Co-Optimization of Fuels & Engines

better fuels | better vehicles | sooner

Fuel Property and Engine Combustion Research of the US Co-Optima Initiative

Mark Musculus
Combustion Research Facility
Sandia National Laboratories

Contributing PIs:

Scott Curran, ORNL
John Dec, SNL
Andrew Ickes, ANL
Paul Miles, SNL
Chuck Mueller, SNL
Jim Szybist, ORNL

SAND2017-6420C

Tailor-Made Fuels From Production to Propulsion

5th International Conference

June 20th – 22nd 2017
Eurogress, Aachen Germany

Co-Optima Leadership Team: John Farrell (NREL), John Holladay (PNNL), Chris Moen (SNL), Robert Wagner (ORNL)

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

US Department of Energy (DOE) Bioenergy Technologies Office Program Managers: Alicia Lindauer, Borka Kostova
US DOE Vehicle Technologies Office Program Managers: Gurpreet Singh, Kevin Stork, Leo Breton & Michael Weismiller

US DOE Co-Optimization of Fuels & Engines (Co-Optima): increase efficiency, diversify fuels

Light-duty

Up to 15% fuel economy (FE) improvement*
Phase 1: boosted SI; Phase 2: multi-mode SI/ACI

Heavy-duty

Up to 1-4% FE improvement (worth $1-5B/year)*

Potential lower cost path to meeting next tier of criteria emissions regulations

Fuels

Diversifying resource base

Providing economic options to fuel providers to accommodate changing global fuel demands

Increasing supply of domestically sourced fuel by up to 25 billion gallons/year

Cross-cutting goals

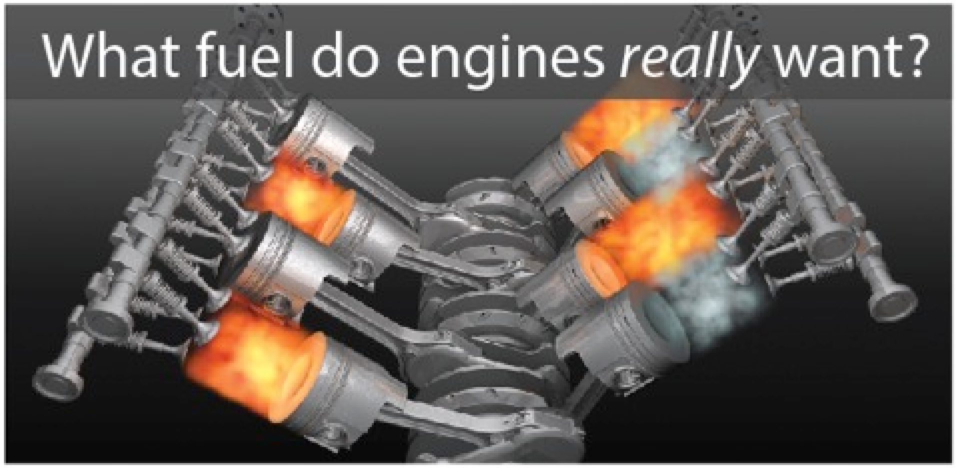
Stimulate domestic economy

Adding up to 500,000 new jobs

Providing clean-energy options

* Beyond projected results of current R&D efforts. The team is actively engaging with OEMs, fuel providers, and other key stakeholders to refine goals and approaches to measuring fuel economy improvements

Primary technical challenges of Co-Optima: Target fuel properties? How to make them?



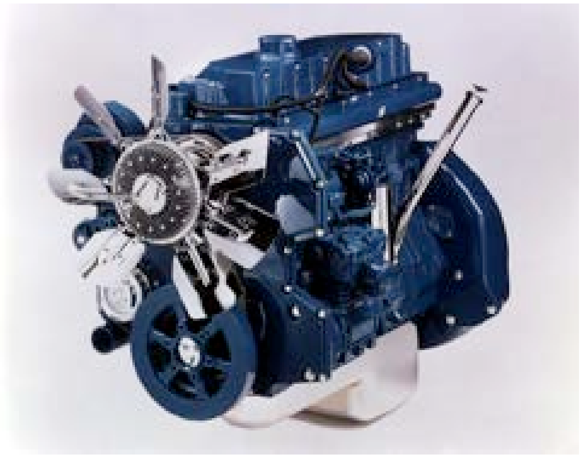
Identifying key fuel properties that impact efficiency for advanced spark ignition and compression ignition combustion approaches

Identifying fuel formulations that provide target ranges of key fuel properties when blended with petroleum blendstocks

Co-Optima research is structured around two guiding hypotheses on engines and fuels

Central Engine Hypothesis

There are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range

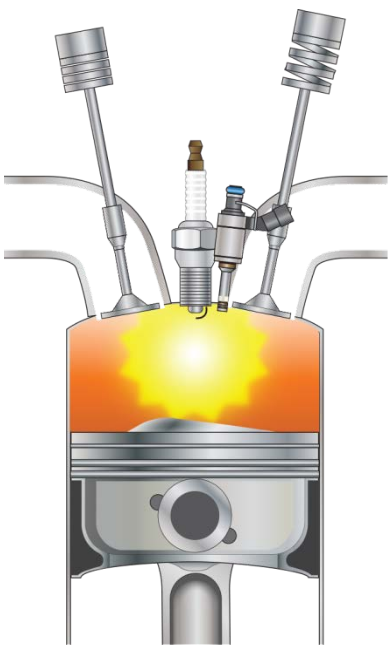


Central Fuel Hypothesis

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

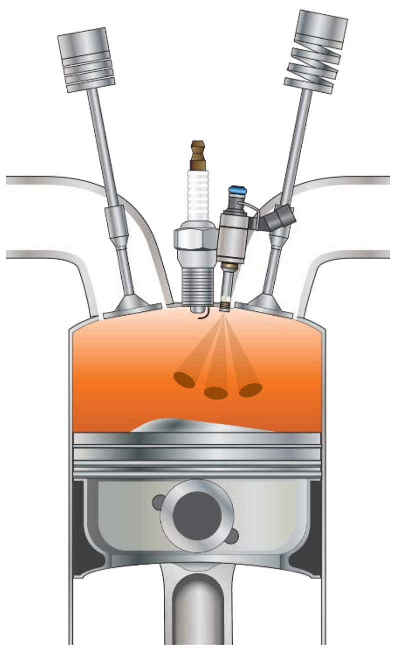
Co-Optima engine & fuel research proceeds along two parallel application/mode tracks

Light-Duty



Boosted SI

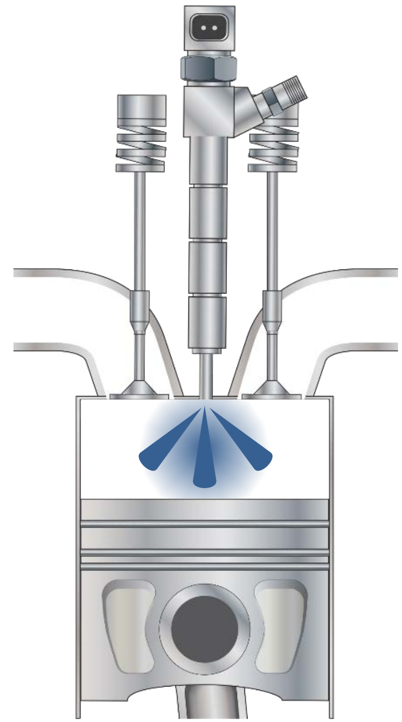
Near-term



Multi-mode SI / ACI

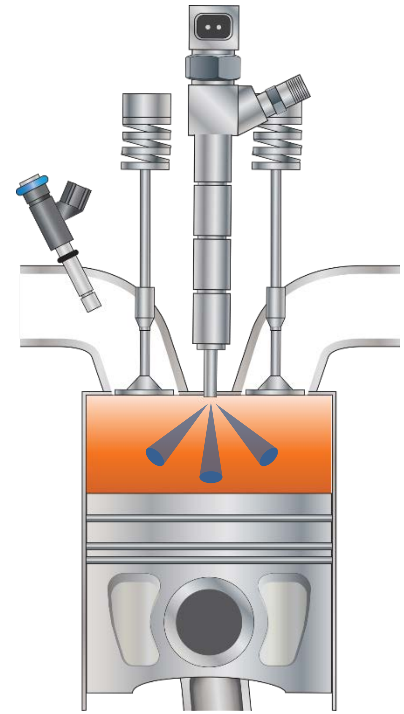
Mid-term

Medium and Heavy-Duty



Mixing Controlled

Near-term



Kinetically Controlled

Longer-term

Three-tiered approach to screen, measure, analyze, and evaluate candidate blendstocks

Tier 1

> 470 blendstocks

14 chemical families

Identify broad range of potential hydrocarbon and oxygenated blendstocks

Utilize property information on blendstocks from literature or estimates to identify Tier 2 blendstocks

Tier 2

41 blendstocks

10 chemical families

Measure blendstock properties

Evaluate blendstock performance in BOBs at 10-30% blend levels

Remove candidates from list if improved data indicate they do not meet criteria

Add new candidates as our under-standing improves of how fuel structure impacts key properties

Tier 3

8 representative* blendstocks

5 chemical families

Refine property measurements

Develop improved blending models

Produce/procure blendstocks in quantity for testing and validate engine and fuel economy performance

Characterize/compare benefits and identify challenges for commercial introduction

*These blendstocks constitute a representative subset of a broader range of molecules/mixtures that meet the Tier 3 criteria

Properties of many Tier 1 blendstock candidates are catalogued in a publicly accessible database*

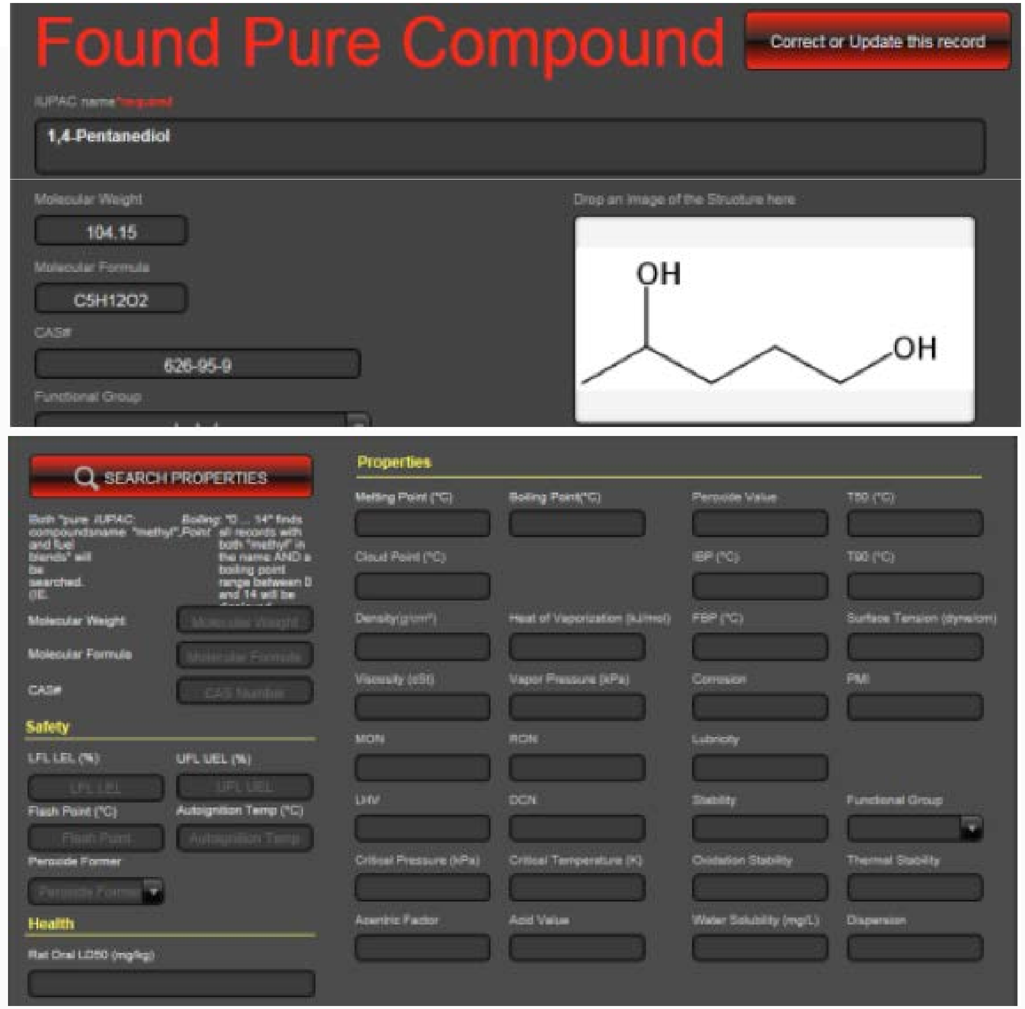
Tier 1

> 470 blendstocks

14 chemical families

Identify broad range of potential hydrocarbon and oxygenated blendstocks

Utilize property information on blendstocks from literature or estimates to identify Tier 2 blendstocks



* Available at: https://fuelsdb.nrel.gov/fmi/webd#FuelEngineCoOptimization

41/470 candidate blendstocks passed through Tier 1 screening for boosted SI engines

- Tier 1 screening applies criteria based on boiling point, melting point, solubility, corrosion, toxicity, fuel handling safety, biodegradation, and autoignition characteristics (e.g., RON for boosted SI)

	Alcohols (9)
1	Methanol
2	Ethanol
3	1-Propanol
4	Isopropanol
5	1-Butanol
6	2-Butanol
7	Isobutanol
8	2-Methylbutan-1-ol
9	2-Pentanol

	Ethers
10	Anisole

	Esters (13)
11	Methyl acetate
12	Methyl butanoate
13	Methyl pentanoate
14	Methyl isobutanoate
15	Methyl-2-methylbutanoate

	Esters (13)
16	Ethyl acetate
17	Ethyl butanoate
18	Ethyl isobutanoate
19	Isopropyl acetate
20	Butyl acetate
21	2-Methylpropyl acetate
22	3-Methylpropyl acetate
23	mixed esters

	Ketones (9)
24	2-Butanone
25	2-Pentanone
26	3-Pentanone
27	Cyclopentanone
28	3-Hexanone
29	4-Methyl-2-Pentanone
30	2,4-Dimethyl-3-Pentanone
31	3-Methyl-2-butanone
32	Ketone mixture

	Furans
33	2,5-Dimethylfuran/2-methylfuran

	Branched alkanes
34	2,2,3-Trimethylbutane

	Alkenes
35	Diisobutylene

	Multicomponent mixtures (6)
36	Methanol-to-gasoline
37	Ethanol-to-gasoline
38	Bioreformate via multistage pyrolysis
39	Bioreformate via catalytic conversion of sugar
40	Mixed aromatics via catalytic fast pyrolysis
41	Aromatics and olefins via pyrolysis-derived sugars

The "merit function" is an algebraic expression for determining what fuel properties engines want

Project Lead: Paul Miles, Sandia National Laboratories

The overall engine and emissions-control system thermal efficiency can be expressed as a product of sub-efficiencies

$$\eta_{th} = \eta_{ideal} * \eta_{glh} * \eta_{comb} * \eta_{pump} * \eta_{ht} * \eta_{emiss} \cdots$$

$$\eta_{ideal} = 1 - \frac{1}{CR^{\gamma-1}}$$

η_{glh} = combustion phasing ("degree of constant V combustion")

η_{comb} = combustion efficiency

η_{pump} = pumping losses

η_{ht} = heat transer losses

η_{emiss} = emission control losses

Fuel properties play roles in many of the sub-efficiency terms of the merit function

Project Lead: Paul Miles, Sandia National Laboratories

Since we are interested in relative efficiency, we can differentiate to get:

$$\frac{d\eta_{th}}{\eta_{th}} = \frac{d\eta_{CR}}{\eta_{CR}} + \frac{d\eta_{\gamma}}{\eta_{\gamma}} + \frac{d\eta_{glh}}{\eta_{glh}} + \frac{d\eta_{comb}}{\eta_{comb}} + \frac{d\eta_{pump}}{\eta_{pump}} + \frac{d\eta_{ht}}{\eta_{ht}} + \frac{d\eta_{emiss}}{\eta_{emiss}} + \ldots$$

PMI, $T_{c,90}$

HOV

Flame Speed

RON, octane sensitivity, HOV

How can we quantify these in terms of fuel properties for each combustion mode?

Boosted SI merit function quantifies engine & fuel effects on percentage change in efficiency

Project Lead: Paul Miles, Sandia National Laboratories

- First term is based on the Octane Index (OI), where K is indicative of the engine operating condition
  - K=0: “Research Octane Number” (RON) test condition (cold)
  - K=1: “Motor Octane Number” (MON) test condition (hot)
  - K<0: “beyond RON,” e.g., boosted spark ignition (SI)
  - K>1: “beyond MON,” e.g., advanced compression ignition

$$OI = RON - K \cdot S = RON - K \cdot (RON - MON)$$

$$Merit\,[\Delta\%] = \frac{(RON_{mix} - 91)}{1.6} - K\frac{(S_{mix} - 8)}{1.6} + \frac{0.085[ON/kJ/kg] \cdot ((HoV_{mix}/(AFR_{mix}+1)) - (415[kJ/kg]/(14.0[-]+1)))}{1.6} + \frac{((HoV_{mix}/(AFR_{mix}+1)) - (415[kJ/kg]/(14.0[-]+1)))}{15.2} + \frac{(S_{L\,mix} - 46[cm/s])}{5.4} - H(PMI_{mix} - 1.6)[0.7 + 0.5(PMI_{mix} - 1.4)] + 0.008°C^{-1}(T_{c,90,conv} - T_{c,90,mix})$$

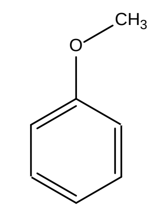
Boosted SI fuel matrix designed to determine if octane index can predict engine efficiency limits

Project Lead: Jim Szybist, Oak Ridge National Laboratory

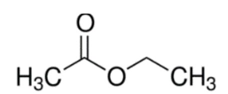
	Co-Optima "Alkylate"	Co-Optima "Aromatic"	Co-Optima "E30"	"Tier III" E10 EEE	25 mol% Methyl Butyrate Blend "MB"	25 mol% Ethyl Acetate Blend "EA"	25 mol% "Anisole" Blend
RON	97.9	98	98.3	91.8	98.1	98.5	98.8
MON	96.7	87.3	87.6	84.2	90.9	92.6	90.5
S	1.2	10.7	10.7	7.6	7.2	5.9	8.3
Aromatic	0	35.8	8.1	22.6	23 mol%	23 mol%	23 mol%
Saturates	100	65	57.1	71.2	47 mol%	47 mol%	47 mol%
Olefins	0	4.2	5	5.2	5 mol%	5 mol%	5 mol%
Ethanol	0	0	29.95	9.8	0	0	0
T10	93.1	59.4	60.7	54.6	-	-	-
T50	100.3	108.1	74.3	89.9	-	-	-
T90	105.9	157.9	155.2	157.9	-	-	-
C (wt%)	83.75	87.22	74.78	82.63	79.37	79.18	83.95
H (wt%)	15.80	13.12	13.79	13.66	12.89	12.85	12.23
O (wt%)	0	0	11.19	3.71	7.74	7.97	3.82

Fuels: Co-Optima "core" fuels, tier III cert gasoline, and 3 bio-blendstock candidates

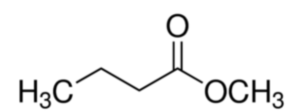
Anisole
RON = 103
S = 12



Ethyl Acetate
RON = 118
S = -2



Methyl Butyrate
RON = 107
S = 2

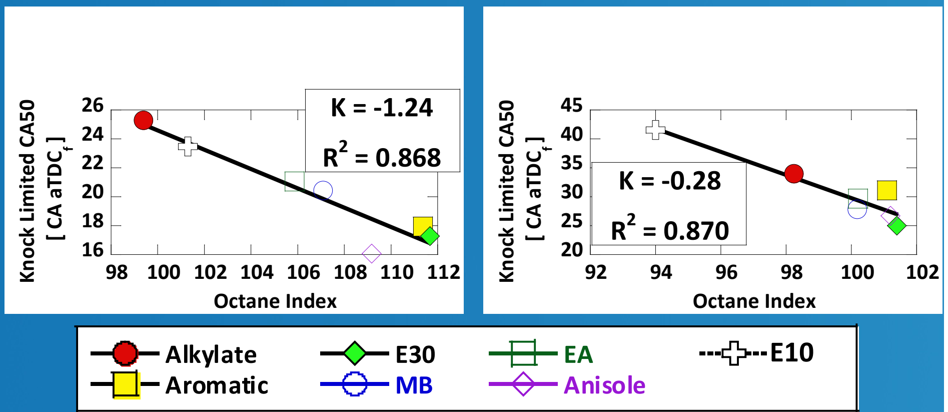


Operating Conditions: Constant fueling rate (14.5-19.0 bar IMEP), varying intake temperature, backpressure, and EGR

	Sweep 1	Sweep 2	Sweep 3	Sweep 4	Sweep 5	Sweep 6	Sweep 7	Sweep 8
Intake T [°C]	35	35	35	35	90	90	90	90
Manifold DP [kPa]	>20	8	8	8	>20	8	8	8
EGR [%]	0	0	10	20	0	0	10	20

Boosted SI: For ϕ≈1, octane index correlates well with knock-limited combustion phasing

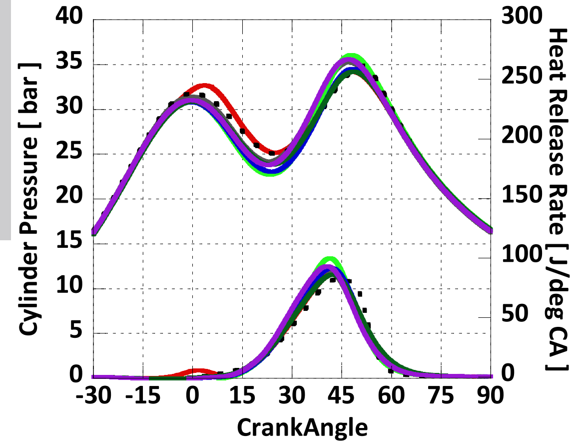
Project Lead: Jim Szybist, Oak Ridge National Laboratory

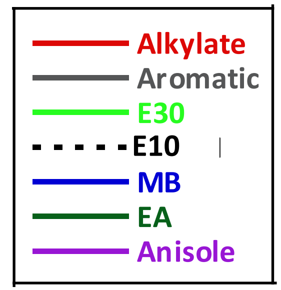


*OI = RON – K*S*

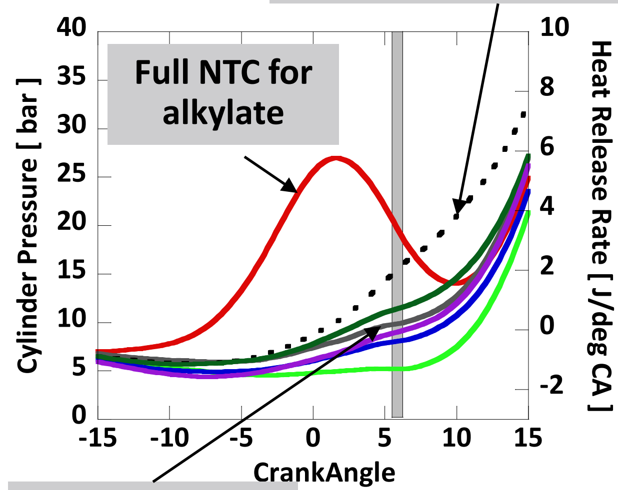
- Octane index includes the two most impactful terms in the merit function
- Experiments confirm that OI correlates with knock-limited phasing much better than AKI, RON, or MON
- Despite good correlation coefficients, significant outliers were observed
  - Anisole fuel blend generally out-performs OI prediction (earlier knock-limited CA50)
  - Aromatic fuel blend under-performs with high intake manifold temperature

Focusing on retarded phasing, significant differences in early combustion phases are apparent





Pre-Spark Heat Release (PSHR) for E10 Fuel is between alkylate & aromatic



Some PSHR for aromatic

Premixed ACI: at ϕ = 0.4, different CA50 for fuels with same RON & S; "O_2" OI analysis works well

Project Lead: John Dec, Sandia National Laboratories

Advanced Compression Ignition (ACI)

- Designed fuel test matrix with five fuels with RON ≈ 98, four with S ≈ 10.5, one with S ≈ 1

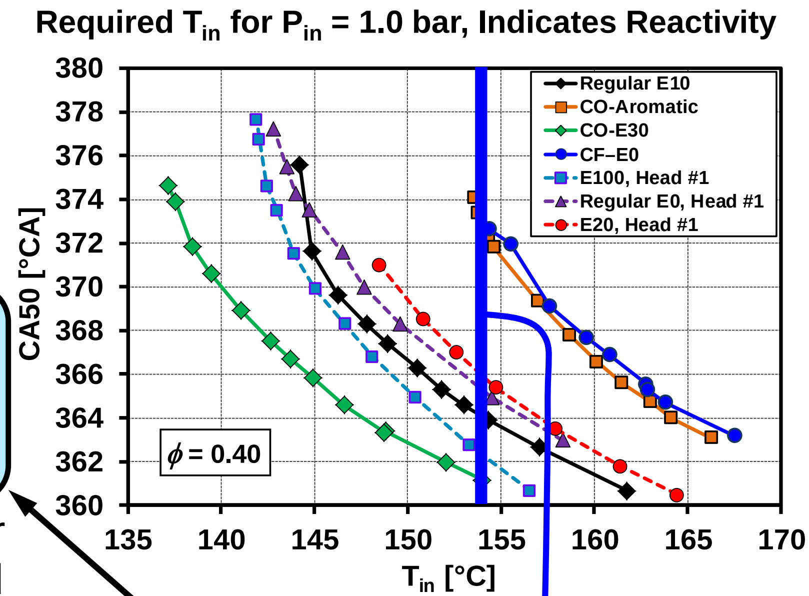
Co-Optima Core Fuels	Alkylate	E30	Aromatic	Olefin	Cyclo-alkane
RON	98.0	97.4	98.1	98.2	98.0
MON	96.6	86.6	87.8	88.0	87.1
S	1.4	10.8	10.3	10.2	10.9
Aromatics	0.7	13.8	39.8	13.4	33.2
n+i-Paraffin	98.1	40.5	46.2	56.4	40.6
Cycloalkane	0.0	7.0	8.0	2.9	24.2
Olefins	0.1	6.0	4.5	26.5	1.6
Ethanol	0.0	30.4	0.0	0.0	0.0

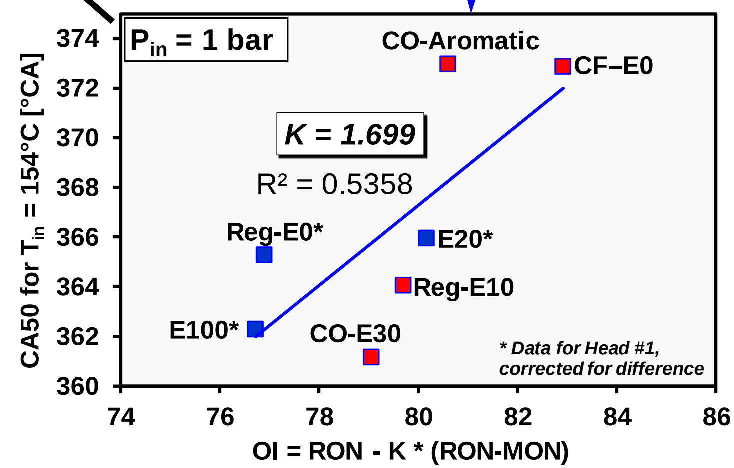
Premixed ACI: at ϕ = 0.4, different CA50 for fuels with same RON & S; "O_2" OI" analysis works well

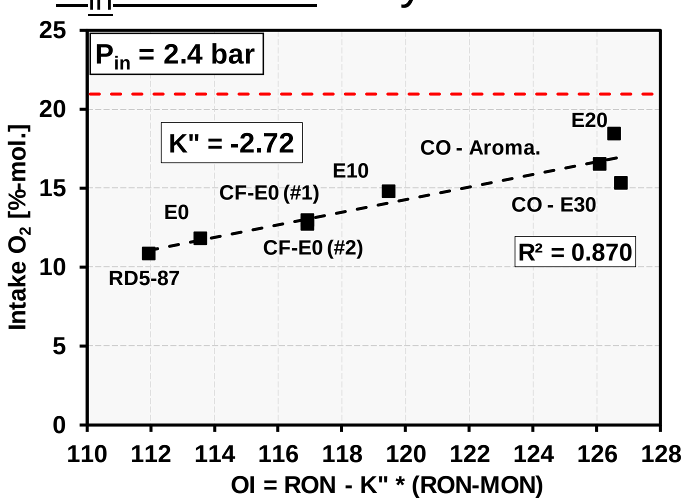
Project Lead: John Dec, Sandia National Laboratories

Advanced Compression Ignition (ACI)

- Designed fuel test matrix with five fuels with RON ≈ 98, four with S ≈ 10.5, one with S ≈ 1
- P_{in} = 1.0 bar: Surprisingly, reactivity varies among matched RON&S fuels: E30>>Aromatic
  - For LTGC at P_{in} = 1 bar with these fuels, Octane Index (OI) gives poor correlation (R^2 =0.536)
  - RON and MON appear insufficient for specifying fuel reactivity for lean LTGC (ϕ = 0.4) at this cond.
  - Perhaps this is because E30 is less ϕ-sensitive, or differences in HOV ⇒ Further studies are planned
- P_{in} = 2.4 bar: Try OI" based on intake O_2, since T_{in} = 60°C for all
  - OI" correlates fuels fairly well at P_{in}=2.4 bar, R^2 =0.870
  - Improved understanding of this intake-O_2 based OI" is needed







Premixed ACI: Reactivity of E30 (high RON & S) similar to E0, correlates with ITHR & ϕ-sensitivity

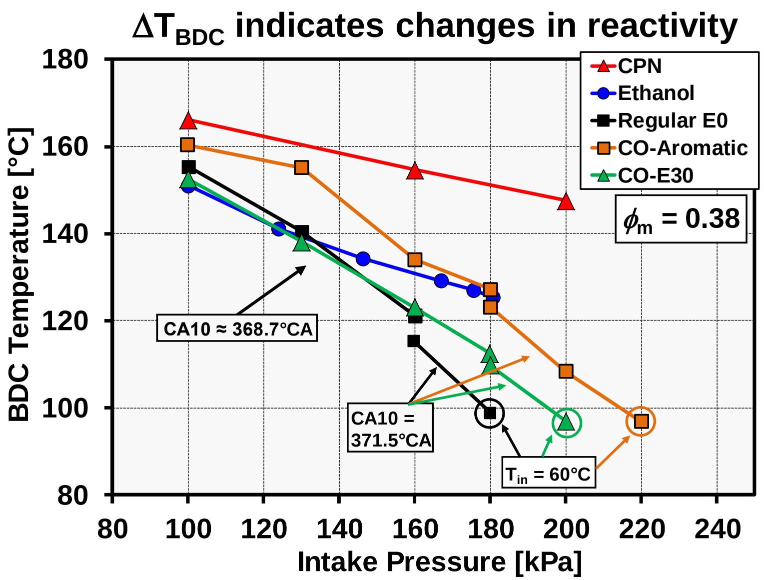
Project Lead: John Dec, Sandia National Laboratories

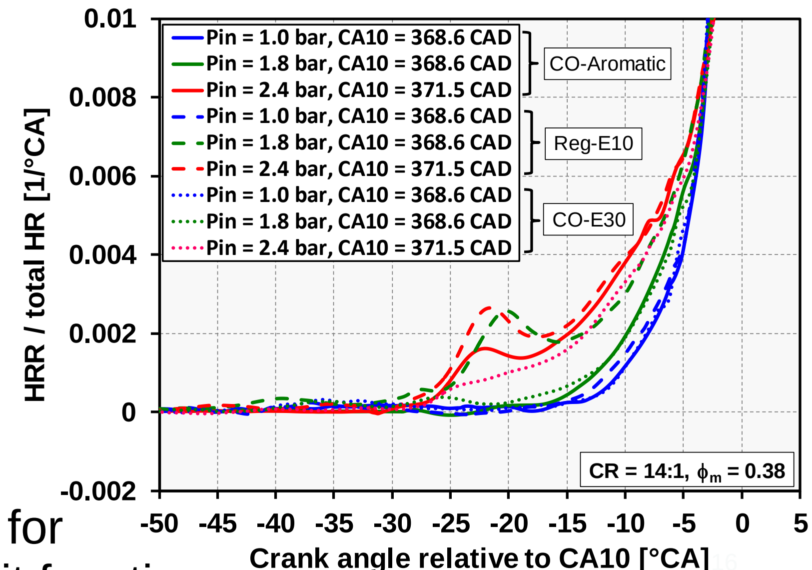
Reactivity Changes w/ Boost

- Increased fuel autoignition reactivity with boost is a key challenge for both LTGC and SI
  - LTGC: High EGR required for CA50 control limits O_2.
  - SI: Increased knock propensity limits CR
- Despite higher RON & S, E30 has similar reactivity to Reg-E0 for P_{in} = 1.0 – 1.6 bar ⇒ Somewhat less reactive for higher P_{in}
- Higher RON & S aromatic fuel is much less reactive than Reg-E0, esp. at $P_{in} \geq 1.8$ bar
  - At P_{in} = 1.8 bar, aromatic & E30 have lower ITHR than Reg-E10 ⇒ may affect reactivity trends
  - Also agrees with lower ϕ-sensitivity (for PFS)

Future Work:

- Evaluate E30 ϕ-sensitivity & high load behavior
- Evaluate the other three fuels in test matrix ⇒ High-Olefin, High-Cycloalkane, & Alkylate
- Investigate Co-Optima fuels with good potential for full-time LTGC-ACI engines ⇒ Support ACI merit function





Reactivity Controlled Compression Ignition (RCCI): LD multi-cyl. metal & HD single-cyl. optical engines

Project Lead: Scott Curran, Oak Ridge National Laboratory

Motivation for Using RCCI in ACI Engines

On-the-fly in-cylinder mixing of two fuels =
Control of combustion phasing & HRR

- Global octane number adjusted by fuel ratio
- Reactivity stratification by injection timing

RCCI Challenges

Peak pressure rise rate (PPRR) limits high load

- E30 extends limit ⇒ not well understood

Incomplete combustion at lowest loads

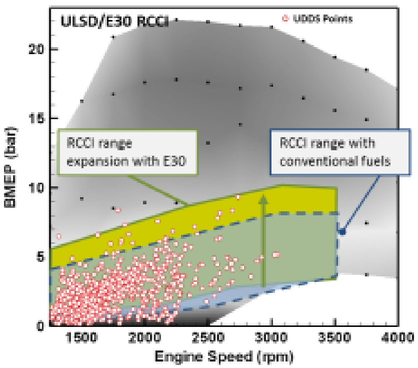
- Reasons are unclear

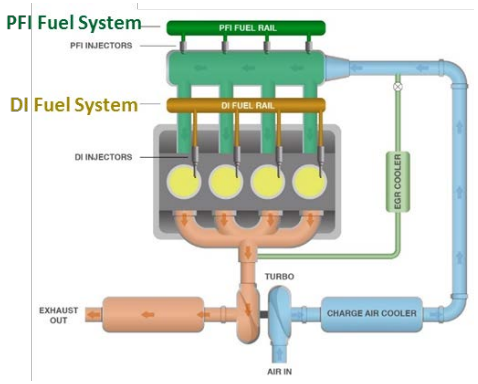
Approach for RCCI Work

- Use ORNL multi-cylinder metal engine to identify key fuel-property & operating-condition combinations where an improved understanding is required
- Use SNL single-cylinder optical engine to image in-cylinder mixing, ignition, and combustion processes at these conditions

ORNL Metal Engine

- Multi-cylinder light-duty diesel engine (PFI + DI)
- Transient capable + emissions characterization

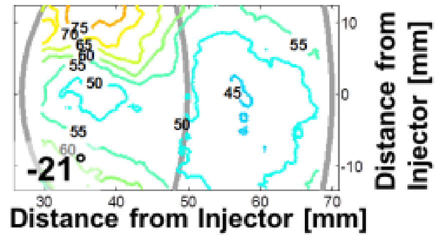


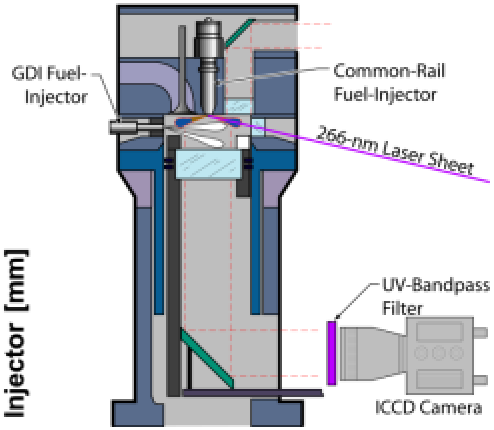


Project Lead: Mark Musculus, Sandia National Laboratories

SNL Optical Engine

- Single-cylinder heavy-duty diesel engine (GDI + DI)
- Image combustion & in-cylinder mixing (PRF)

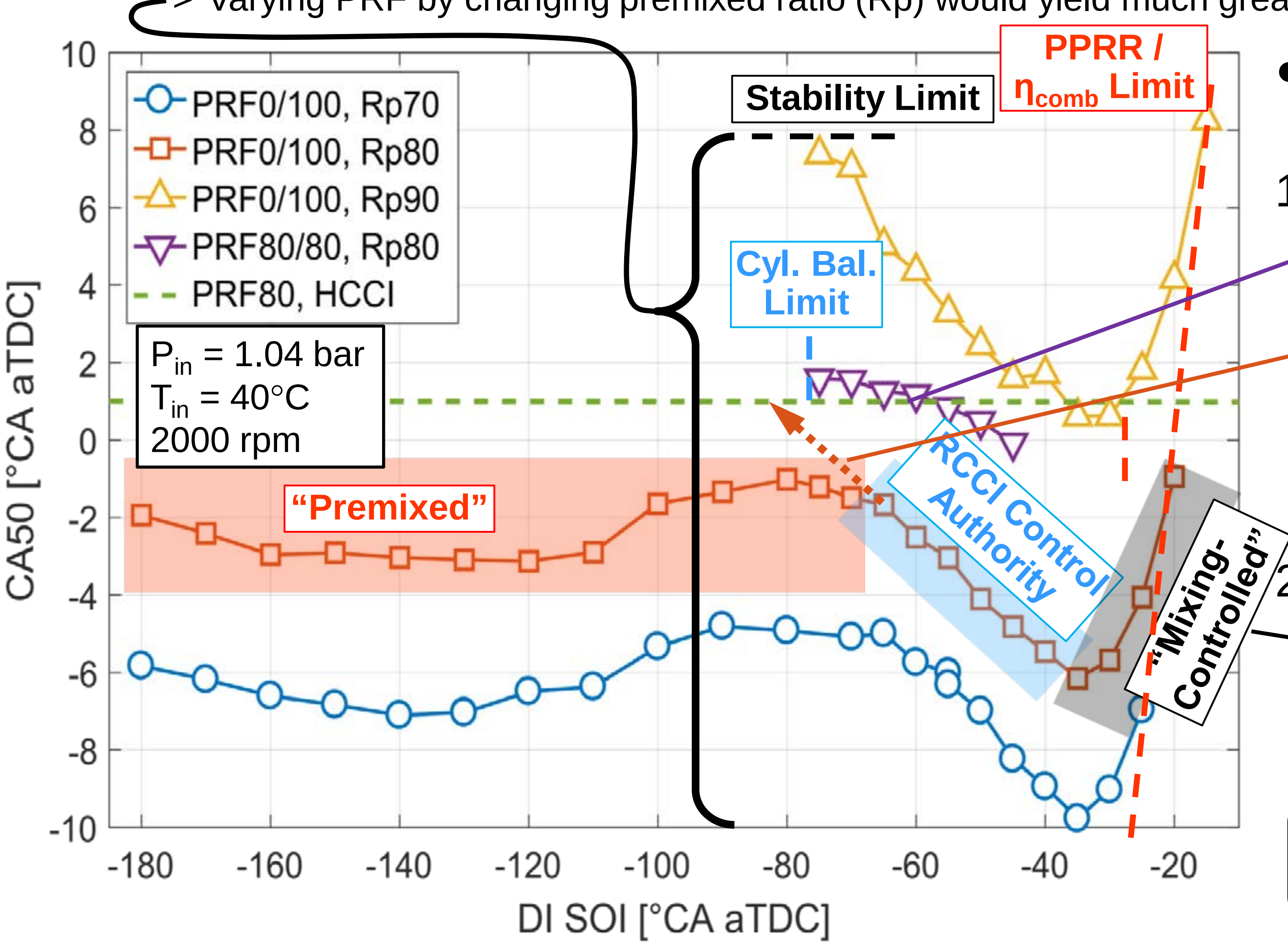




RCCI: At constant PRF, CA50 control authority limits approach premixed & mixing-controlled

Project Lead: Scott Curran, Oak Ridge National Laboratory

- Use PRFs (iso-octane & n-heptane): similar physical properties, different reactivity
  - DI SOI from -70 to -35 °CA aTDC have characteristic RCCI CA50 control authority
  - Control authority is limited by constant PRF in each sweep
    - > Varying PRF by changing premixed ratio (Rp) would yield much greater CA 50 control



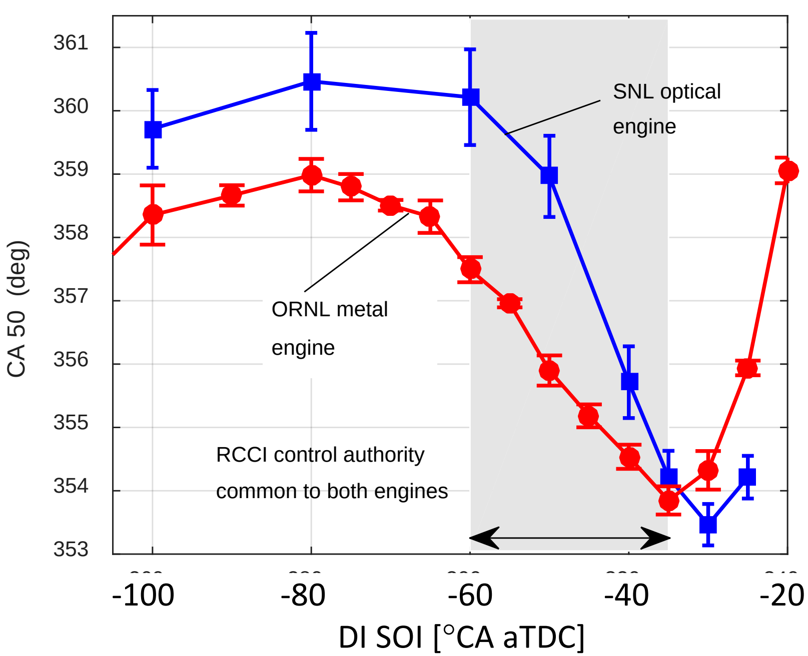
- Two limits of control authority range:
  1. "Premixed"
     - Premixed + DI PRF80 reaches premixed "HCCI"
     - Premixed PRF100 + DI PRF0 does not reach premixed "HCCI" CA50
       - > Wall wetting?
       - > Incomplete mixing?
  2. "Mixing-Controlled"
     - Late DI SOI: control authority trend reverses
       - > Fuel-rich mixing-controlled combustion?

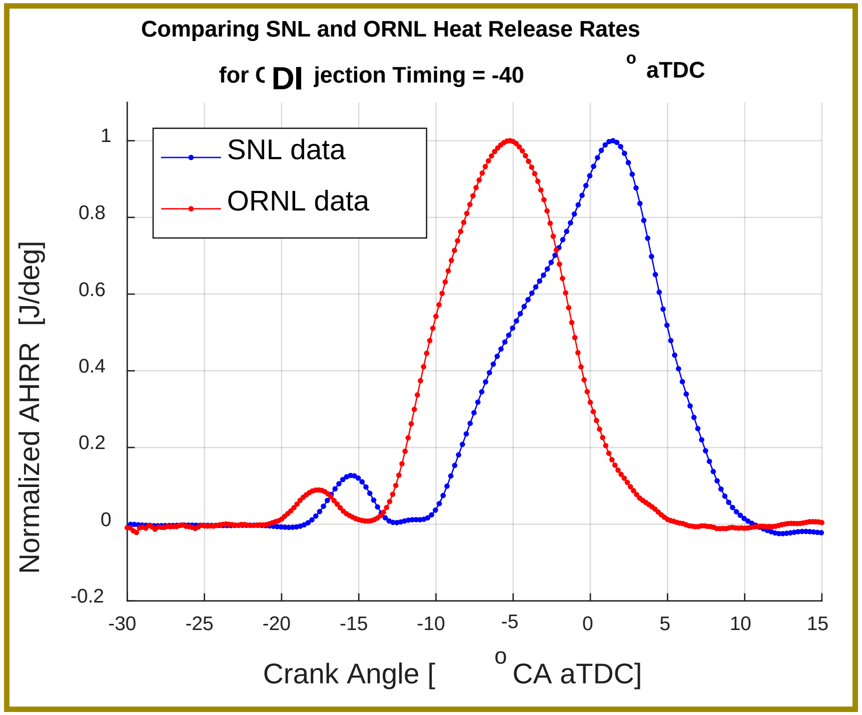
Gain insight from optical diagnostics

RCCI: Good matching of combustion phasing & control authority in optical & metal engines

Project Lead: Mark Musculus, Sandia National Laboratories

The mid-point of combustion heat release (CA50) depends on the injection timing of high-reactivity (PRF 0) fuel from the common rail (CR) DI injector



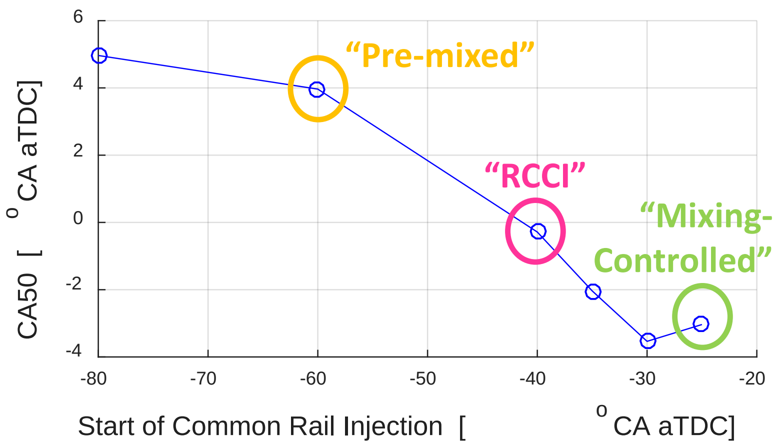


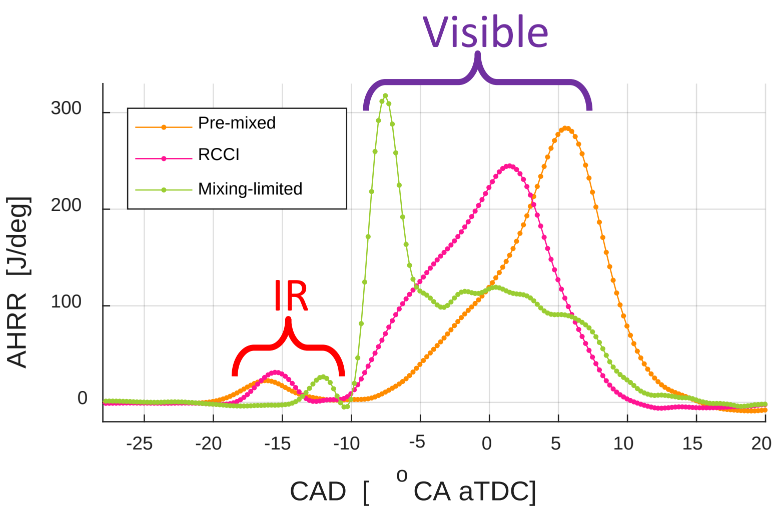
Heat release phasing is shifted, but the 2 engines yield the same characteristic shapes

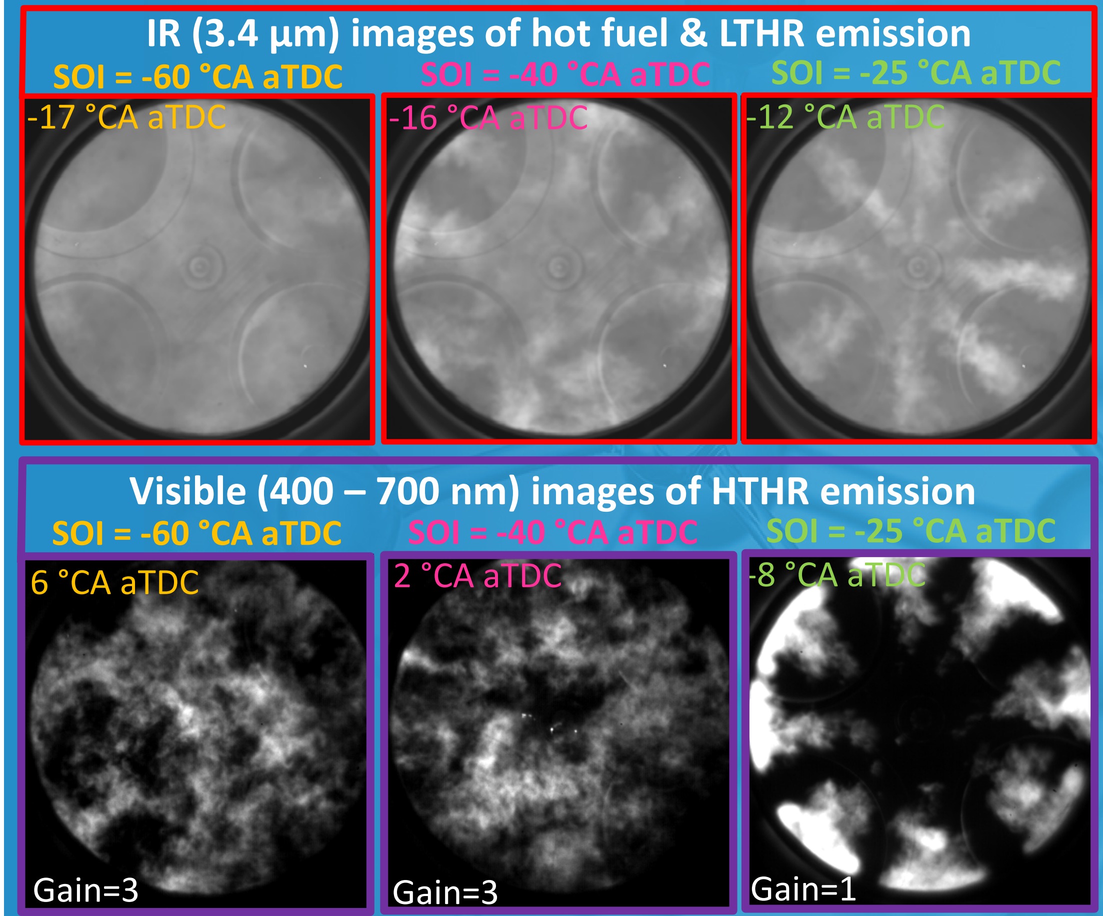
- Matching SNL HD optical engine with ORNL LD metal engine: **1. charge-gas ρ & T @ mid-control-authority DI injection, 2. premixed iso-octane (80%), 3. global Φ (0.35)**
- Even with different engine displacement (heavy-duty vs light-duty), compression ratios, and piston geometry, the **combustion characteristics are similar**, with three CA50 regimes (pre-mixed, RCCI, & mixing-controlled) and similar heat release shapes

Fundamental Stratified ACI (SNL, Musculus): Structure in IR & visible images (=incomplete mixing?), bright @ late DI (=rich?)

Project Lead: Mark Musculus, Sandia National Laboratories







- **Structure in IR imaging of 1st-stage and visible imaging of 2nd-stage ignition at all conditions – incomplete mixing?**
- **Brightening jet structure in visible imaging indicates transition to richer mixtures**

Next steps

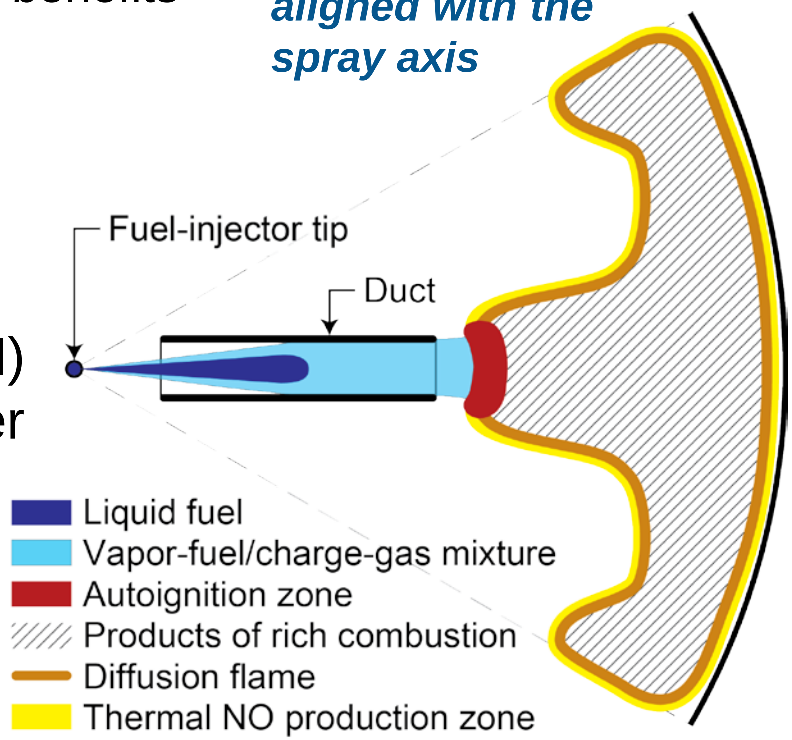
- Follow up with laser-sheet mixing diagnostics to quantify mixing effects for these PRFs
- Image combustion phenomena for ORNL fuels with different physical properties

Mixing-Controlled Compression Ignition (MCCI): Ducted fuel injection for high efficiency, low soot

Project Lead: Chuck Mueller, Sandia National Laboratories

- Mixing-controlled CI combustion is desirable for many reasons
  - > Inherently high efficiencies, low HC & CO emissions
  - > Ignition timing easily controlled by injection timing
  - > Inherently fuel-flexible (cetane # is key fuel parameter)
  - – Soot is a barrier to fully achieving the above benefits
    - > Soot is a potent toxin
    - > 2nd only to CO_2 as a climate-forcing species
    - > Limits amount of EGR possible for NO_x control
    - > Aftertreatment is expensive, has efficiency penalties (backpressure, regeneration)
- **Approach:** Use Ducted Fuel Injection (DFI) to make richest autoigniting mixtures leaner
  - – **Effective at lowering soot** (next slide)
  - – Geometrically & conceptually simple
  - – Tolerant to dilution for NO_x control
  - – Synergistic with Co-Optima oxygenated fuels, but does not require oxygenation
  - – Might increase comb. efficiency by limiting over-mixing at spray periphery

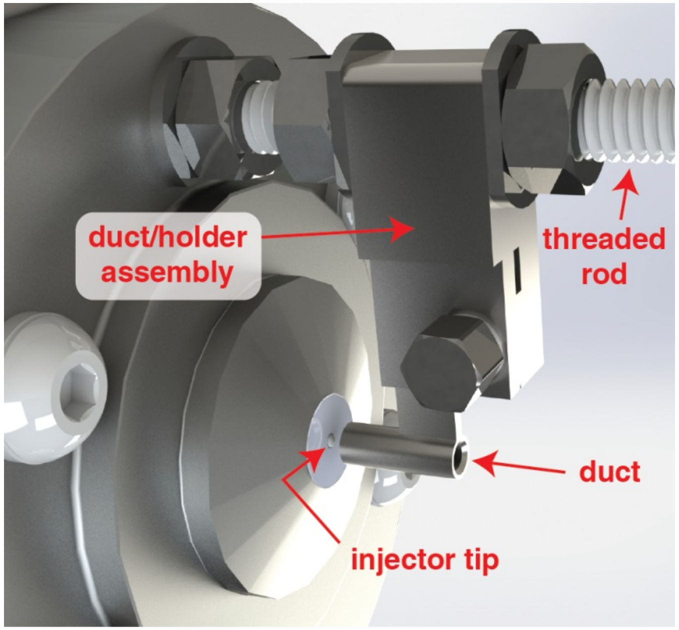
DFI Concept: Inject fuel down a small tube/duct aligned with the spray axis

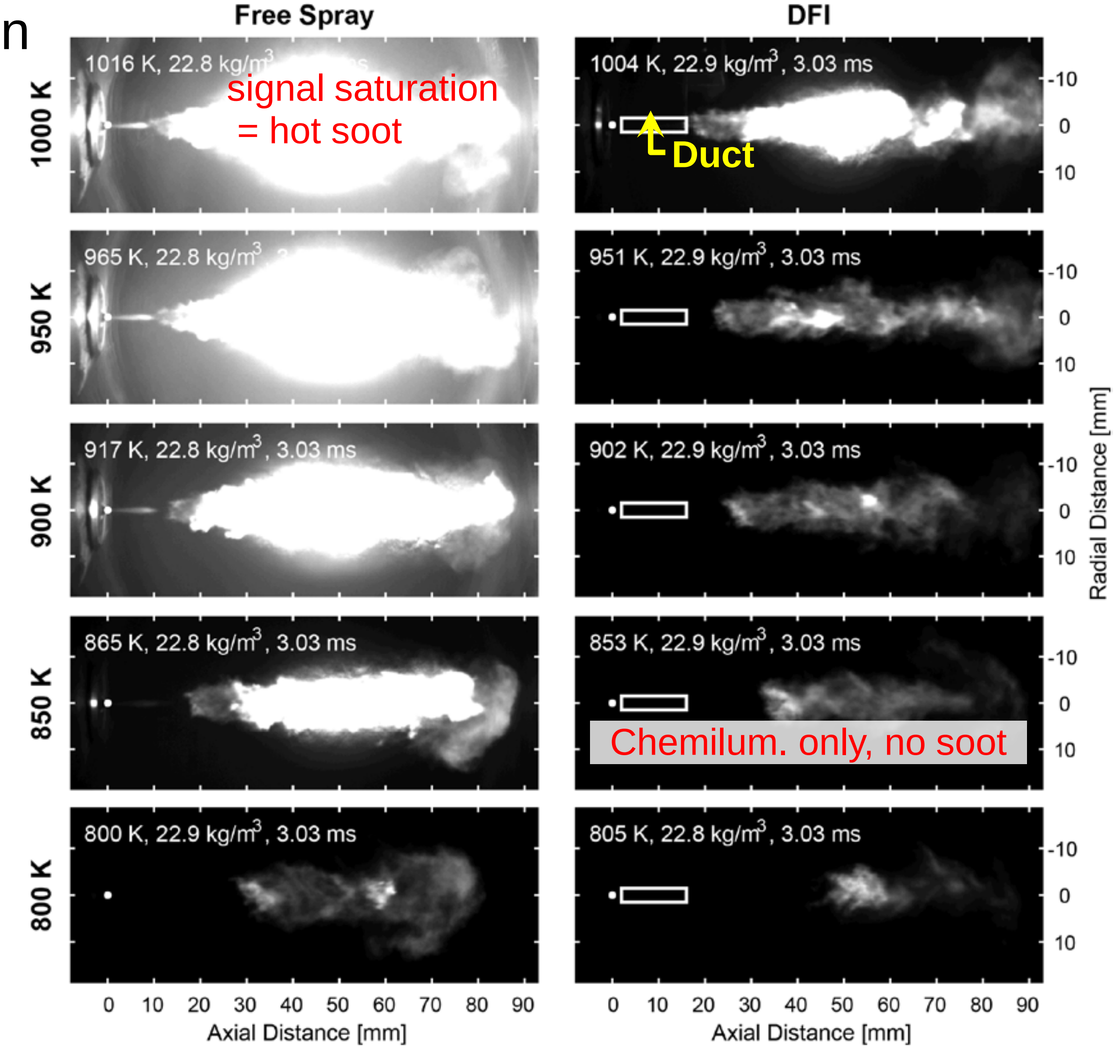


MCCI: Initial DFI data show considerable soot reduction even with non-oxygenated fuel, no EGR

Project Lead: Chuck Mueller, Sandia National Laboratories

- Ducted Fuel Injection (DFI) in Sandia constant-volume combustion vessel
  - 90 µm orifice diameter
  - 1500 bar injection pressure
  - 21 mol% oxygen (no EGR)
  - n-dodecane fuel (not oxygenated)

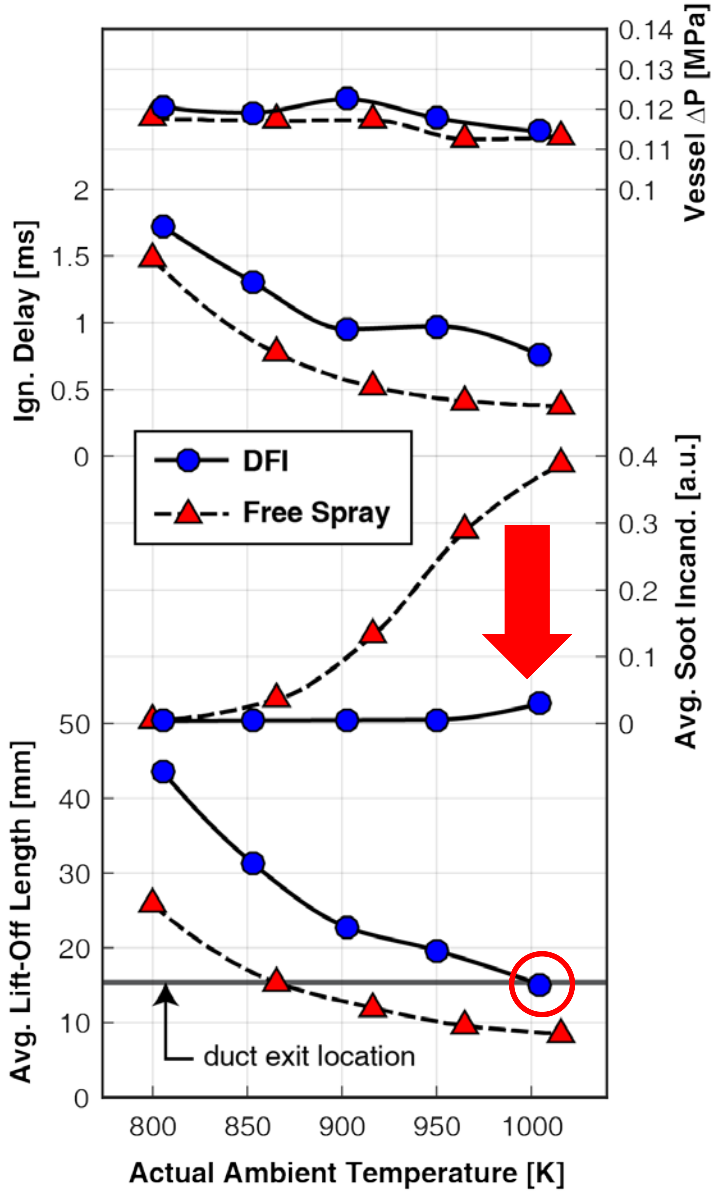




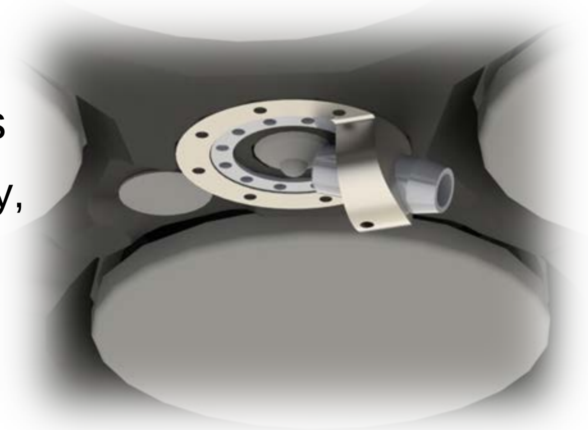
DFI is effective at lowering or preventing soot incandescence over a range of temperatures

MCCI: DFI reduces in-cylinder soot by factor of ~10, longer lift-off, higher pressure rise

Project Lead: Chuck Mueller, Sandia National Laboratories



- Effects of DFI on combustion observables
  - Lift-off lengths increase with DFI
    - > Flame anchors to duct exit at 1000 K
    - > Longer ignition delay could increase noise
  - Soot incandescence decreases by 10×
    - > Similar for quantitative in-cylinder soot
  - Total pressure rise (ΔP) in vessel is slightly, but consistently larger with DFI
    - > Higher combustion efficiency?
    - > Reduce over-mixing at spray periphery?
- <u>Future Work</u>:
  - Optical engine tests
    - > emissions, efficiency, & fuel effects
    - > Vertical-sheet LII
  - Develop merit function



ACI Merit Function: Quantify how fuel properties & engine conditions enable high-efficiency ACI

Project Lead: Andrew Ickes, Argonne National Laboratory

- ACI merit function: quantify enabling engine conditions & fuel properties
  - Boosted SI merit function quantifies efficiency effects to guide fuel and engine co-optimization
  - ACI approaches already have high efficiency; quantify enabling fuel & engine effects to guide co-optimization
- Will synthesize results from multiple Co-Optima ACI approaches
  - > Highlight key enabling fuel properties for each combustion approach
  - > Relate fuel properties to engine features that affect operating range and efficiency
- Design engine and fuel experiments to inform merit function(s) across the suite of ACI combustion concepts

LTGC | RCCI | GCI | LLFC | SI-based

(Industry solutions incorporated based on published literature and industry support/guidance)

↓

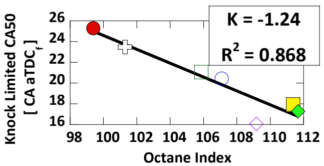
Identify enabling fuel properties and engine features and quantify their effects for each ACI approach

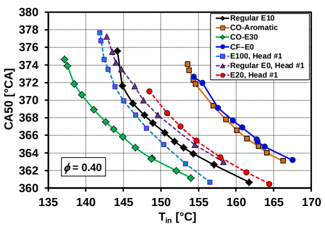
Specific focus on properties/ranges that preclude each ACI approach

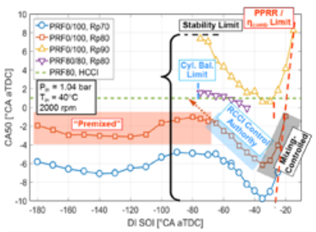
↓

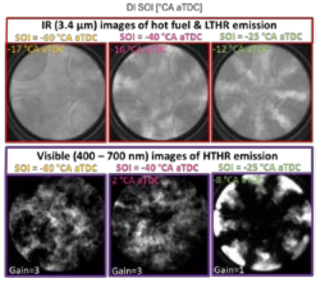
Property guidance and merit function to direct ACI engine & fuel co-optimization

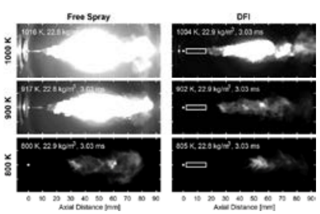
Summary: US DOE Co-Optimization of Fuels & Engines (Co-Optima) Initiative











SI MF
- SNL lead
- Miles

Blendstock screening focuses on optimal fuel properties
SI merit function quantifies fuel property effects on efficiency

SI
- ORNL
- Szybist

At $\phi \approx 1$, octane index correlates well with knock-limited CA50
Large pre-spark heat release variations among fuels tested

ACI
- SNL
- Dec

At $\phi = 0.4$, same RON & S, diverging CA50; "O2" OI works well
E30 reactivity similar to E0, correlates w/ ITHR & ϕ-sensitivity

RCCI
- ORNL
- Curran

Const. PRF control-authority limits = premixed, mixing-control
Wall-wetting/incomplete-mixing may narrow premixed limit

RCCI
- SNL
- Musculus

Matched optical/metal engine comb. phasing & control auth.
Image struct. (=incomplete mixing?), bright @ late DI (=rich?)

MCCI
- SNL
- Mueller

DFI reduces in-cyl. soot 10X w/ non-oxygenated fuel, no EGR
Longer lift-off & ignition delay (noise?), higher ΔP (efficiency?)

ACI MF
- ANL lead
- Ickes

Identify/quantify fuel properties enabling high-efficiency ACI
Merit function to guide ACI engine & fuel co-optimization

Acknowledgement

- Portions of the work on boosted SI merit function development, premixed ACI, Stratified ACI (RCCI), and MCCI were performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA.

  Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Backup Slides

Tiered Blendstock Identification

Tier 1

> 470 blendstocks

14 chemical families

Identify broad range of potential hydrocarbon and oxygenated blendstocks

Utilize property information on blendstocks from literature or estimates to identify Tier 2 blendstocks

- Hydrocarbons
  - Normal paraffins
  - Iso-paraffins
  - Cycloparaffins
  - Olefins
  - Aromatics
  - Multi-ring aromatics
- Alcohols

Present in commercial fuels

- Furans
- Ethers
- Carbonyls
  - Ketones
  - Aldehydes
- Esters
  - Volatile fatty acid esters
  - Fatty esters
- Carboxylic Acids

Not present in commercial fuels

A major goal of Co-Optima is to conduct a comprehensive and consistent survey of blendstock options:

What blendstocks are able to increase boosted SI performance?

Tiered Blendstock Identification

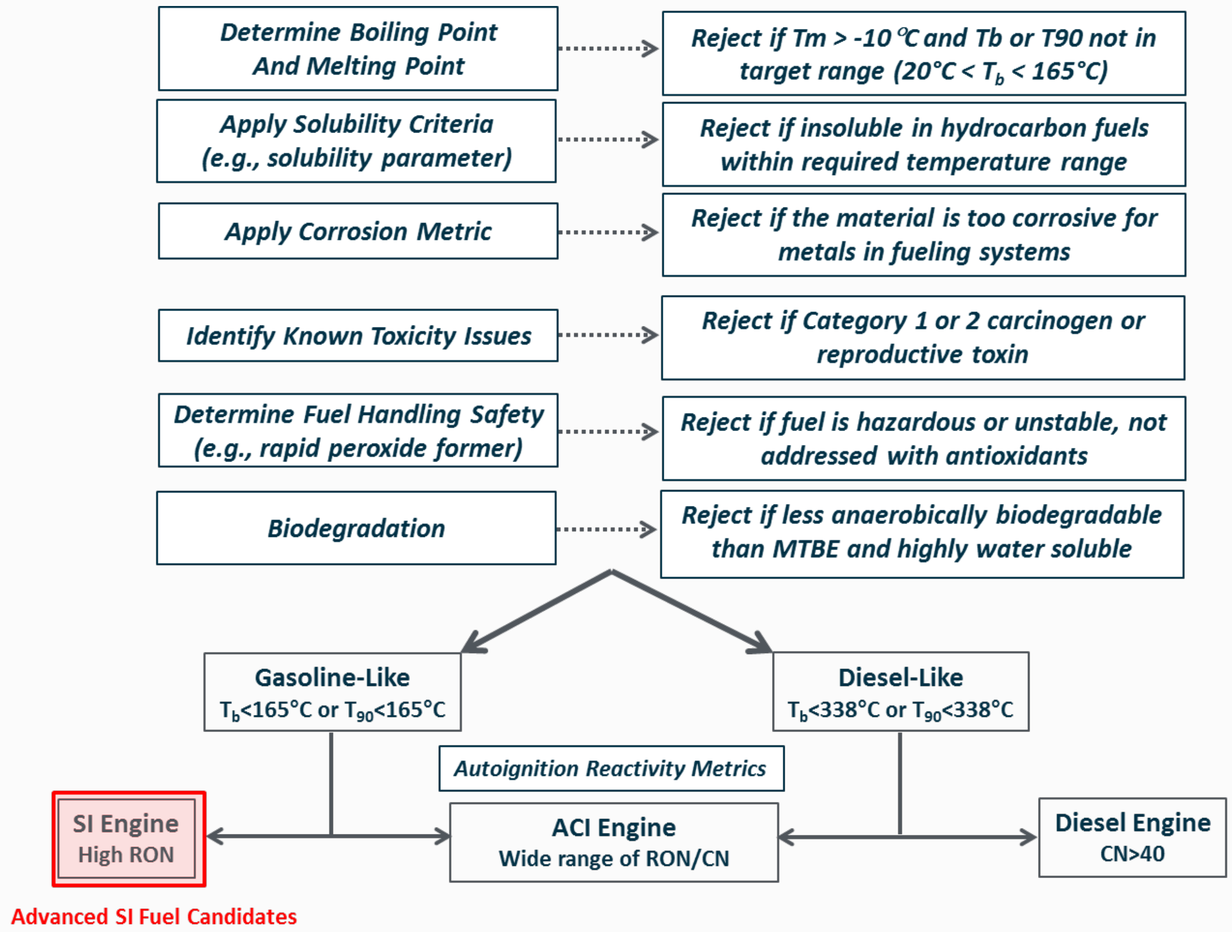
Tier 1

> 470 blendstocks

14 chemical families

Identify broad range of potential hydrocarbon and oxygenated blendstocks

Utilize property information on blendstocks from literature or estimates to identify Tier 2 blendstocks



Tier 1: Blendstock Screening

Tier 1

> 470 blendstocks

14 chemical families

Identify broad range of potential hydrocarbon and oxygenated blendstocks

Utilize property information on blendstocks from literature or estimates to identify Tier 2 blendstocks

- Hydrocarbons
  - Normal paraffins
  - Iso-paraffins
  - Cycloparaffins
  - Olefins
  - Multi-ring aromatics
- Alcohols
- Furans
- Ethers
- Carbonyls
  - Ketones
  - Aldehydes
- Esters
  - Volatile fatty acid esters
  - Fatty esters
- Carboxylic Acids

YES →
Normal paraffins
Iso-paraffins
Cycloparaffins
Olefins
Alcohols

YES FOR SOME →
Aromatics
Ketones
Volatile fatty acid esters
Furans
Ethers

NO →
Multi-ring aromatics
Aldehydes
Fatty esters
Carboxylic acids