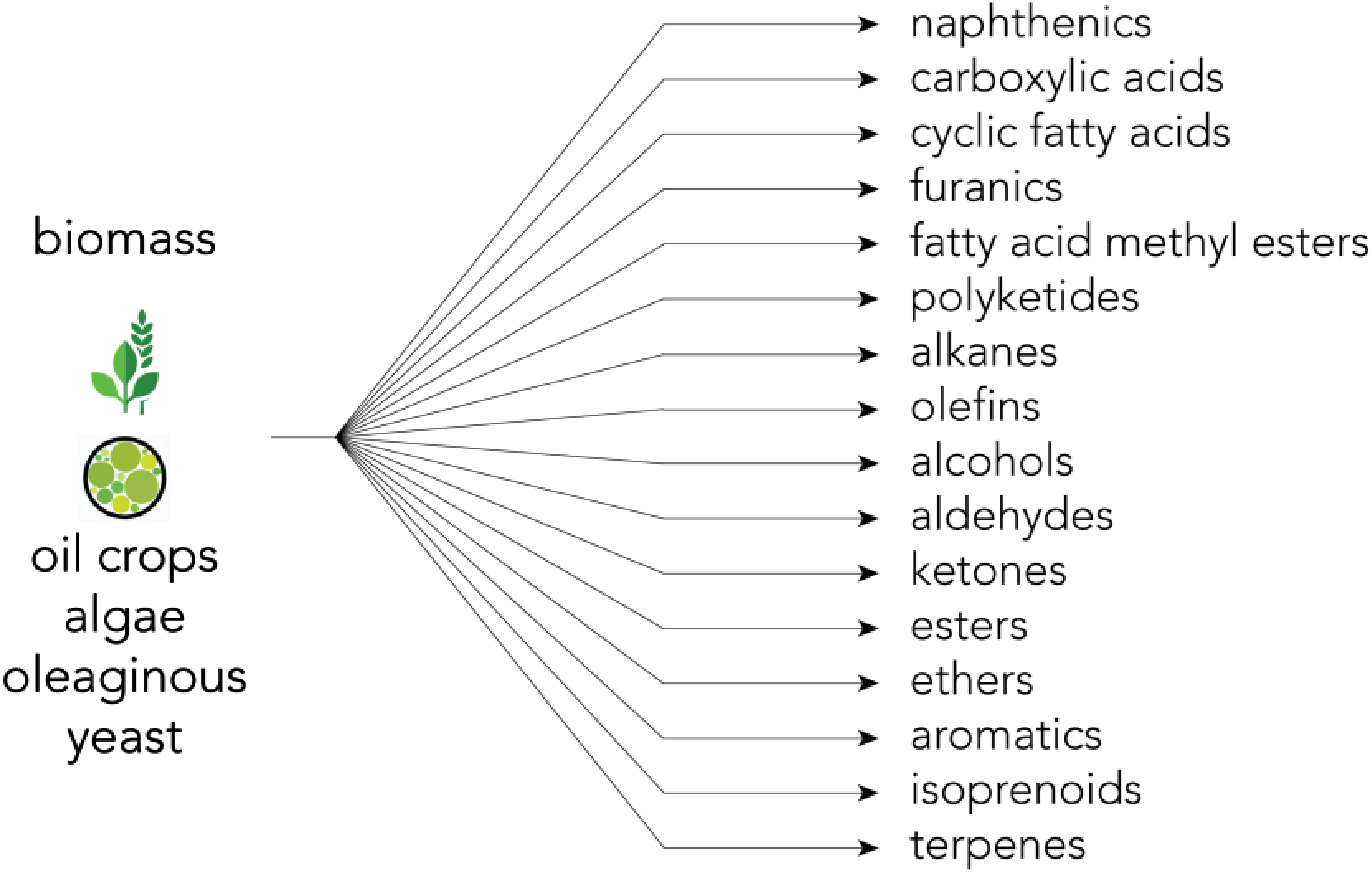
Analysis of Sustainability, Scale, Economics, Risk, and Trade

Market Transformation

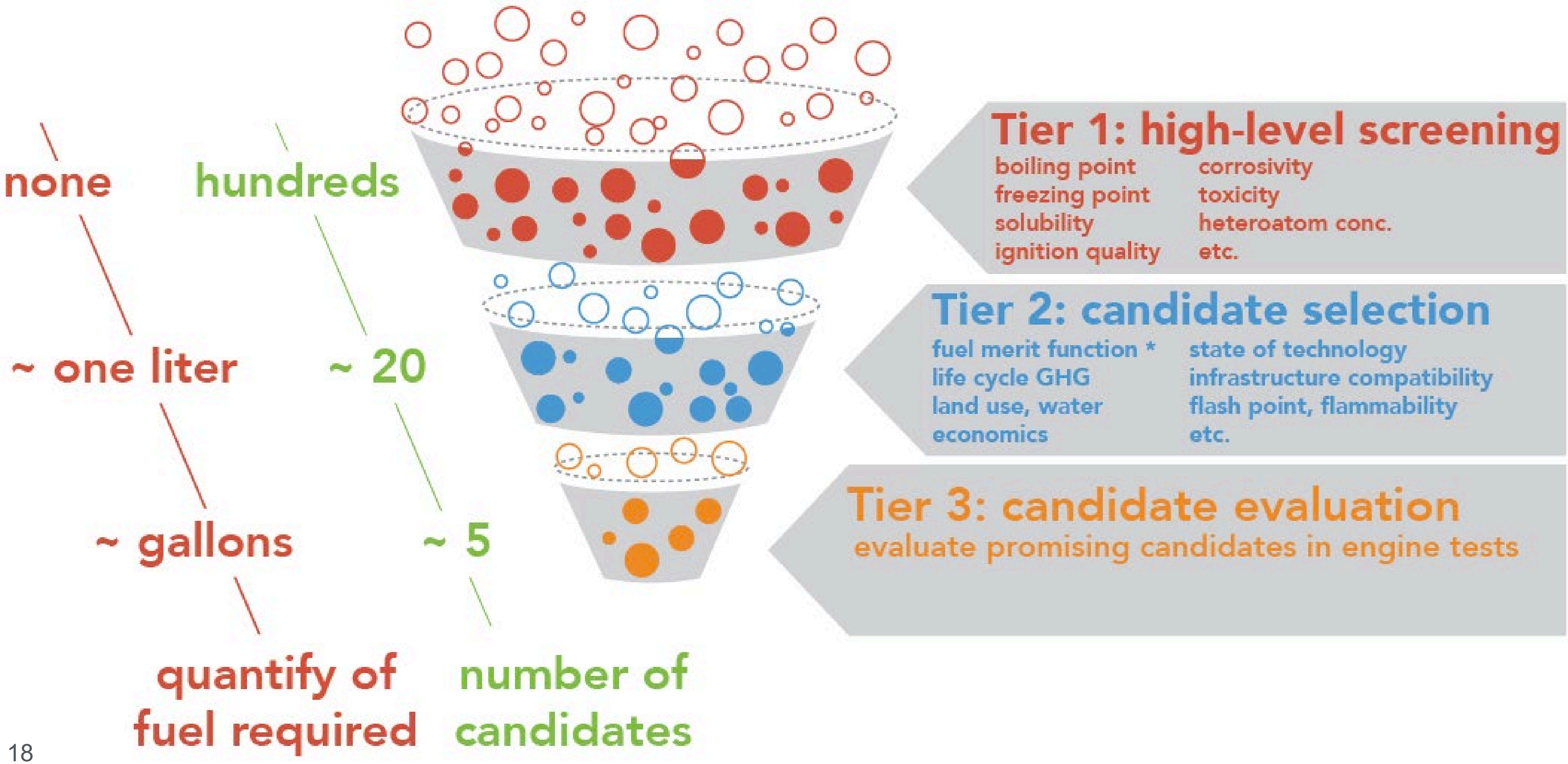

commercialization targets
R&D milestones
Thrust I market introduction
Thrust II market introduction
R&D begins
Thrust I R&D complete
Thrust II R&D complete
18 month decision point
thrust 2 decision point
2015
2020
2025
2030
Year

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")



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

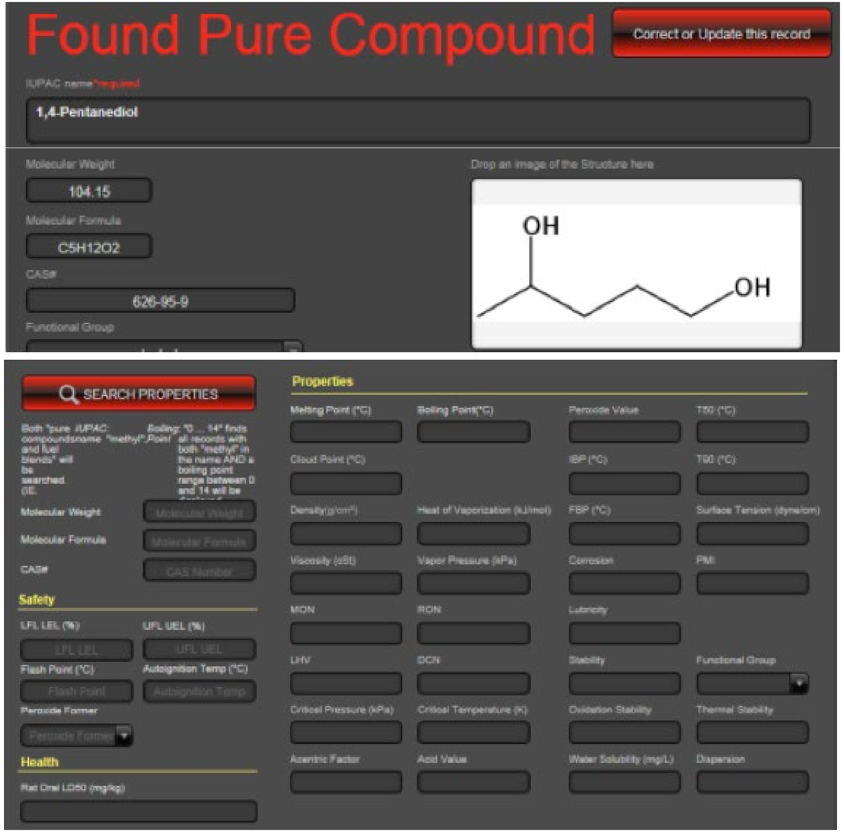
366 molecules, 12 mixtures (at present)

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

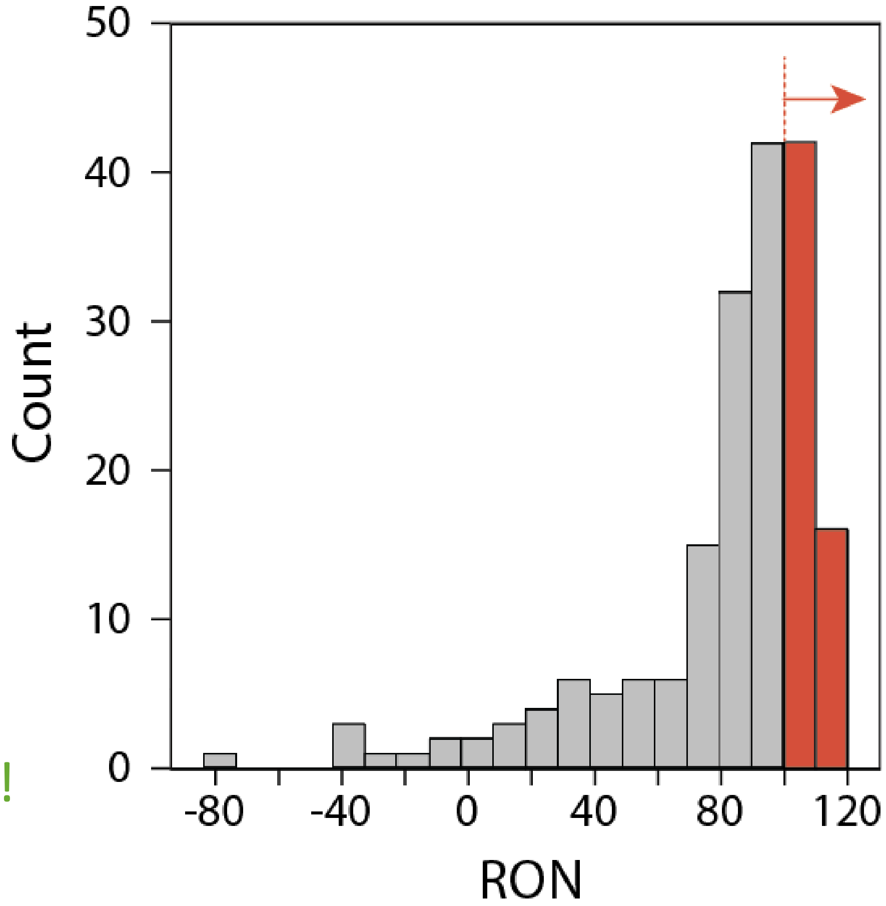
Boiling point between 20°C and 165°C

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

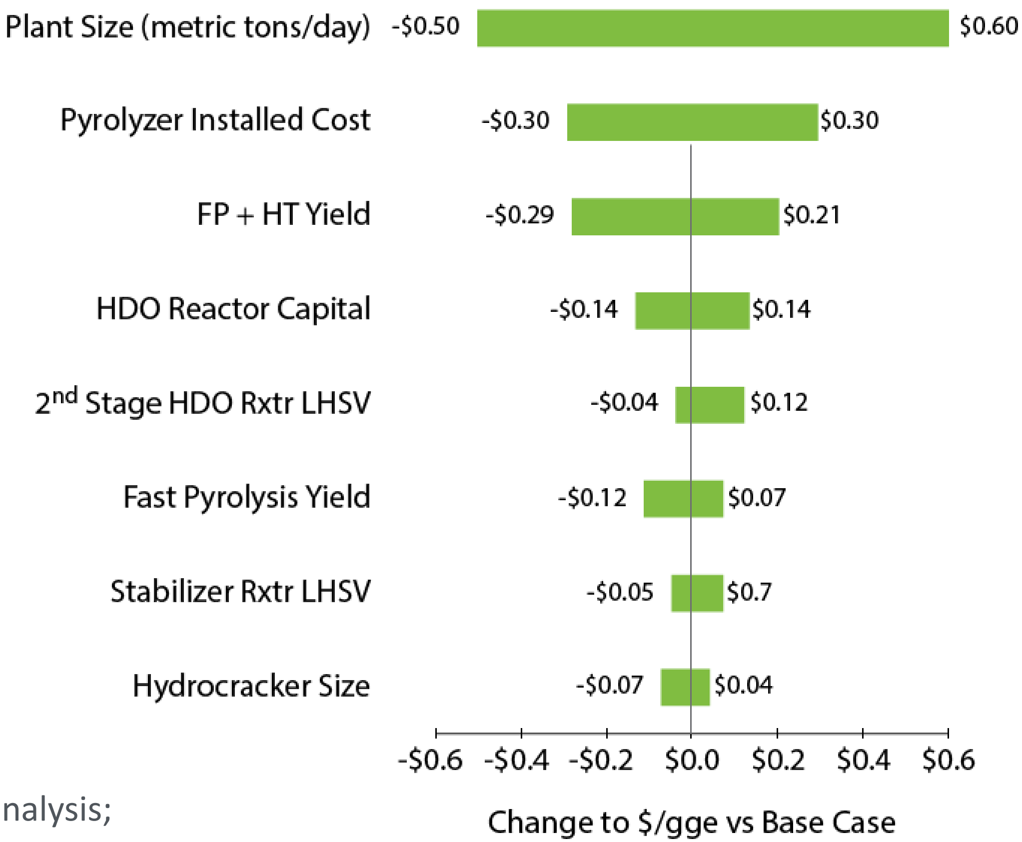
High-level LCA, TEA,* feedstock availability analyses

Identify cost/environmental/scale attributes

Fifteen key metrics identified

GHG, water, economics, TRL

Evaluation of 20 Thrust I blendstocks underway



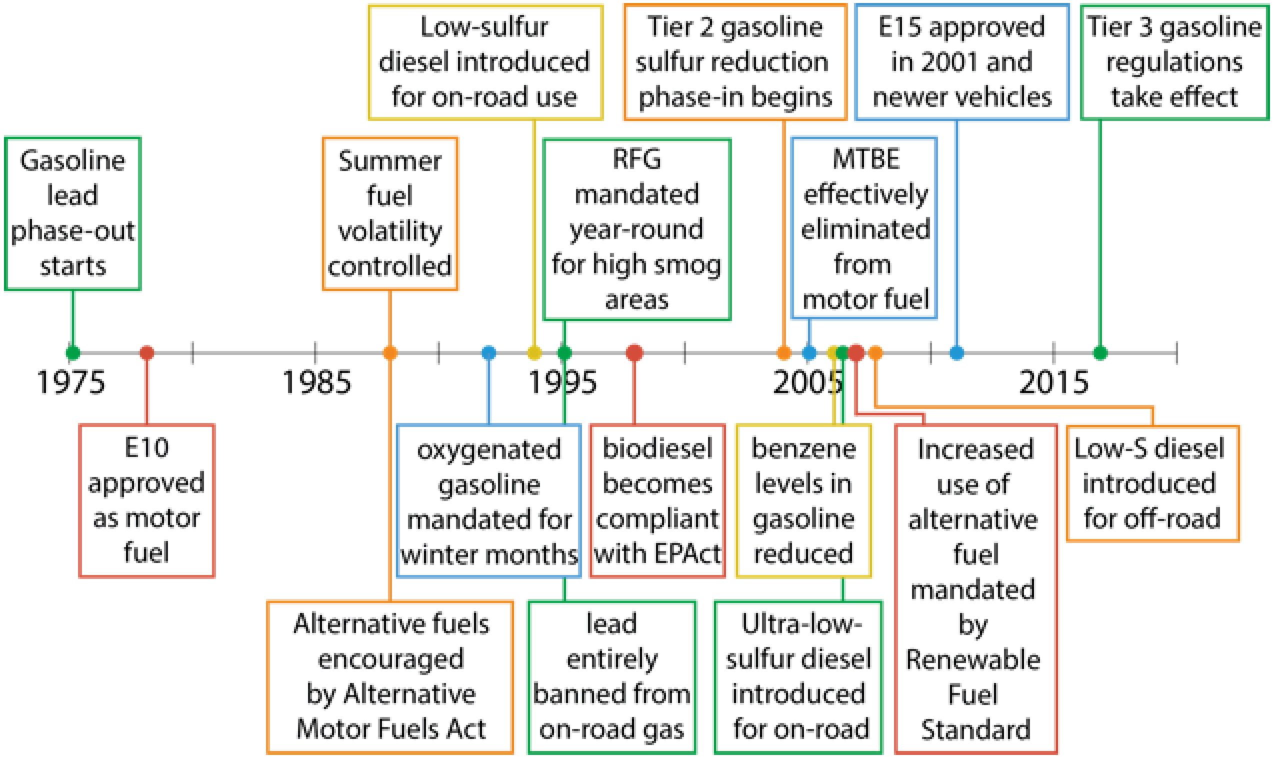
* LCA = Life cycle analysis; TEA = techno-economic analysis; TRL = technology readiness level

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

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

Fuel-related tasks (continued)

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

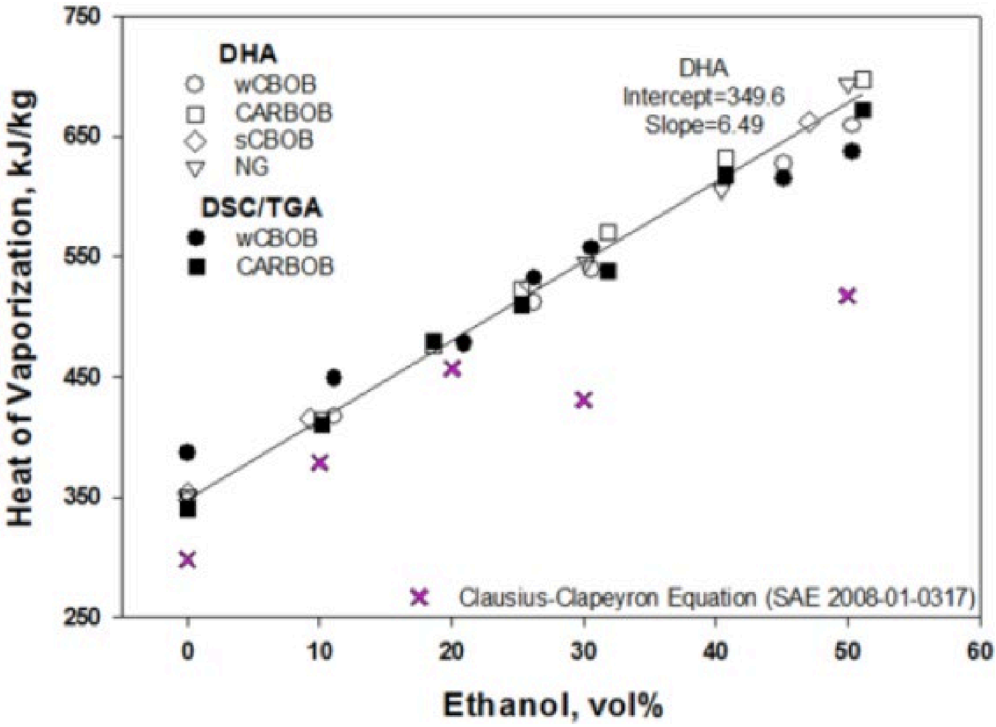
Heat of vaporization (HOV): complex mixtures

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

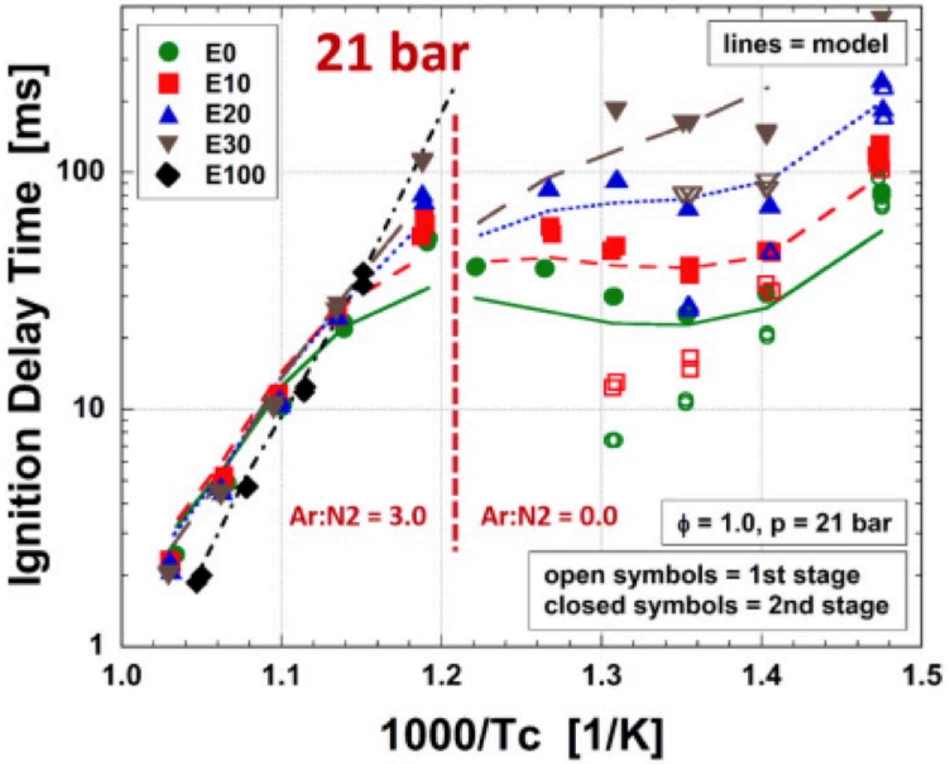
Kinetics and SI autoignition behavior

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)



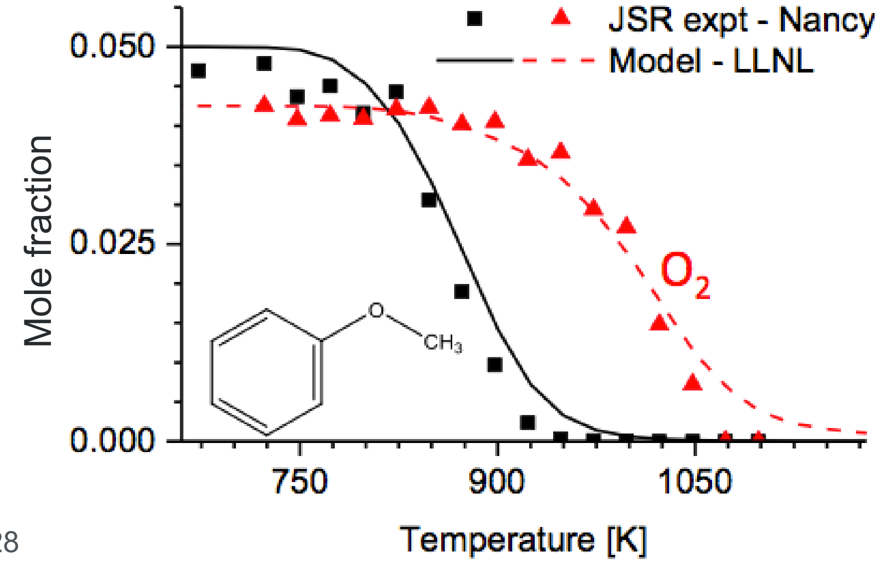
Goldsborough, ANL

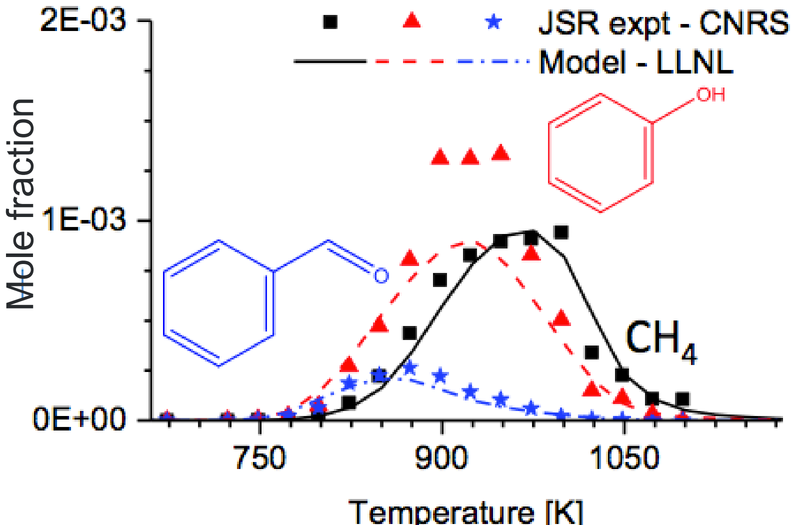
Kinetic mechanism development

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)





Thrust I tasks

Topic	Lead PI (Lab)
Thrust I	
Merit Function Definition	Miles (SNL) et al.
Efficiency Benefits of High Octane Fuels	Sluder (ORNL)
Effects of RON, HoV, and Octane Sensitivity	Ratcliff (NREL)
	Kolodziej/Ickes (ANL)
Dilution Limits on SI Combustion	Szybist (ORNL)
	Kolodziej/Wallner (ANL)
Fuel Effects on LSPI	Splitter (ORNL)
Advanced LD SI Engine Fuels Research	Sjöberg (SNL)
CFD of Thrust I Experiments	Som (ANL)

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

Relationship between sensitivity and HOV

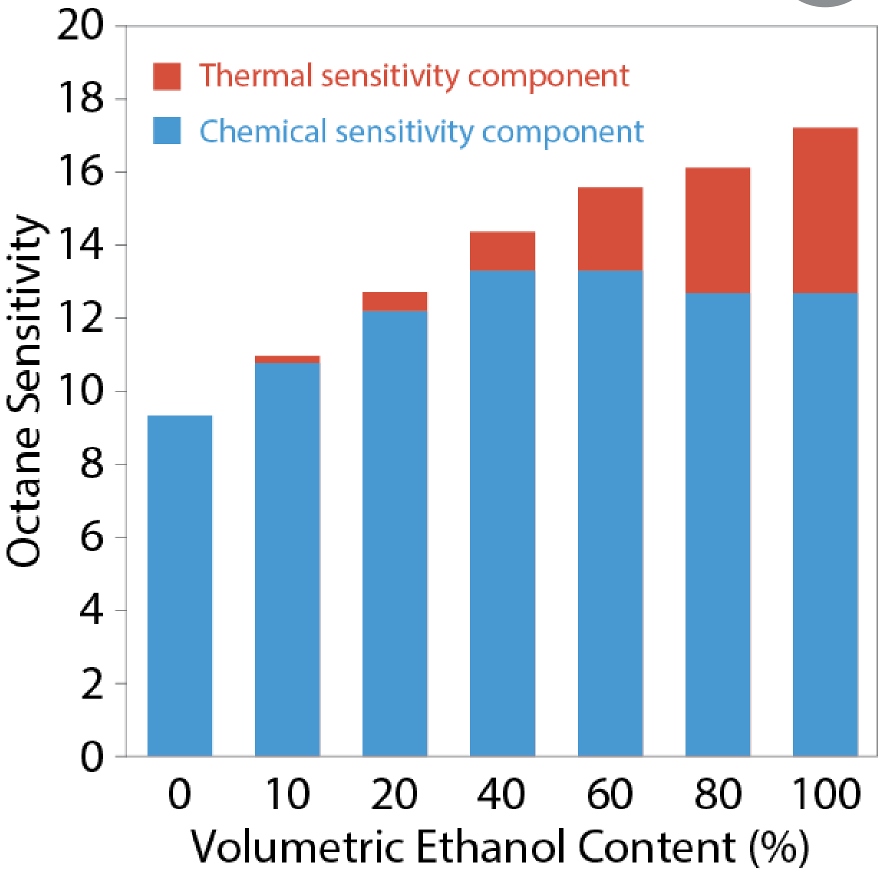
Inconsistencies in literature regarding HOV impact on knock

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

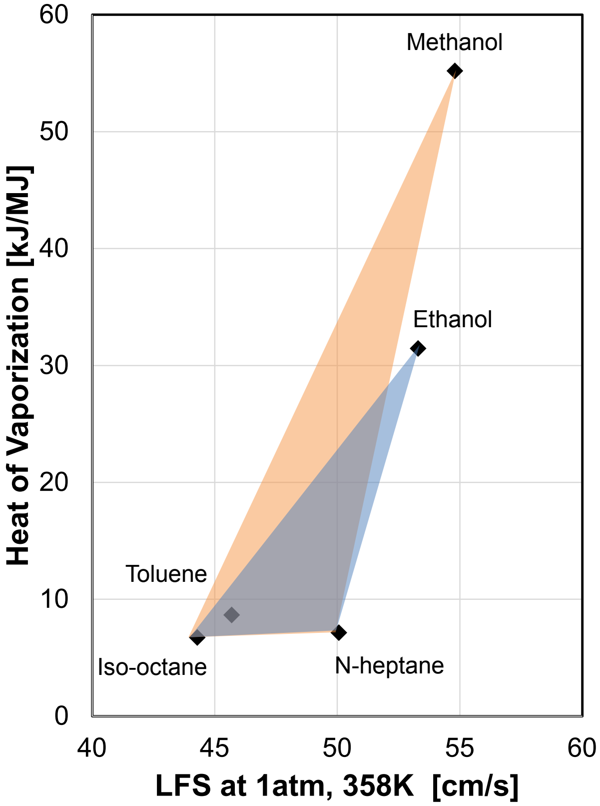
Quantify relative fuel impact on dilution tolerance and compare vs engine parameters

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



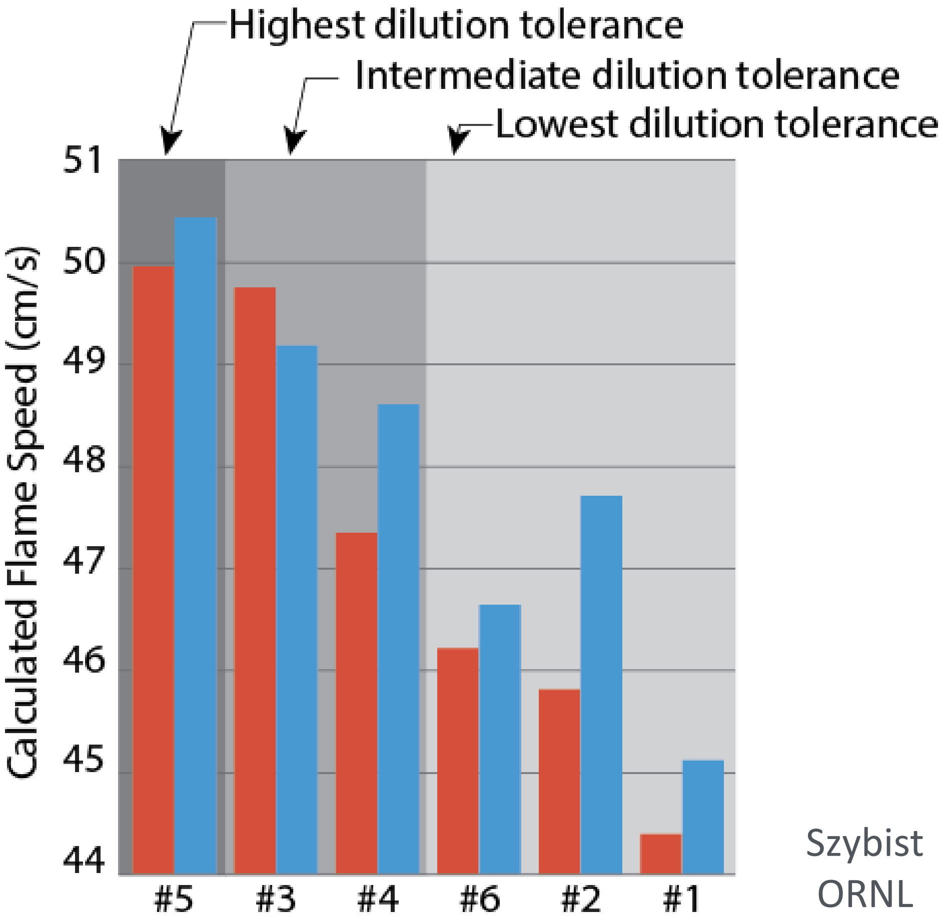
Wallner ANL

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



Szybist
ORNL

Thrust II tasks

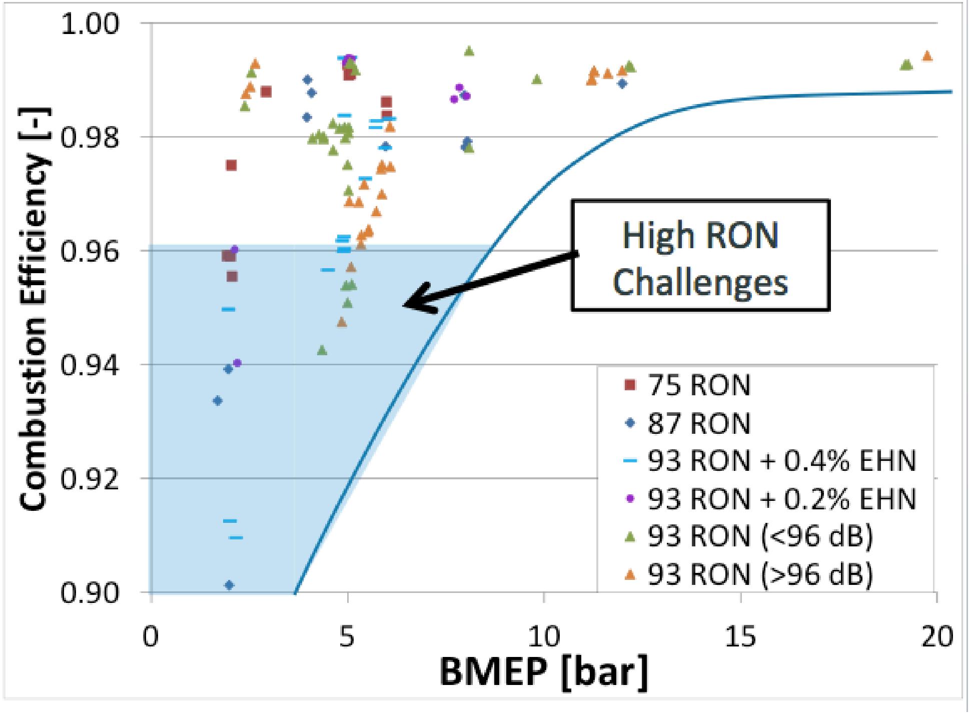
Topic	Lead PI (Lab)
Thrust II	
Evaluate Thrust I Fuel Compatibility with ACI Strategies	Dec (SNL) - LTGC
	Ciatti (ANL) - GCI
	Curran (ORNL) - GCI
Accelerate ACI Combustion System Development	Curran (ORNL) - RCCI
	Musculus (SNL) - RCCI
	Mueller (SNL) - LLFC
High-throughput spray chamber	Pickett (SNL)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

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



Ciatti ANL

Multi-cylinder RCCI experiments

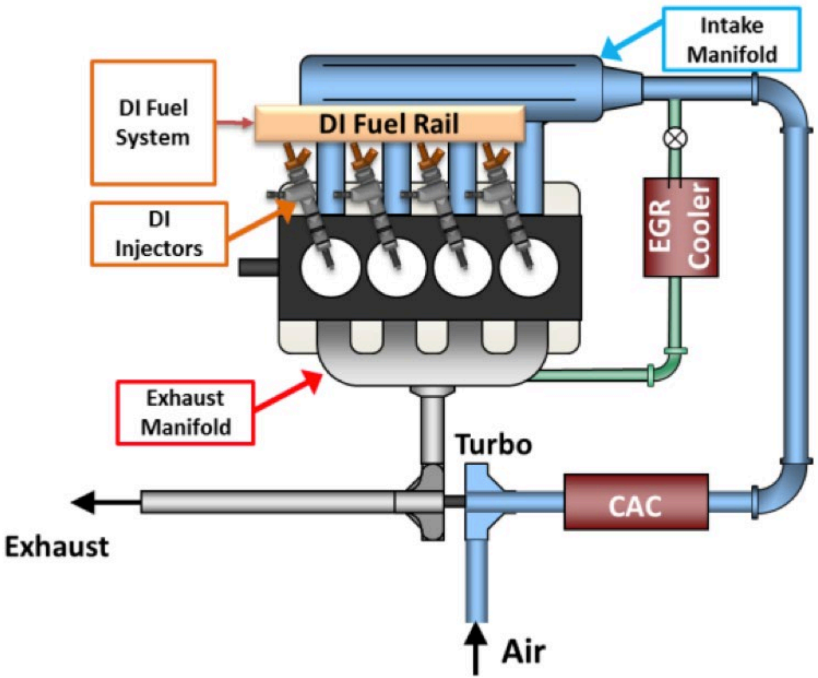
1.9L GM diesel engine platform with production viable hardware

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

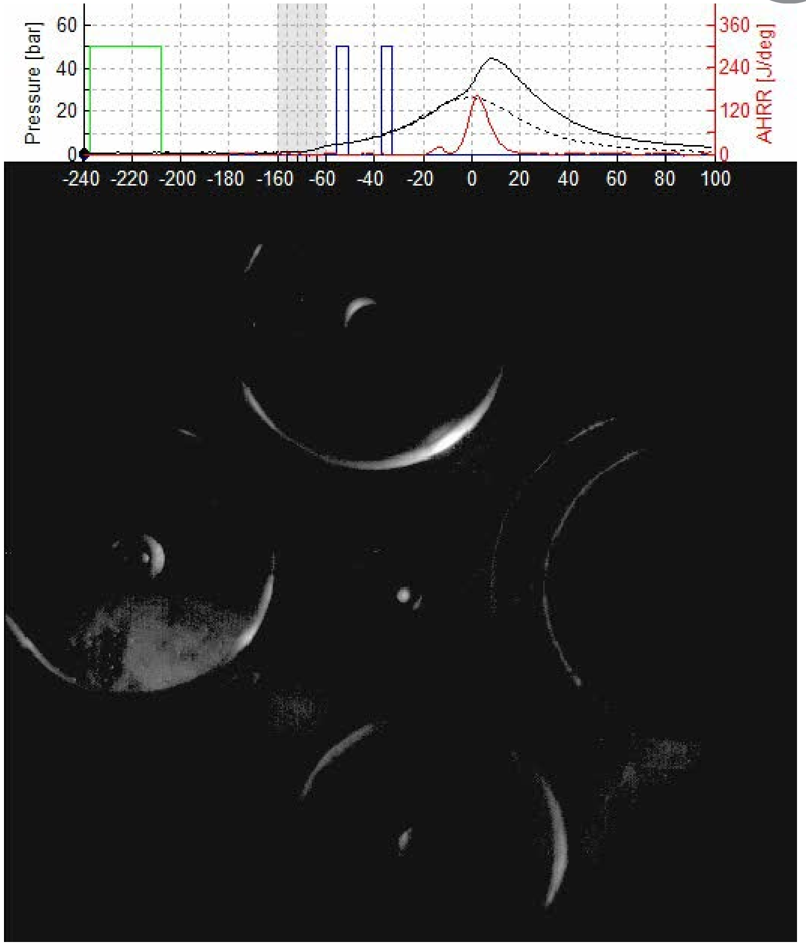
Measure in-cylinder mixing/ kinetics to optimize dual-fuel heat-release

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

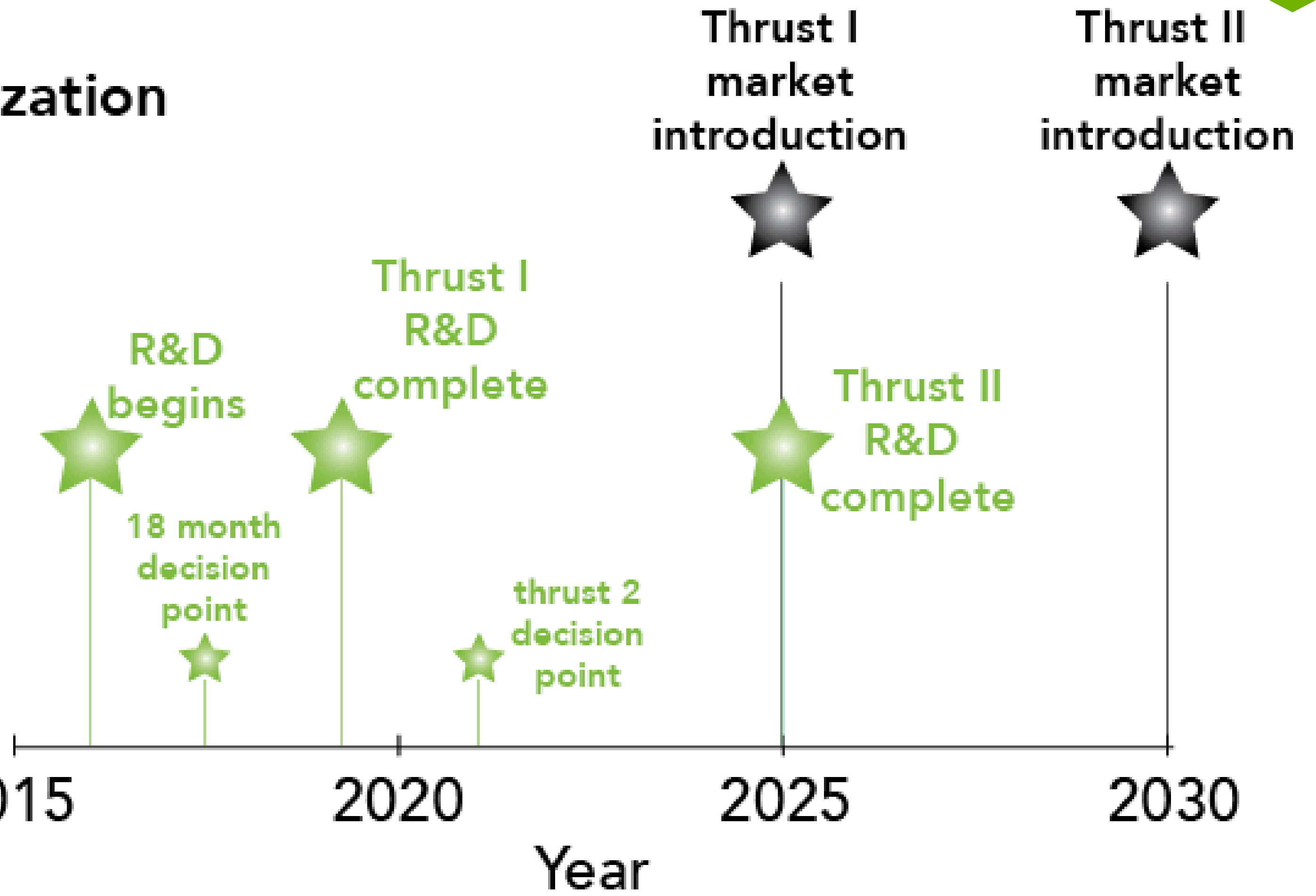


Musculus SNL

18 month decision point

commercialization targets

R&D milestones



First major milestone: 18 month decision point

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

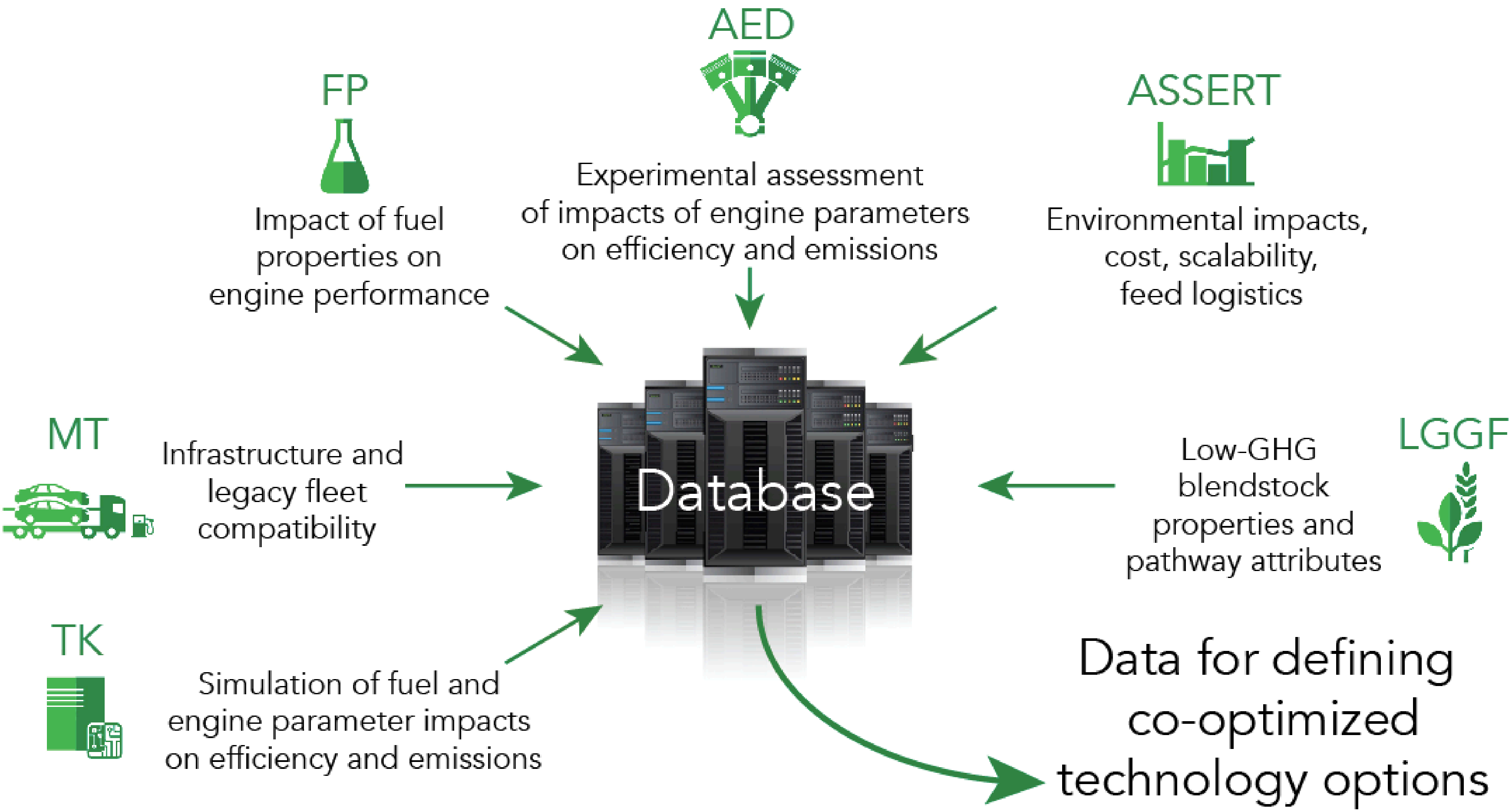
Will conduct rigorous assessment of fuel/engine options and identify promising* low-GHG fuel/engine combinations

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



Approach

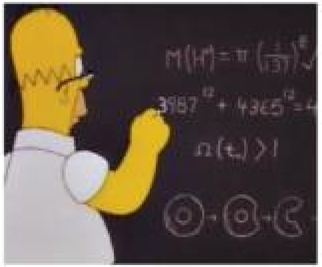
Database: fuel properties, sustainability, affordability, scalability, infrastructure, and retail attributes

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

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		

18 month decision point summary

- Co-Optima team is conducting R&D across wide technology space to identify
  - Properties and attributes of Thrust I blendstock candidates
  - Engine/vehicle merit function to relate properties to performance
- At end of 18 months (3/31/17) we will have surveyed all promising candidates and characterized performance along multiple dimensions
- Decision will address whether promising* low-GHG blendstocks/fuels have been identified that merit further fuel development/scale-up efforts
  - If "no" – shift fuel discovery/development efforts to Thrust II (other Thrust I efforts – engine testing, ASSERT and MT metrics, etc – will likely continue)
  - If answer is "yes" – continue development and scale-up efforts

* Need stakeholder input to define what constitutes "promising"

  - Focus of 2016 Stakeholder Listening Days (stay tuned)

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