SAND2020-4496PE

Co-Optimization of
Fuels & Engines

Heavy-Duty Mixed-Controlled Compression Ignition: Fuel Effects and Ducted Fuel Injection

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Sandia National Laboratories

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Project #FT077

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Overview

Projects

Abbrev.	Description
DFI	E.2.2.4. Fuel effects on ducted fuel injection (DFI): Mueller
Surr.	E.2.2.5. Surrogate fuels for mixing-controlled compression-ignition (MCCI): Mueller
Soot	F.1.5.4. Fuel effects on soot formation: Manin

Timeline

Project	Start	End	% Complete
DFI	Oct. 1, 2018	Sep. 30, 2021	52%
Surr.	Oct. 1, 2018	Sep. 30, 2021	52%
Soot	Oct. 1, 2018	Sep. 30, 2021	52%

Barriers*

- **Need improved MCCI (a.k.a. clean-diesel) combustion modes & understanding of fuel effects thereon**
  - "The research areas of highest priority for clean diesel combustion are: reduced engine-out NO_x and particulate emissions…" P. 2 of [1]
  - "Critical challenges include…improving lifted-flame combustion" [2]
  - "Develop improved engine-out NO_x control using higher levels of exhaust gas recirculation" [1]
  - Inadequate understanding of fuel effects on soot formation & oxidation processes [1]

[1] https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf, Page 2.
[2] https://www.energy.gov/eere/vehicles/advanced-combustion-strategies

Budget

Project	FY20 [$k]	FY19 [$k]	DOE Share
DFI	450	340	100%
Surr.	150	0	100%
Soot	220	160	100%

__Acronyms & other definitions are listed in green, italic text at bottom of this & subsequent slides__: NO_x = nitrogen oxides, FY = fiscal year (runs October 1 – September 30), $k = $1000

Relevance

"The U.S. Department of Energy's Vehicle Technologies Office provides **low cost**, **secure**, and **clean** energy technologies to move people and goods across America."

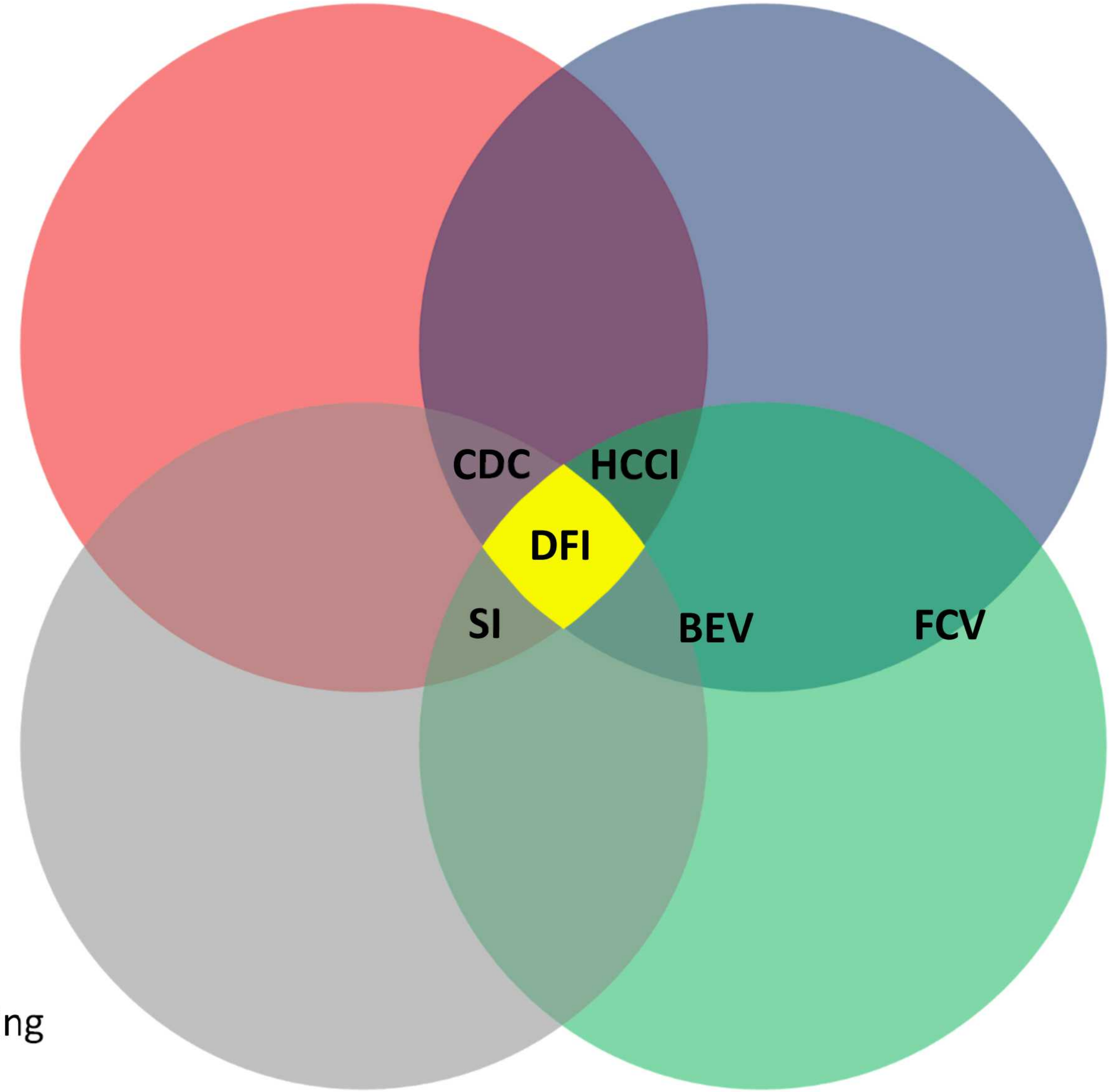
https://www.energy.gov/eere/vehicles/vehicle-technologies-office

Low Cost

- Maintains value of existing production facilities
- Compatible with existing fuels, energy-distribution infrastructure
- Uses abundant, inexpensive materials
- Lower DEF consumption, less costly aftertreatment
- Retrofittable

Technically Viable

- Conceptually simple
- Fuel-flexible
- Wide speed/load range
- Low cyclic variability
- Easy to control ignition timing
- Durable & reliable



Secure

- High efficiency
- Energy security: compatible with domestic fuels/energy
- Climate security: synergistic with sustainable (oxygenated) fuels

Clean

- Low emissions of **soot**, NO_x, HC, & CO
- Reduces aftertreatment requirements
- Extends aftertreatment useful life, lessens regeneration/maintenance
- Less soot in lube oil

DEF = diesel exhaust fluid, NO_x = nitrogen oxides, HC = hydrocarbons, CO = carbon monoxide, SI = spark-ignition, CDC = conventional diesel combustion, HCCI = homogeneous charge compression ignition, DFI = ducted fuel injection, BEV = battery electric vehicle, FCV = fuel cell vehicle

FY20 Milestones

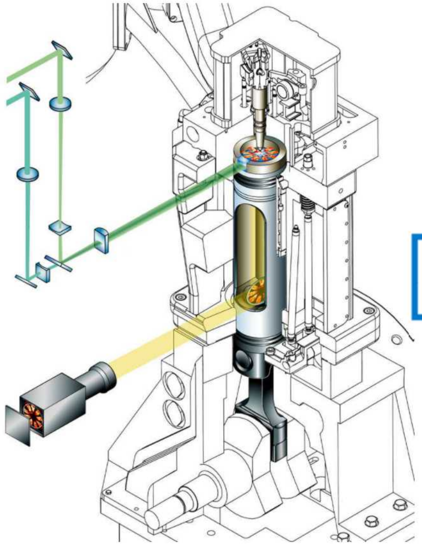
Any proposed future work is subject to change based on funding levels.

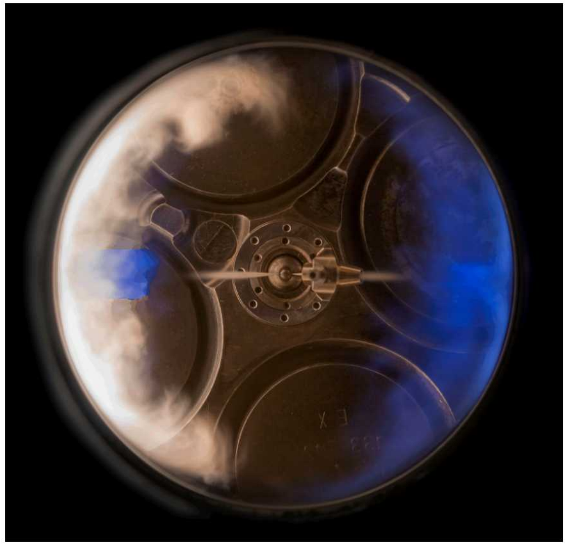
MM/YY	Project	Description of milestone or go/no-go decision	Status
03/20	DFI	Transition from two- to four-duct configuration & complete baseline optical-engine parameter-sweep experiments with four-duct DFI configuration.	**Done**.
06/20	DFI	Complete optical-engine testing of two commercially available oxygenates blended with diesel fuel in four-duct DFI configuration.	On track but delayed by COVID-19 lab closure.
03/20	Surr.	Complete optical-engine testing of all diesel target & surrogate fuels from CRC Project AVFL-18a.	**Done**.
09/20	Surr.	Complete publication summarizing results from optical-engine testing.	On track.
03/20	Soot	Characterize combustion characteristics and soot formation for various target and surrogate fuels selected by CRC partners.	**Done**.
03/20	Soot	Provide time-resolved measurements of soot formation in high-pressure pyrolyzing fuel sprays with multimode-relevant fuel blends.	Delayed by COVID-19 lab closure.

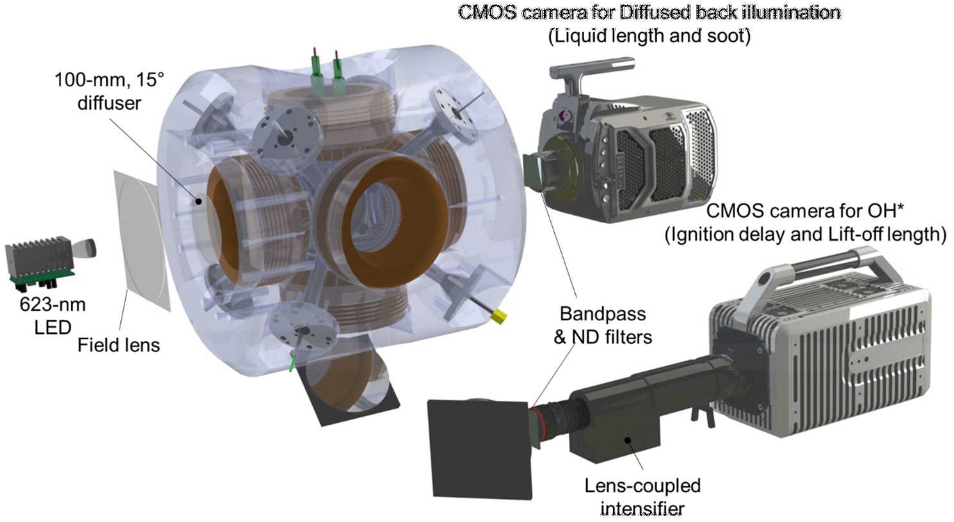
COVID-19 = disease potentially resulting from novel coronavirus infection in a human, CRC = Coordinating Research Council, AVFL = Advanced Vehicles/Fuels/Lubes

Approach

- **Employ unique experimental capabilities & optical diagnostics to develop an enhanced understanding of fuel-property & operating-condition changes on MCCI combustion processes.**







Our focus on soot led us to oxygenated fuels & leaner lifted-flame combustion, which led us to DFI, which enabled us to break the soot/NO_x trade-off, which could enable the next generation of high-efficiency MCCI engines burning sustainable fuels.

Barriers

- Need reduced engine-out NO_x and particulate emissions
- Need improved lifted-flame combustion approaches
- Need better engine-out NO_x control using higher levels of EGR
- Need enhanced understanding of fuel effects on soot processes

Tasks

- Transition to four-duct DFI configuration
- Parameter sweeps with four-duct DFI config.
- Test diesel surrogate fuels in optical engine
- Test surrogate fuels in const.-volume vessel

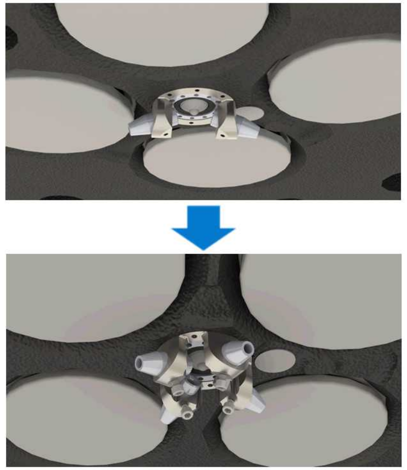
EGR = exhaust-gas recirculation

DFI (Mueller)

Successfully transitioned from two- to four-duct DFI configuration & completed six parameter sweeps.

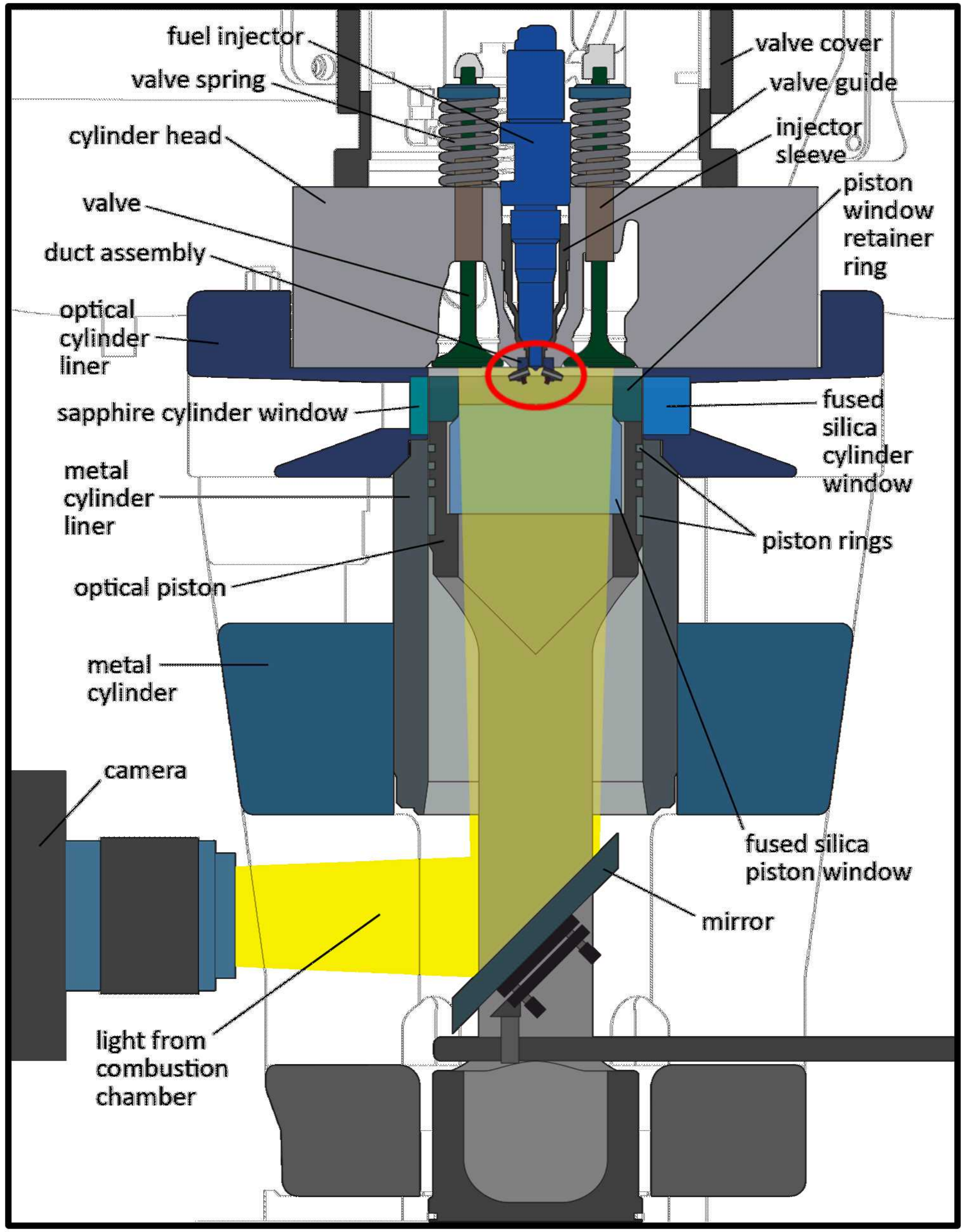
- **Four-duct configuration enabled peak load to be more than tripled relative to FY19 experiments**
  - 2.6 bar $IMEP_g$ with two-duct config. $\rightarrow$ 8.7 bar $IMEP_g$ with four-duct config.
- **Six parameter sweeps were conducted to determine DFI sensitivities to operating-condition changes**

Engine speed	1200 rpm
Load ($IMEP_g$)	2.4 – 8.7 bar
Fuel	No. 2 S15 cert. diesel
Injector tip	4 × 0.108 mm × 140°
Injection pressure	80, **180**, 240 MPa
Intake-O_2 mole fraction	12, 14, **16**, 18, 21%
Inj. duration (commanded)	1.5, 2.5, **3.5**, 4.5 ms
Start of combustion timing	-5.0, **0.0**, +5.0 CAD ATDC
Intake manifold abs. press.	2.0, **2.5**, 3.0 bar
Intake manifold temperature	50, 70, **90** °C
Coolant temperature	50, 70, **90** °C
Fired cycles per run	180
Runs per condition	≥ 3



Roughly corresponding to:
- 1.3, **1.6**, 2.0 bar
- 13, 31, **49** °C

in a metal engine with 17:1 CR

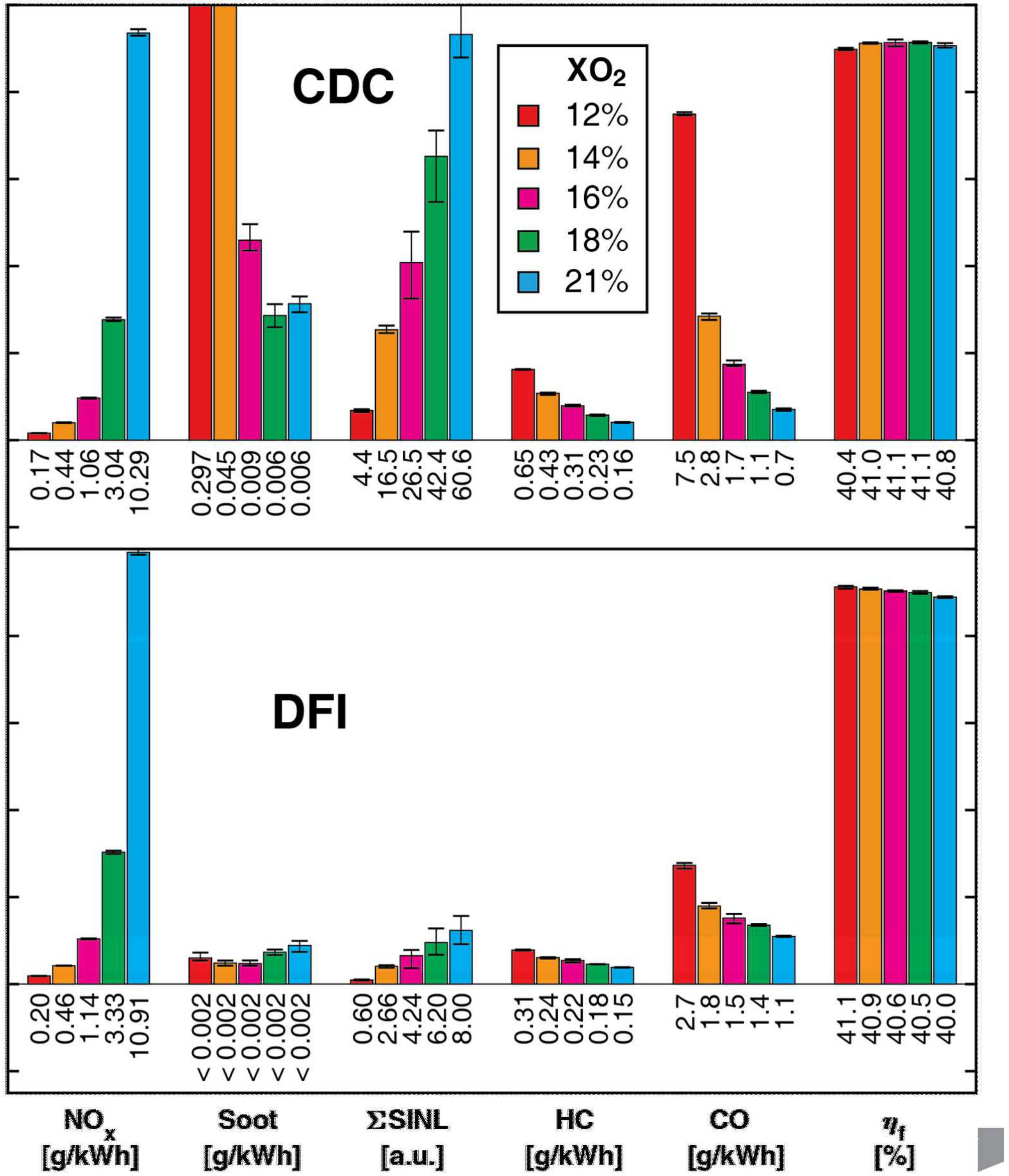


$IMEP_g$ = gross indicated mean effective pressure (measured during compression & expansion strokes only), rpm = revolutions per minute, S15 = 15 parts per million sulfur, MPa = million Pascals, O_2 = molecular oxygen, ms = milliseconds, CAD = crank-angle degrees, ATDC = after top-dead-center, CR = compression ratio

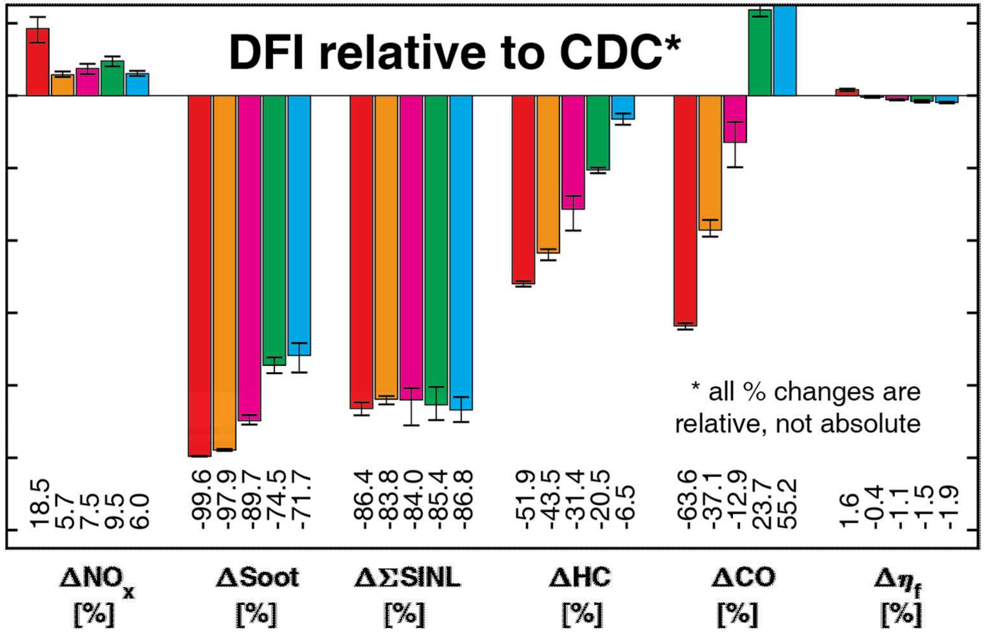
DFI (Mueller)

Baseline experiments show encouraging DFI performance over a range of operating conditions with commercial diesel fuel.

- **Plots show results from intake-O_2 mole-fraction (XO_2) sweep**
- **DFI exhibits generally lower emissions than CDC**
  - DFI has lower soot, HC, & CO emissions at likely XO_2 levels
  - NO_x is much lower for DFI at minimum feasible XO_2
  - ΣSINL = cycle- & spatially integrated natural luminosity = a sensitive measure of hot in-cylinder soot (determined via high-speed imaging)
- **DFI & CDC have similar fuel-conversion efficiencies (η_f)**
  - DFI η_f increases as XO_2 level decreases: DFI is synergistic with dilution



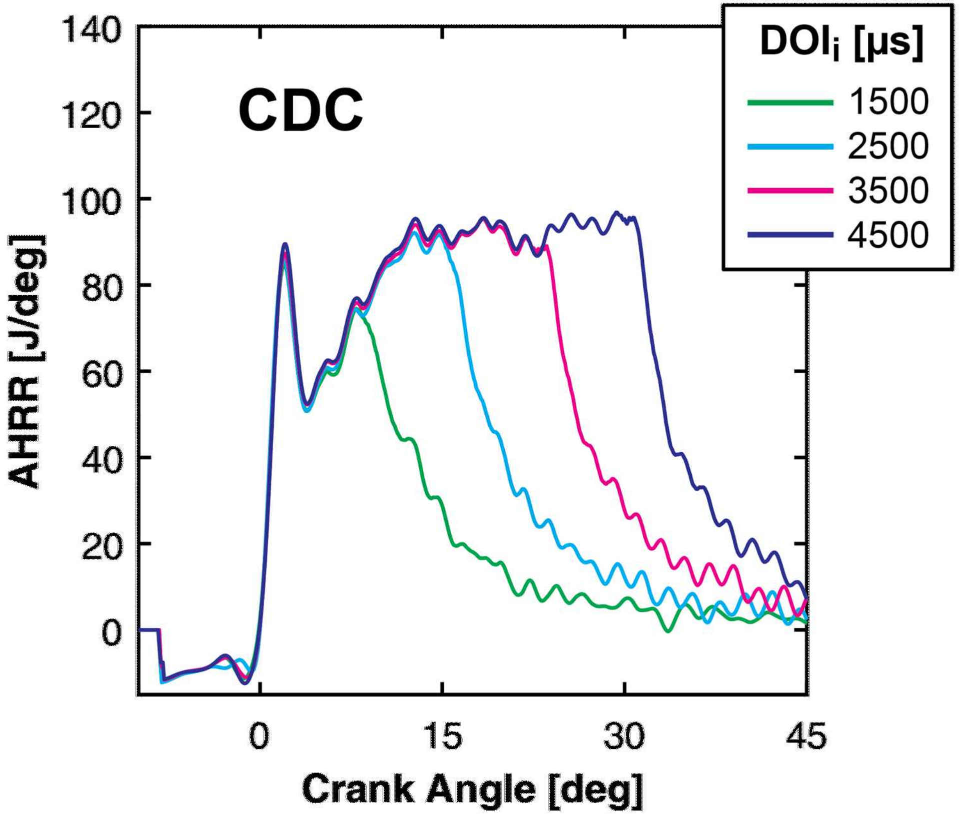
All results from four-duct configuration, 1200 rpm, ~6.7 bar $IMEP_g$

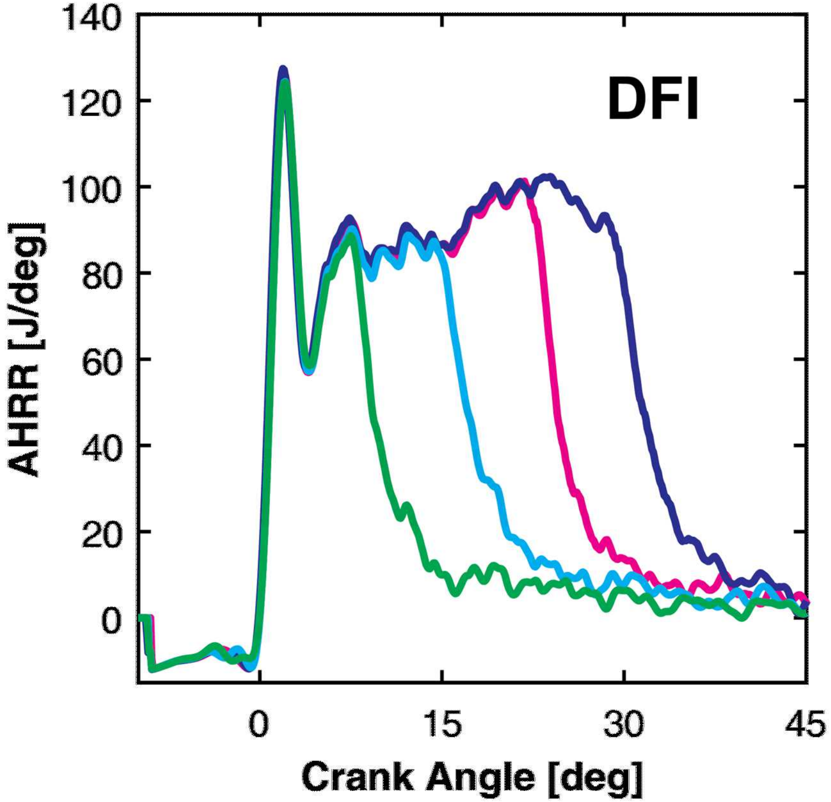


CDC = conventional diesel combustion, g = grams, kWh = kilowatt hour, a.u. = arbitrary units

DFI (Mueller)

DFI ignition timing & load are easily controlled via injection timing, & DFI heat release is similar to CDC.





All results from four-duct configuration, 1200 rpm, 2.4 - 8.7 bar IMEP$_g$

- **Plots show results from sweep of indicated (i.e., electronically commanded) duration of injection = DOI$_i$**
- **DFI has larger premixed burns & shorter combustion durations than CDC**
  - Larger premixed burns may increase combustion noise levels
  - Shorter combustion durations should assist in improving thermal efficiencies

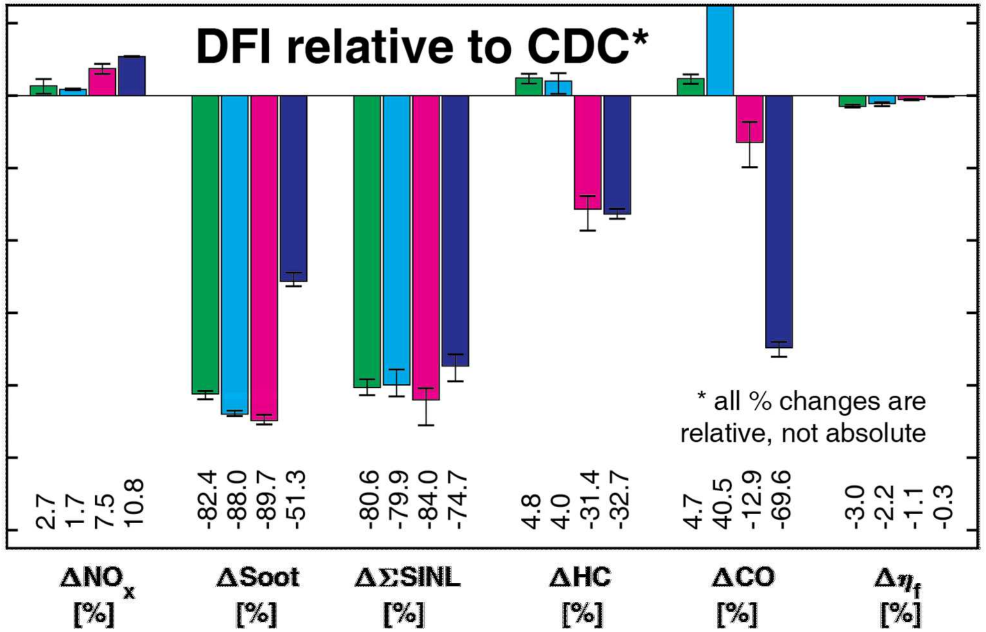
μs = microseconds, AHRR = apparent heat-release rate, J = Joules, deg = degree

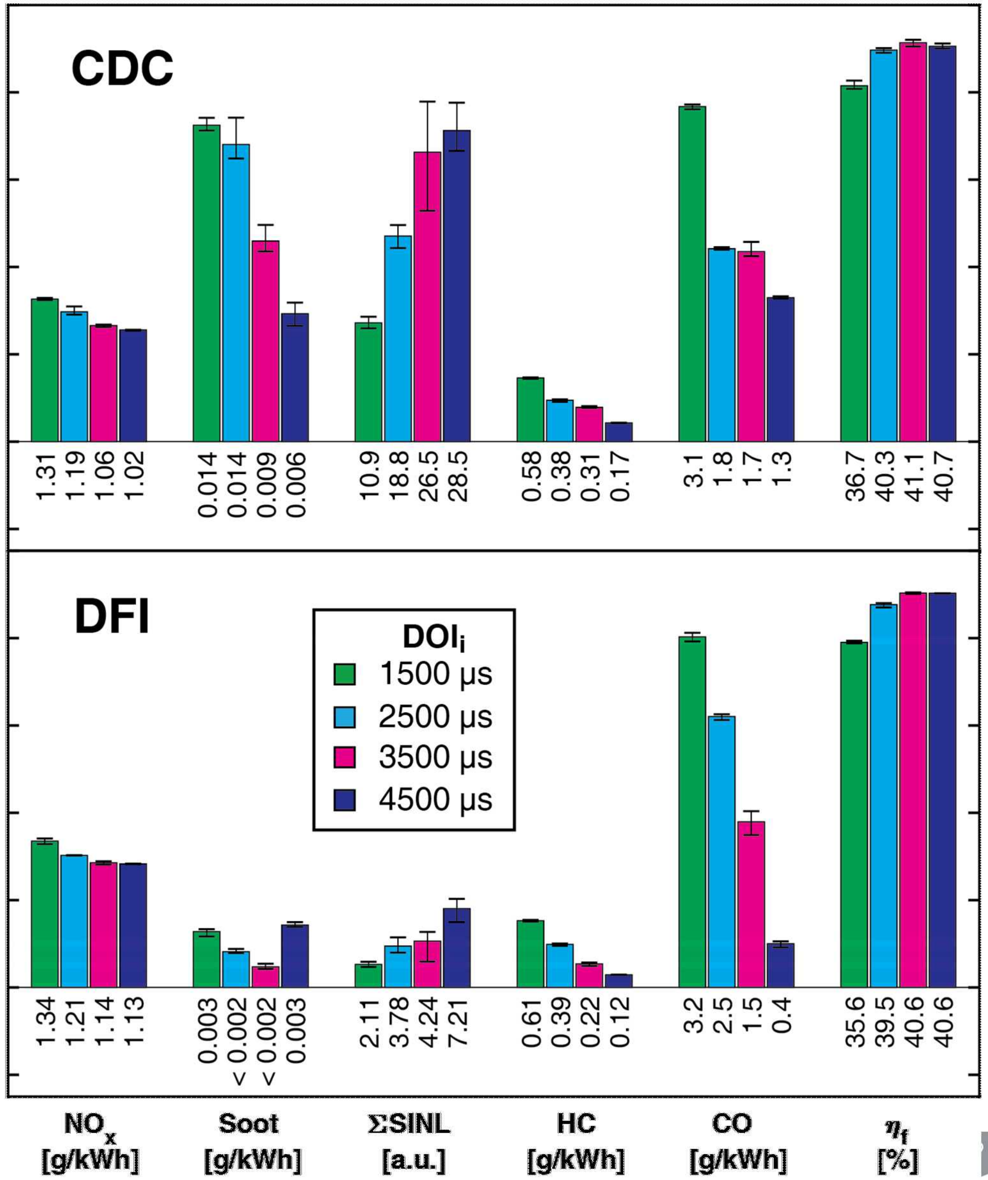
DFI (Mueller)

DFI performs well across a range of loads.

- **Plots show results from DOI_i / load sweep**
- **Emissions**
  - Soot is 50 – 90% lower for DFI across the sweep
  - HC & CO are lower for DFI when DOI_i is longer than 2500 μs
  - NO_x is 2 – 11% higher for DFI
- **Fuel-conversion efficiency (η_f) is 0.3% – 3.0% lower for DFI**
  - η_f and NO_x both can be improved via dilution
- **DFI performance generally improves with longer DOI_i**

All results from four-duct configuration, 1200 rpm, 2.4 - 8.7 bar $IMEP_g$, 16 mol% O_2



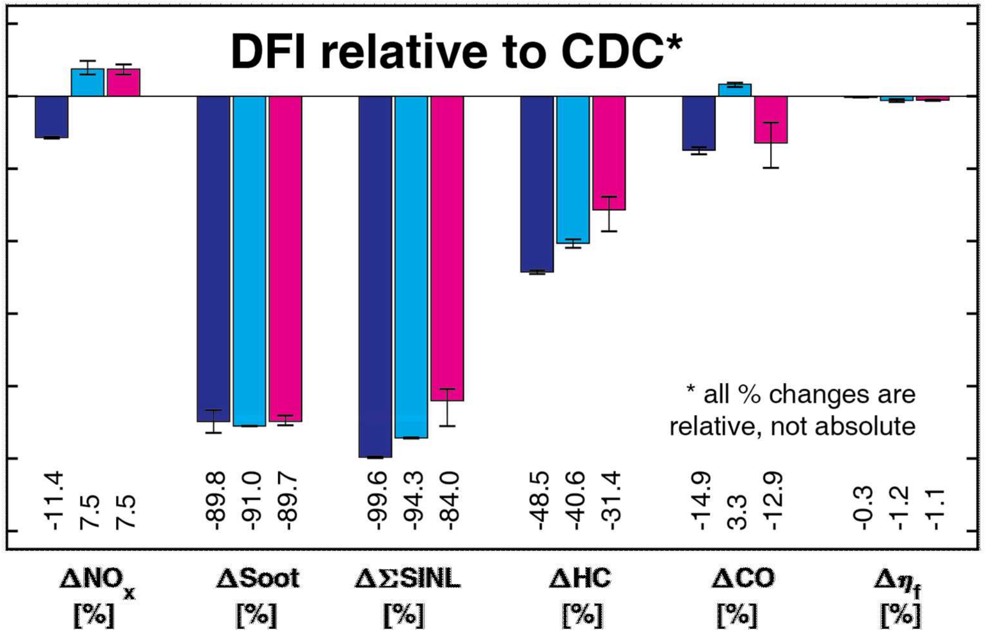


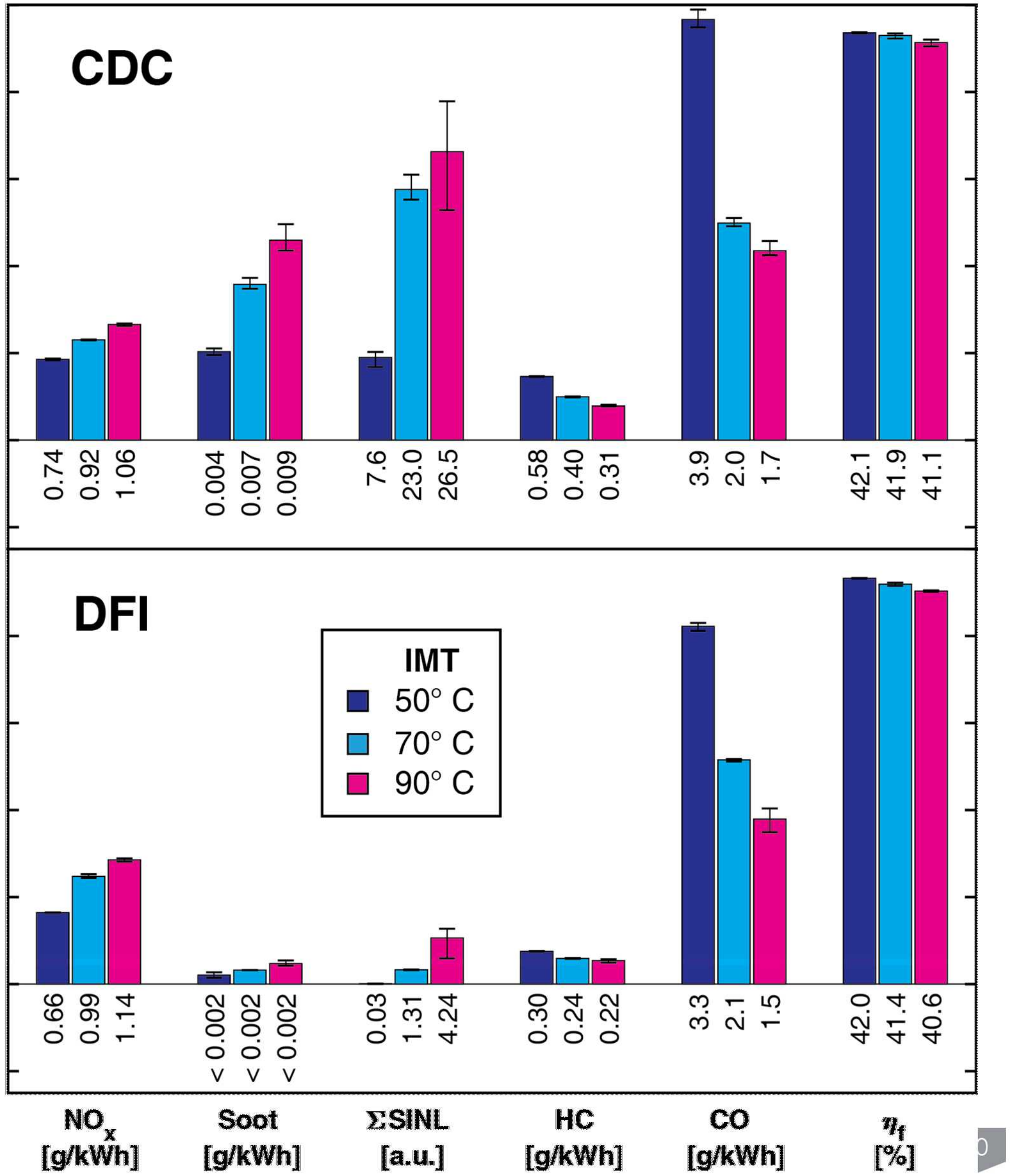
DFI (Mueller)

DFI outperforms CDC at simulated cold-start conditions.

- **Plots show intake manifold temperature (IMT) sweep results**
  - Coolant temperature was maintained at same value as IMT
- **Emissions**
  - DFI has lower soot & HC emissions, lower or similar CO emissions
  - NO_x is lower for DFI at minimum IMT
- **Similar η_fs for CDC & DFI**
- **DFI should work well in applications with frequent cold-starts (e.g., hybrids) & at conditions below catalyst light-off temp.**

All results from four-duct configuration, 1200 rpm, 6.7 – 7.0 bar $IMEP_g$, 16 mol% O_2



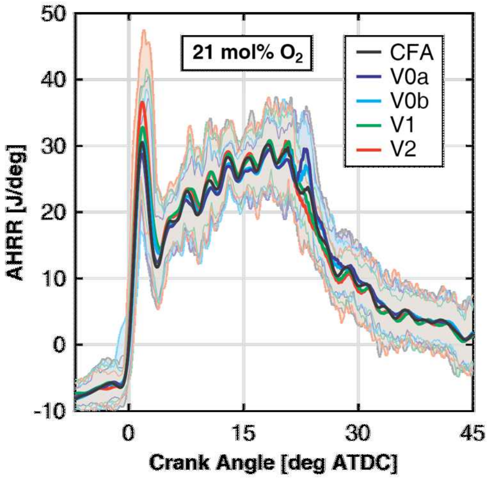


Surr. (Mueller)

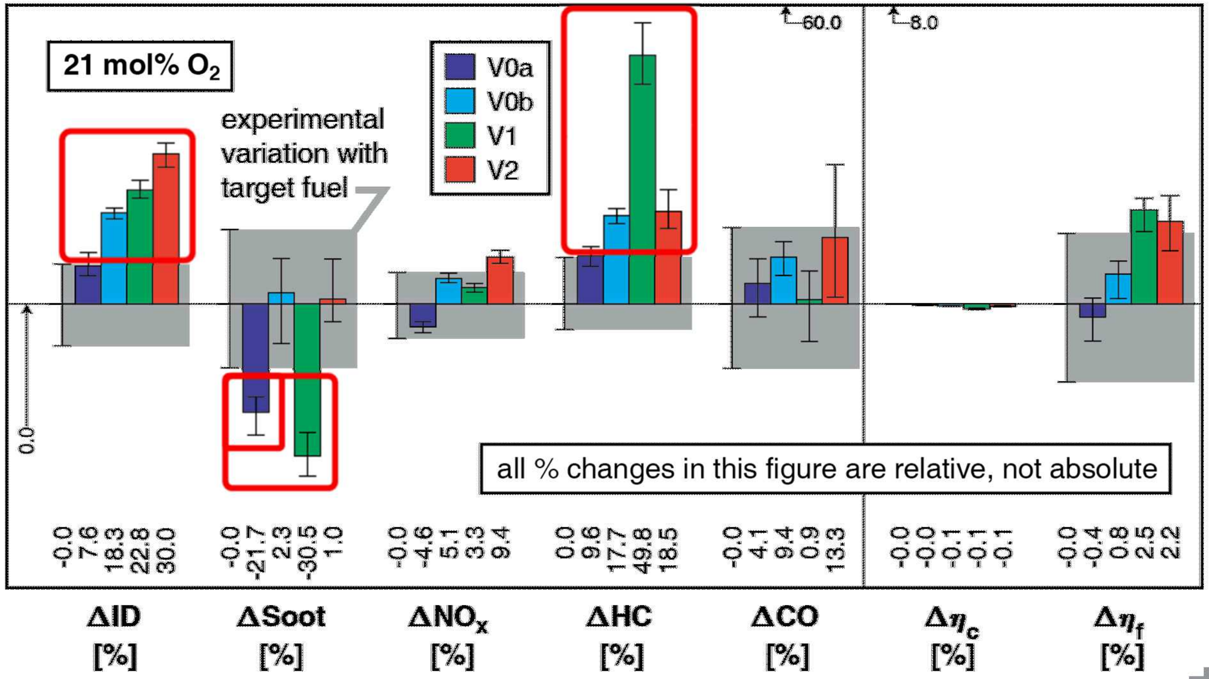
Diesel surrogate fuels may not need to be extremely complex to match commercial diesel performance accurately.

Work conducted under Coordinating Research Council Project AVFL-18a

- **Tested diesel target fuel + four surrogates (4, 5, 8, & 9 components)**
  - All surrogates accurately replicated target-fuel apparent heat-release rate (AHRR)
  - Matching target-fuel cetane # did not necessarily match ignition delays (ID) at engine conditions
  - Simplest surrogate, V0a, matches target-fuel performance within experimental uncertainty for all key metrics except soot (η_c = combustion efficiency)
  - Surrogates tend to have longer IDs, lower soot, & higher HC emissions than target fuel
- **Currently working to understand underlying reasons for performance differences**



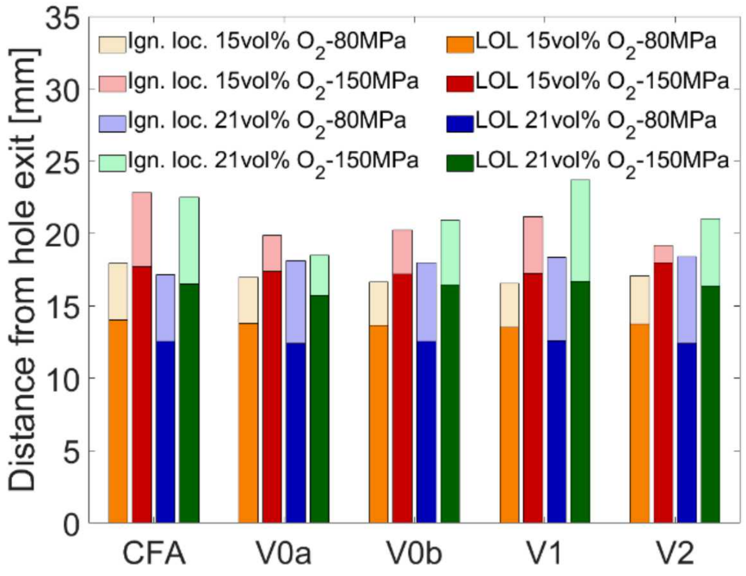
Fuels	**CFA, V0a, V0b, V1, V2**
Intake O_2 mole fractions	**21%, 16%**
Engine speed	1200 rpm
Load (gross IMEP)	1.54 bar
Injector tip	2 × 0.110 mm × 140°
Injection pressure	80 MPa
Injected energy	814 J
Injection schedule	Single inj., ~3.5 ms
Start of combustion timing	TDC
Intake manifold abs. pressure	2.00 bar
Intake manifold temperature	90 °C
Coolant temperature	90 °C

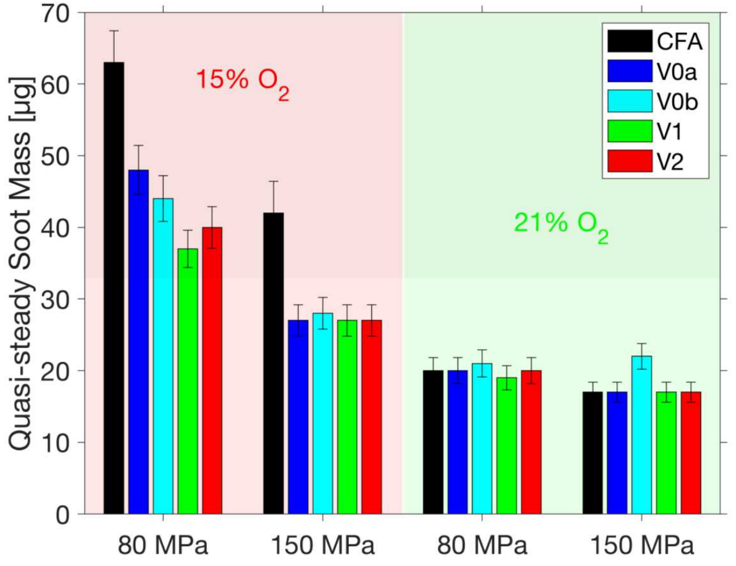


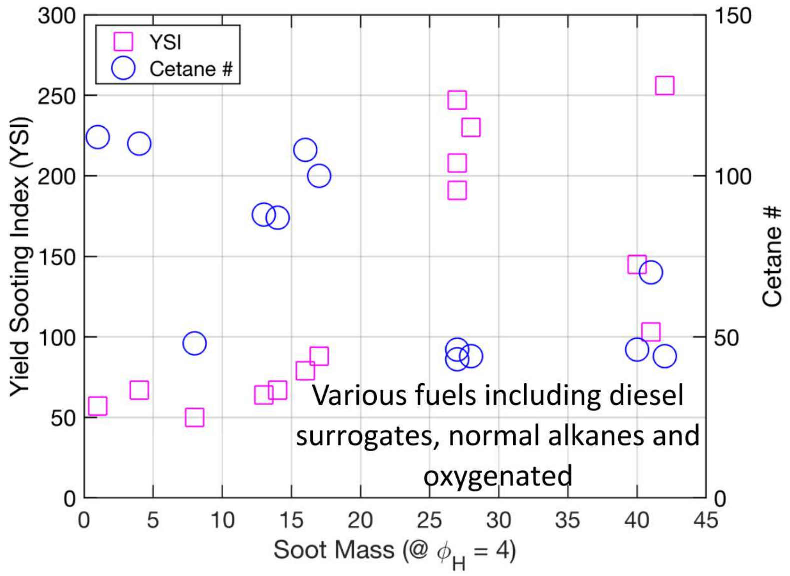
Soot (Manin)

The relationship between the target fuel and the surrogates regarding soot levels appears to be condition-dependent.

- **Ignition delays and lift-off lengths are all within 10% of each other**
  - Expected based on ignition properties (cetane number)
- **All fuels produce similar soot levels at 21% O_2, but differences are significant at lower O_2 concentration**
  - Surrogate fuels remain close (within uncertainty) across all conditions







- **There is no straightforward correlation between sooting tendency (YSI) and measured soot levels**
  - Ignition characteristics also play a major role in measured soot levels
  - Sooting tendencies for the target and surrogate fuels at atmospheric conditions appear to correlate well with their aromatic contents, but not at high pressures
- **Predicting sooting levels at engine-relevant conditions requires more information than sooting tendency (YSI) alone**
  - Including ignition properties is necessary to account for flame-related ϕ
  - Other molecular param's (aromatic content, C/H, O_2-ratio) are also needed

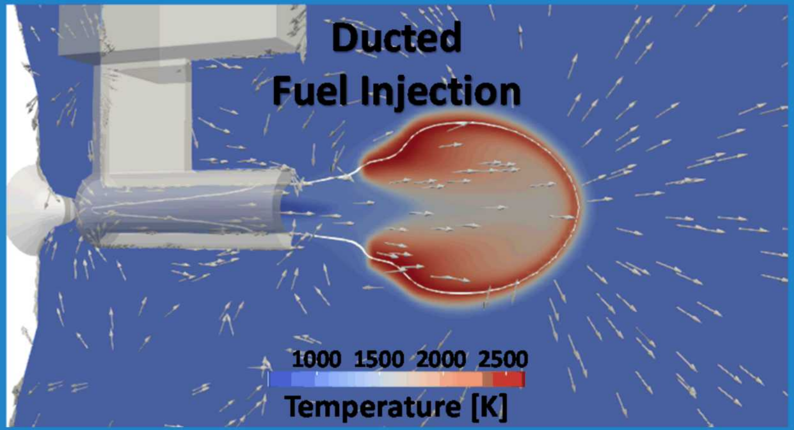
Responses to Previous Year Reviewers' Comments

DFI	**Most feedback was positive; e.g., the "reviewer observed outstanding accomplishments on both the DFI and soot work" and "this project addresses the key barriers in heavy-duty mixing-controlled combustion, thereby offering good support to the Co-Optima goals and overall DOE objectives."** • *Response: We are grateful to the reviewers for their encouraging comments!* **"For DFI, higher load engine testing would be important."** • *Response: Our work since the last AMR meeting has more than tripled the peak load of DFI.* **Testing should "be further extended to different engine speed, engine load, and EGR dilution conditions in the future to provide a more comprehensive picture."** • *Response: We have studied & reported on higher loads & a much more comprehensive range of dilution conditions. We plan to study engine speed effects in the future.* **The reviewer "encouraged the quick addition of...the impact of injection strategies that reflect real engine operation (cold starting, transient, etc.)"** • *Response: We have studied & reported on simulated cold-start conditions. Unfortunately, we do not currently have the ability to do transient testing with the optical engine.* **"The reviewer would like to have seen one of the modeling laboratories brought in to try and bring analytical tools to bear on the DFI system."** • *Response: We have established an initial collaboration with ANL & are teaming to respond to DOE FOAs for future funding.*
Surr.	• No reviewer comments – this project was not discussed at the FY19 AMR meeting due to timing of funding.
Soot	• No reviewer comments – this project was a new start in FY20.

ANL = Argonne National Lab., FOA = Funding Opportunity Announcement, AMR = Annual Merit Review

Collaboration & Coordination with Other Institutions

DFI	• Advanced Engine Combustion Memorandum of Understanding • NREL/LBNL/JBEI (Vardon, George): Novel oxygenate selection • Caterpillar & Ford: Technology Commercialization Fund CRADA • ANL (Som, Magnotti): DFI simulation • ANL (Powell): DFI spray characterization via x-ray diagnostics • Univ. of Minnesota (Northrop et al.): DFI particulate mass & particle number characterization
Surr.	• Coordinating Research Council Project AVFL-18a & FACE Working Group • LLNL (Pitz, Kukkadapu): Kinetic model development for hydrocarbon & oxygenated MCCI fuels • LLNL (McNenly): Quantitative in-cylinder soot evolution mapping via vertical laser-induced incandescence
Soot	• LLNL (Pitz): Kinetic model development/testing, reaction analysis • NREL (Kim): Kinetic model, soot metric analysis • Caterpillar: Injector hardware, simulations • IFPEN: Simulations, soot model development • CMT: Simulations, soot metric and model evaluation



NREL = National Renewable Energy Lab., LBNL = Lawrence Berkeley National Lab., JBEI = Joint BioEnergy Institute, CRADA = Cooperative Research and Development Agreement, ANL = Argonne National Lab., AVFL = Advanced Vehicles/Fuels/Lubes, FACE = Fuels for Advanced Combustion Engines, LLNL = Lawrence Livermore National Lab., IFPEN = Institut Francais du Petrol Energies Nouvelles (France), CMT = CMT-Motores Térmicos, Universitat Politècnica de València (Spain)

Remaining Challenges & Barriers

DFI	• Unquantified potential for oxygenated fuels with DFI to curtail total cost of ownership & net CO_2 emissions • Unknown whether DFI can be extended to full load at high efficiency • Current optical-engine test facilities are limited by relatively low peak cylinder pressures (~120 bar), precluding full-load testing at high efficiency • Particulate matter & particle number characteristics of DFI (including fuel effects thereon) are largely unknown • Unknown whether DFI can be successfully extended to configurations with more than four ducts • Need an improved fundamental understanding of DFI • Accurate relations for scaling DFI to various engine sizes are not available • Tools for accurate simulation of DFI are currently lacking • Lots of different groups are working on DFI (& DFI-related) activities with little or no coordination
Surr.	• Unknown whether even simpler surrogates can be formulated to replicate target-fuel performance accurately • Relative influences of key surrogate-fuel properties have yet to be quantified
Soot	• CFD simulations do not yet capture soot under (fundamental) pyrolysis conditions • Existing/current soot metrics do not match soot measurements at engine-relevant conditions • Additional soot data for fuels of various (relevant) chemistry needed to develop MCCI soot metric • Pyrolysis experiments need time-resolved quantitative mixing measurements for full potential • Accurate control over small-quantity injection into high-pressure facility

CO_2 = carbon dioxide

Proposed Future Research

Any proposed future work is subject to change based on funding levels.

DFI	**FY21** • Test two novel, Co-Optima bioblendstocks in diesel & biodiesel base fuels at idle & moderate-load conditions to explore performance & potential net CO_2 reduction. • Conduct experiments to quantify particulate matter & particle number characteristics of DFI. • Increase peak cylinder pressure capability of the optical engine to enable in-cylinder diagnostics at higher loads & at higher efficiencies (requires new cylinder head & new optical piston). • Test DFI configurations with more than four ducts. • Collaborate with modeling & simulation team(s) to develop DFI design tools for industry.
Surr.	**FY21** • Continue engagement with CRC Project AVFL-18a; no new experimental tasks currently planned.
Soot	**FY20** • Time-resolved measurements of pyrolyzing sprays with multi-mode-relevant fuel blends. **FY21** • Pyrolysis experiments with sprays of n-dodecane fuel doped with aromatics and relevant fuels. • Ignition/soot experiments for select MCCI Co-Optima fuels. • Propose fuel-dependent soot metric for MCCI operation.

Summary

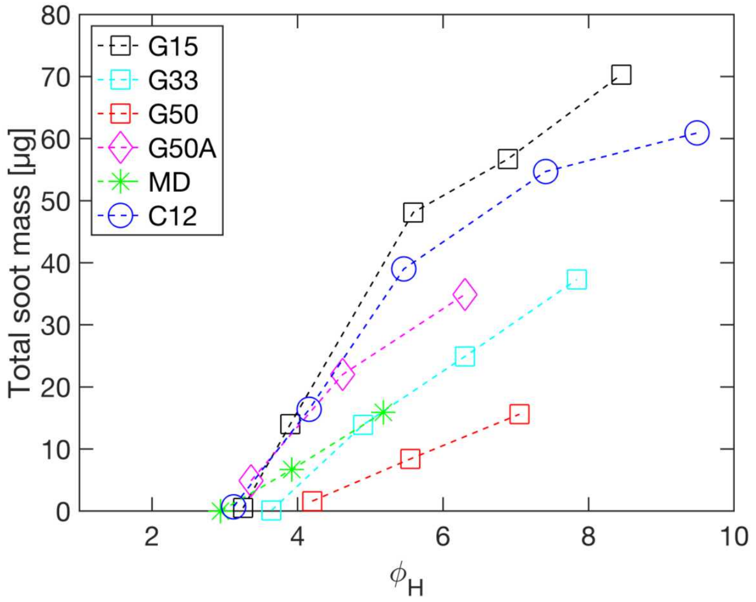
Relevance	This research directly supports the DOE Vehicle Technologies Office mission of providing "low cost, secure, and clean energy technologies to move people and goods across America" & a key industry objective of enabling clean diesel combustion by lowering NO_x, soot, & other emissions, while maintaining efficiency & performance.
Approach	• Optical-engine & combustion-vessel experiments are utilized to lead DFI development & enhance understanding of fuel effects on soot. • Tasks are extensively cross-linked, complementary, & focused on overcoming barriers identified by DOE & industry. • All milestones are either completed or on track (pending the evolving COVID-19 situation).
Technical Accomplishments	• Successfully transitioned from two- to four-duct DFI configuration & completed six operating-parameter sweeps. • More than tripled the peak-load capability of DFI relative to FY19 experiments. • Baseline experiments with commercial diesel fuel show encouraging DFI performance over a range of operating conditions & loads with a four-duct DFI configuration. • DFI outperforms CDC in applica'ns with frequent cold-starts (e.g., hybrids) & at cond's below catalyst light-off temp. • Diesel surrogate fuels may not need to be extremely complex to match commercial diesel performance accurately. • Surrogate fuels present similar ignition & combustion characteristics but different sooting levels in vessel testing. • Existing soot metric (YSI) does not capture sooting levels/tendencies under high-pressure spray-flame conditions.
Collaboration & Coordination	The work is closely integrated with Co-Optima, the Advanced Engine Combustion MOU, the Engine Combustion Network, domestic & international labs, academia, & industry via a CRADA.
Future Research	• Addresses key technical barriers to DFI implementation with sustainable fuels by enhancing understanding of: fuel effects on performance & net CO_2, DFI particulate matter characteristics, approaches for increasing load & optical-engine testing at higher loads, & requirements for accurate & cost-effective simulation tools. • Pyrolysis experiments with other fuels & aromatics to understand their sooting behaviors at high pressures. • Develop & propose a fuel-based soot metric for relevant MCCI fuels & engine operating conditions.

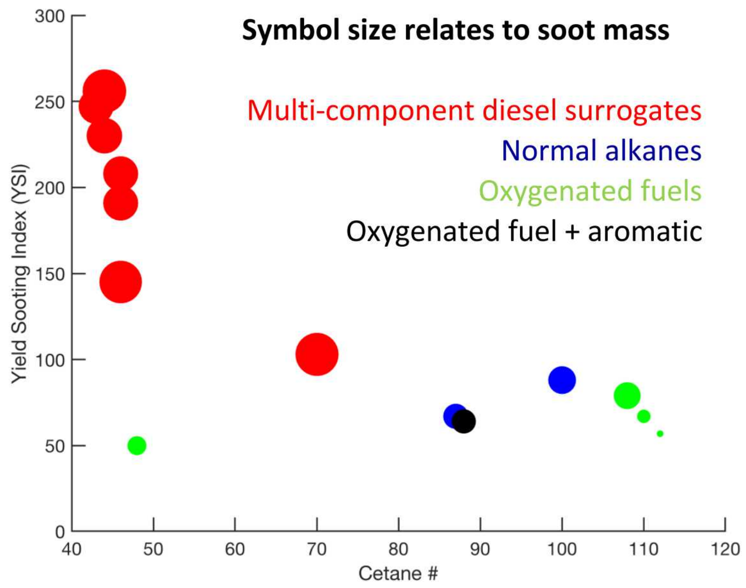
Technical Back-Up Slides

Soot (Manin)

Fuels' sooting levels are closely related to their ignition/flame stabilization behaviors.

- **Soot levels normalized to isolate fuel sooting propensity**
  - Estimated at constant equivalence ratio ($\phi = 4$) at the lift-off length
- **Different fuels exhibit different behavior**
  - This alone highlights the importance of mixing and chemistry, for fuels with different ignition/combustion properties
  - Past observations showed a correlation between soot levels vs. equivalence ratio and YSI, not confirmed by further testing





- **Mild trend between YSI and soot mass, with far outliers**
  - Molecular composition, including aromatics content, or oxygenate content (if applicable) need to be accounted for
- **Ignition properties also bear a mild effect on soot levels**
  - Other effects appear to be more important based on this limited fuel selection

Reviewer-Only Slides

Publications & Presentations

DFI

Journal Publications

1. Nilsen, C.W., Biles, D.E., Yraguen, B.F., and Mueller, C.J., "Ducted Fuel Injection vs. Conventional Diesel Combustion: An Operating-Parameter Sensitivity Study Conducted in an Optical Engine with a Four-Orifice Fuel Injector," *SAE Int. J. Engines*, in press, 2020.
2. Nilsen, C.W., Biles, D.E., and Mueller, C.J., "Using Ducted Fuel Injection to Attenuate Soot Formation in a Mixing-Controlled Compression-Ignition Engine," *SAE Int. J. Engines* **12**(3):309-322, doi:10.4271/03-12-03-0021, 2019.

Other Publications/Releases

- Mueller, C.J., "Sandia National Laboratories R&D 100 Award Video: Ducted Fuel Injection," SAND2019-4135V, https://youtu.be/1dijtRUZeLw, May 2019.
- Sandia FY19 press release, https://share-ng.sandia.gov/news/resources/news_releases/ducted_injection/, Oct. 2019.
- Ashley, S., "Can Diesel Finally Come Clean?" *Scientific American*, https://www.scientificamerican.com/article/can-diesel-finally-come-clean/, Dec. 2019.
- Mueller, C.J., "Mixing-Controlled CI Combustion and Fuel-Effects Research," *DOE Vehicle Technologies Office FY 2019 Annual Progress Report, Advanced Combustion Systems and Fuels*, 2020.
- Mueller, C.J., "Combination of Ducted Fuel Injection with Oxygenated Fuel Indicates Promising Path for Future Engines and Fuels," *Co-Optimization of Fuels & Engines FY19 Year in Review*, 2020.
- Sandia National Laboratories Innovation Marketplace: "Ducted Fuel Injection," http://www.sandia.gov/working_with_sandia/technology_partnerships/_assets/documents/Innovation%20Marketplace_March2020_Smaller.pdf.

Presentations: 14 from this project since 2019 DOE Annual Merit Review meeting, two invited.

Award

2019 R&D 100 Special Recognition Silver Medal in Green Technology category for "Ducted Fuel Injection."

Surr.

Presentations: Three from this project since 2019 DOE Annual Merit Review meeting.

Soot

Journal and/or Other Publications

- Since June 2019

Presentations: Three from this project since 2019 DOE Annual Merit Review meeting. Or list the presentations with titles & dates…

Critical Assumptions & Issues

DFI	1. The potential barriers to the commercial implementation of DFI can be overcome, including: • *Limited physical understanding of fuel effects on performance (how to optimize?)* • *Duct durability (thermal/mechanical fatigue, deposits)* • *Full-load operation (scaling to more ducts & larger orifices)* • *Spray/duct alignment (establishing initially & maintaining over life of engine)* • *Combustion noise (maintaining within established limits)* • *Cold-start performance (maintaining stability & low emissions)* • *Thermal efficiency loss (modify combustion chamber design?)* 2. Co-Optima fuels can be produced in sufficient volumes & at costs that will enable market penetration. 3. Full electrification will not replace internal-combustion engines before DFI with Co-Optima fuels is implemented. 4. Optical-engine results are adequately representative of results from production/metal engines.
Surr.	• Computationally tractable & accurate predictions of fuel effects on soot emissions can be obtained using current and/or future kinetic-modeling approaches & surrogate-fuel components.
Soot	• Fuel physical properties are assumed to have a secondary impact on mixing during pyrolyzing experiments. • Mixture properties may need to be measured and/or modeled to understand their true impact. • The addition of aromatics to n-dodecane in sufficiently small quantities is assumed to have minimal impact on ignition and flame lift-off characteristics while demonstrating a quantifiable effect on soot formation. • Additional data must be collected to inform the development of the empirical correlation.