US DOE Co-Optimization of Fuels and Engines (Co-Optima) Initiative: Recent progress on advanced compression-ignition

Mark Musculus
Combustion Research Facility
Sandia National Laboratories

Team PIs:
Steven Ciatti, ANL  Andrew Ickes, ANL
Scott Curran, ORNL  Chuck Mueller, SNL
John Dec, SNL  Mark Musculus, SNL

ERC – 2017 SYMPOSIUM
Impact of Future Regulations on Engine Technology

June 14th and 15th, 2017
Engine Research Center
University of Wisconsin, Madison, WI

VTO Program Managers: Gurpreet Singh, Kevin Stork, Leo Breton & Michael Weismiller
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
Co-Optima’s application/mode tracks use merit functions to guide fuel & engine research

- Merit functions quantify engine & fuel property effects to guide engine & fuel R&D for each combustion approach
  - Boosted SI, multimode ACI, mixing-controlled CI, etc.
- Boosted SI merit function quantifies engine & fuel effects as percentage-point decrease in fuel consumption
  - Actively updated – recently: adjusted many coefficients; removed LSPI term (too uncertain); added cold-start term

\[
\text{Merit}[\Delta\%] = \frac{(RON_{mix} - 91)}{1.6} - K \frac{(S_{mix} - 8)}{1.6} \\
+ \frac{0.085[ON / kJ / kg] \cdot ((HoV_{mix} / (AFR_{mix} + 1)) - (415[kJ / kg] / (14.0[-] + 1))))}{1.6} \\
+ \frac{((HoV_{mix} / (AFR_{mix} + 1)) - (415[kJ / kg] / (14.0[-] + 1))))}{15.2} \text{ } + \frac{(S_{Lmix} - 46[cm / s])}{5.4} \\
- H(PMI_{mix} - 1.6)[0.7 + 0.5(PMI_{mix} - 1.4)] + 0.008^\circ C^{-1}(T_{c,90,conv} - T_{c,90,mix})
\]
Overview: Co-Optima Engine & Fuel Tasks for Advanced Compression Ignition (ACI)

Co-Optima ACI projects use both gasoline-like & diesel-like fuels

- **ACI approaches using “boosted-SI” gasoline-like fuels**
  - Low-Temperature Gasoline Combustion (LTGC): pre-vaporized, premixed
    Sandia National Laboratories, John Dec
  - Gasoline Compression Ignition (GCI): 2\textsuperscript{nd} injection near TDC, stratified
    Argonne National Laboratory, Steve Ciatti

- **ACI approaches using diesel-like or dual-fuel with gasoline-like fuel**
  - Development of Stratified ACI: Reactivity-Controlled CI (RCCI)
    Oak Ridge National Lab., Scott Curran (multi-cylinder LD metal engine)
  - Fundamental Processes of Stratified ACI: RCCI, “optical” fuels
    Sandia National Labs., Mark Musculus (single-cyl. HD optical engine)
  - Mixing-Controlled CI Combustion (MCCI): ducted fuel injection (diesel)
    Sandia National Laboratories, Chuck Mueller

- **ACI merit function development**
  - ANL/ NREL/ ORNL/ SNL – Andrew Ickes (lead, ANL)
LTGC (SNL, Dec): Determine optimal properties to allow both LTGC and boosted SI, evaluate fuel metrics

**Motivation:** LTGC provides efficiencies at or above those of diesel engines
- Substantial reduction in fuel consumption vs. SI ⇒ use light-distillates efficiently for more effective use of crude oil supplies
- Ultra-low NOx and PM minimize aftertreatment and cost

**Project Objective:** Determine / develop optimal LTGC fuel

- **FY17 Objectives:** Investigate the performance of “booted-SI” fuels for LTGC and the validity of the Central Fuel Hypothesis
  ⇒ Are RON & MON sufficient metrics for LTGC?
  ⇒ Also provide well-characterized data for kinetic model development

**Approach:** Use Sandia single-cylinder LTGC engine
- Well-controlled experiments for premixed fueling (also G-DI, PFS fueling, though not used here)
- Work w/ Co-Optima Fuel Properties Team & Boosted-SI engine researchers to develop fuel test matrix
LTGC (SNL, Dec): at $\phi = 0.4$, identical RON & S fuels have diverging CA50; alternative “$O_2$” OI works well

Accomplishments – Fuel Reactivity

- Designed fuel test matrix with five fuels with $\text{RON} \approx 98$, four with $S \approx 10.5$, one with $S \approx 1$

<table>
<thead>
<tr>
<th>Co-Optima Core Fuels</th>
<th>Alkylate</th>
<th>E30</th>
<th>Aromatic</th>
<th>Olefin</th>
<th>Cycloalkane</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON</td>
<td>98.0</td>
<td>97.4</td>
<td>98.1</td>
<td>98.2</td>
<td>98.0</td>
</tr>
<tr>
<td>MON</td>
<td>96.6</td>
<td>86.6</td>
<td>87.8</td>
<td>88.0</td>
<td>87.1</td>
</tr>
<tr>
<td>S</td>
<td>1.4</td>
<td>10.8</td>
<td>10.3</td>
<td>10.2</td>
<td>10.9</td>
</tr>
<tr>
<td>Aromatics</td>
<td>0.7</td>
<td>13.8</td>
<td>39.8</td>
<td>13.4</td>
<td>33.2</td>
</tr>
<tr>
<td>n+i-Paraffin</td>
<td>98.1</td>
<td>40.5</td>
<td>46.2</td>
<td>56.4</td>
<td>40.6</td>
</tr>
<tr>
<td>Cycloalkane</td>
<td>0.0</td>
<td>7.0</td>
<td>8.0</td>
<td>2.9</td>
<td>24.2</td>
</tr>
<tr>
<td>Olefins</td>
<td>0.1</td>
<td>6.0</td>
<td>4.5</td>
<td>26.5</td>
<td>1.6</td>
</tr>
<tr>
<td>Ethanol</td>
<td>0.0</td>
<td>30.4</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Accomplishments – Fuel Reactivity

- 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 ($\phi = 0.4$) at this cond.
  - Perhaps this is because E30 is less $\phi$-sensitive, or differences in HOV $\Rightarrow$ Further studies are planned
- $P_{in} = 2.4$ bar: Try OI" based on intake $O_2$, since $T_{in} = 60^\circ C$ for all
  - OI" correlates fuels fairly well at $P_{in}=2.4$ bar, $R^2 = 0.870$
  - Further understanding of this intake-$O_2$ based OI" is needed

LTGC (SNL, Dec): at $\phi = 0.4$, identical RON & S fuels have diverging CA50; alternative "O₂" OI works well
LTGC (SNL, Dec): Reactivity of E30 (high RON & S) is similar to E0, correlates with ITHR & φ-sensitivity

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 O₂.
  - 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
  $\Rightarrow$ 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 $\Rightarrow$ may affect reactivity trends
  - Also agrees with lower $\phi$-sensitivity (for PFS)

Future Work:

- Evaluate E30 $\phi$-sensitivity & high load behavior
- Evaluate the other three fuels in test matrix $\Rightarrow$ High-Olefin, High-Cycloalkane, & Alkylate
- Investigate Co-Optima fuels with good potential for full-time LTGC-ACI engines $\Rightarrow$ Support ACI merit function
GCI (ANL, Ciatti): Minimize pollutant emissions, noise, fuel consumption for three 98 RON “boosted-SI” fuels

- **Objective:**
  - Demonstrate Gasoline Compression Ignition (GCI) combustion with high RON, high S Boosted-SI fuels in a 1.9L GM engine
  - Investigate parameters that affect engine performance and emission; and identify condition with desirable outputs (i.e. pollutant emissions, noise, efficiency)

- **Approach:** double injection strategy to control combustion phasing (CA50 ~ 5 aTDC) while maintaining combustion stability (COV_{IMEP}<3%) and noise (<90 dB), low FSN (<0.1). Parametric study of:
  - Exhaust Gas Recirculation
  - Global lambda

### Parameter | Value
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine 1.9L GM 4-cylinder (17.8:1 CR)</td>
<td></td>
</tr>
<tr>
<td>Engine Speed [rpm]</td>
<td>1000</td>
</tr>
<tr>
<td>Engine Load [bar BMEP]</td>
<td>3-6</td>
</tr>
<tr>
<td>Fuel – 98 RON: Aromatic, Alkylate, E30</td>
<td></td>
</tr>
<tr>
<td>Injection Pressure [bar]</td>
<td>600</td>
</tr>
<tr>
<td>Start of Injection [°aTDC]</td>
<td>-50/varied</td>
</tr>
<tr>
<td>Fuel Split (~ % by duration)</td>
<td>55/45</td>
</tr>
<tr>
<td>EGR [%]</td>
<td>20 (0-30)</td>
</tr>
<tr>
<td>Boost Pressure [bar(a)]</td>
<td>1.4 (1.0-1.7)</td>
</tr>
<tr>
<td>Intake Air Temp [°C]</td>
<td>55 (35-85)</td>
</tr>
<tr>
<td>Global λ (= 1/Φ)</td>
<td>1.8 (1.6, 2.0)</td>
</tr>
</tbody>
</table>
GCI (ANL, Ciatti): Co-Optima core fuels with CA50, noise, & COV const., $\uparrow$EGR $\Rightarrow \downarrow$FSN & NOx, $\uparrow$CO & HC

- For Co-Optima core fuels, as EGR is increased to 20%:
  - FSN decreases ~70%, with FSN Aromatic > Alkylate > E30
  - NOx emissions are halved, while CO and HC emissions increase 20-50%
  - Exhaust emissions control still required
- BSFC/ISFC are larger than expected due to turbocharger issues
- $\lambda=1.8$, EGR=20% point selected for endoscope imaging

<table>
<thead>
<tr>
<th>Co-Optima Core Fuels</th>
<th>Alkylate</th>
<th>Aromatic</th>
<th>E30</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON</td>
<td>98</td>
<td>98</td>
<td>98</td>
</tr>
<tr>
<td>MON</td>
<td>97</td>
<td>87</td>
<td>88</td>
</tr>
<tr>
<td>S</td>
<td>1</td>
<td>11</td>
<td>11</td>
</tr>
<tr>
<td>Aromatics</td>
<td>0</td>
<td>36</td>
<td>8</td>
</tr>
<tr>
<td>Saturates</td>
<td>100</td>
<td>65</td>
<td>57</td>
</tr>
<tr>
<td>Olefins</td>
<td>0</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>Ethanol</td>
<td>0</td>
<td>0</td>
<td>30</td>
</tr>
</tbody>
</table>

Global Lambda and EGR Sweep

![Graph showing fuel consumption and EGR sweep](image)
GCI (ANL, Ciatti): at 20% EGR & $\lambda=1.8$, E30 has fastest burn, highest in-cyl. soot, low late-cycle soot (& FSN)

- Soot luminosity appears near second HRR peak, akin to conv. diesel
- E30: highest peak soot KL integral, but lowest late-cycle (& lowest FSN)

Future work:
- Improve engine efficiency and BSFC with turbocharger operation and injection strategy (higher BMEP points)
- Endoscope imaging for OH* chemiluminescence in low HRR region where soot is absent
- PM measurement for GCI soot characteristics
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)

SNL Optical Engine
• Single-cylinder heavy-duty diesel engine (GDI + DI)
• Image combustion & in-cylinder mixing (PRF)
Stratified ACI (ORNL, Curran): Constant PRF limits of RCCI CA50 control authority approach premixed & mixing-control

- 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
Fundamental Stratified ACI (SNL, Musculus): Good matching of combustion phasing & control authority in optical & metal engines

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.

- Matching SNL HD optical engine with ORNL LD metal engine: 1. charge-gas $\rho$ & $T$ @ mid-control-authority DI injection, 2. premixed iso-octane (80%), 3. global $\Phi$ (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.

For a DI injection in the “RCCI regime,” the heat release phasing is shifted, but the curves have the same characteristic shapes.
Fundamental Stratified ACI (SNL, Musculus): Structure in IR & visible images (=incomplete mixing?), bright @ late DI (=rich?)

- Structure in IR imaging of 1\textsuperscript{st}-stage and visible imaging of 2\textsuperscript{nd}-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
MCCI (SNL, Mueller): Maintain high efficiency, control, & fuel flexibility of diesel; use ducted injection for soot

- 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 CO₂ as a climate-forcing species
  > Limits amount of EGR possible for NOₓ 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 NOₓ 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 (SNL, Mueller): Initial DFI data show considerable soot reduction even with non-oxygenated fuel, no EGR

- 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 (SNL, Mueller): DFI reduces in-cylinder soot by factor of ~10, longer lift-off, higher pressure rise

- **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?

- **Future Work:**
  - Optical engine tests
    - emissions, efficiency, & fuel effects
    - Vertical-sheet LII
  - Develop merit function
ACI Merit Function (NREL/ORNL/SNL + ANL-Ickes): Quantify fuel properties enabling high-efficiency ACI

- 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

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

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

(Industry solutions incorporated based on published literature and industry support/guidance)
ACI approaches using “boosted-SI” gasoline-like fuels

**LTGC**
- **SNL**
- **Dec**

Identical RON & S fuels: diverging CA50, “O2” OI works well

**GCI**
- **ANL**
- **Ciatti**

W/ CA50, noise, COV const., ↑EGR ⇒ ↓FSN&NOx, ↑CO&HC

20% EGR & λ=1.8: E30=highest in-cyl. soot, low late-cyc. soot

ACI approaches using diesel-like fuel or dual fuels

**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 merit function development

**ACI MF**
- **ANL lead**
- **Ickes**

Identify/quantify fuel properties enabling high-efficiency ACI

Merit function to guide ACI engine & fuel co-optimization
The work on LTGC, Fundamentals of Stratified ACI (RCCI), and MCCI was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA.

Publications and Presentations – 1

ANL, Ciatti – GCI (Gasoline Compression Ignition)

SNL, Dec – LTGC (Low-Temperature Gasoline Combustion)

ORNL, Curran – RCCI Metal Engine
- Wissink, M et al., ” Performance and emissions of RCCI with iso-octane and n-heptane on a light-duty multi-cylinder engine,” Oral only presentation at the SAE World Congress, April 2017.

SNL, Musculus – RCCI Optical Engine
Publications and Presentations – 2

SNL, Mueller – Mixing-Controlled CI Combustion and Fuels Research

● Publications


● Presentations

- 16 presentations from this project since last DOE Annual Merit Review (AMR) meeting, 3 invited.

● Patents


● Award

- Coordinating Research Council (CRC) Advanced Vehicles, Fuels, and Lubricants (AVFL) Committee Special Recognition Award (Feb. 7, 2017).