Co-Optimization of Fuels and Engines
Advanced Engine Development Team

Thrust II engine projects

June 9th, 2016

Paul Miles,[4] Magnus Sjöberg,[4] John Dec,[4] Steve Ciatti,[1] Chris Kolodziej,[1] Scott Curran,[3] Mark Musculus,[4] Charles Mueller[4]

1. Argonne National Laboratory
2. National Renewable Energy Laboratory
3. Oak Ridge National Laboratory
4. Sandia National Laboratories

Co-Optima DOE VTO Management Team: Kevin Stork, Gurpreet Singh, & Leo Breton

Overview: Thrust II engine projects

Thrust II engine projects focus on mainly on Advanced Compression Ignition (ACI) Strategies using both gasoline-like and diesel-like fuels

- **Examine Thrust I fuel compatibility with advanced SI combustion strategies**
  - Fuel effects on lean/dilute, well-mixed & stratified combustion (**SNL Sjöberg**)
- **Test Thrust I fuel compatibility with ACI strategies**
  - Partially stratified Low Temperature Gasoline Combustion (LTGC) (SNL Dec)
  - Gasoline Compression Ignition – GCI (ANL Ciatti/Kolodziej)
- **Accelerate ACI Combustion System Development**
  - Reactivity-Controlled Compression Ignition – dual fuel. Multi-cylinder (**ORNL Curran)**, Mixture formation (SNL Musculus)
  - Leaner Lifted Flame Combustion (**SNL Mueller**)

Bold text designates legacy projects with significant results to present; others are new-starts under Co-Optima

Co-Optima Milestones:
Thrust II engine projects

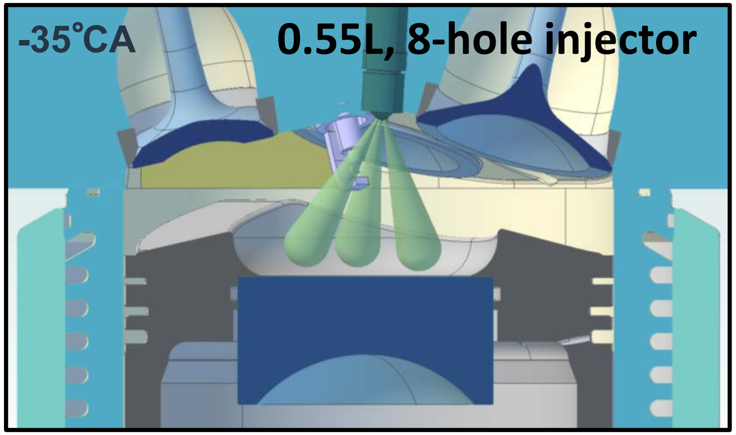
Tracked Co-Optima Milestones

Milestone	Date
Dilute & Stratified SI Combustion Systems	
SNL: Assess reasons for differences in fuel-economy gain using mixed-mode combustion between E30 and gasoline for well-mixed lean and dilute SI operation	12/31/2015 ✓
Accelerate ACI Combustion System Development	
ORNL: Quantify the increase in the RCCI operating range due to the use of renewable fuels with transient hardware-in-the-loop experiments	9/30/2016
SNL: Document fuel effects on LLFC with and without the use of ducted fuel injection	9/30/2016
Test Thrust I Fuel Compatibility with ACI	
ANL: Test Thrust I fuel behavior in GCI combustion systems and characterize necessary engine adaptations	9/30/2016

SNL (Sjöberg) $652k: Continuing advanced light-duty SI engine fuels research + $300k new Co-Optima fuels

Objective

- Contribute to science-base needed for:
  - Spray-guided stratified charge combustion
  - Well-mixed lean/dilute combustion
- Maximize fuel-economy benefits by utilizing unique properties of alternative fuels



Approach

Combine performance testing, optical diagnostics, and complementary modeling

- High-speed optical diagnostics: PIV – Flows, Mie – Liquid Spray, IR & PLIF – Fuel Vapor, Ignition plasma & flame imaging
- Apply enhanced ignition when it increases relevance of the fuels research by stabilizing ultra-lean operation
- Synthesize experimental findings into conceptual understanding
- Provide validation data for CFD models and collaborate on kinetic model development

Fuels

- High-octane E0–E85; additional fuels in coordination with other Co-Optima tasks

Sjöberg: Advanced ignition enables homogeneous, EGR-diluted mixed-mode combustion

Motivation

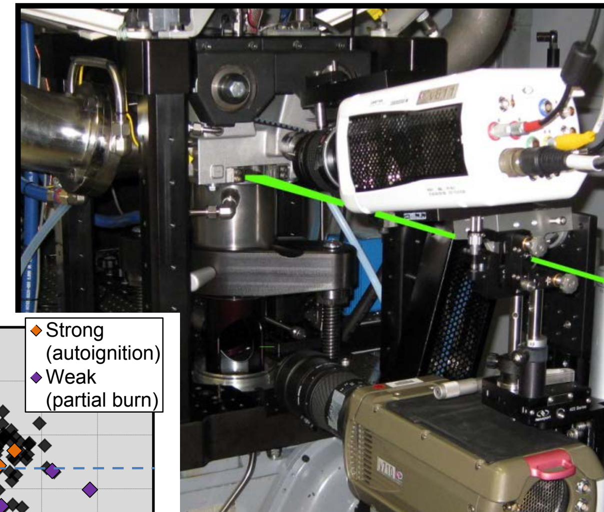
Combustion instability and excessive burn duration limit benefits of lean, well-mixed operation

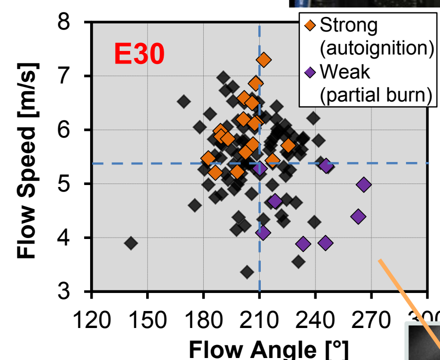
Method

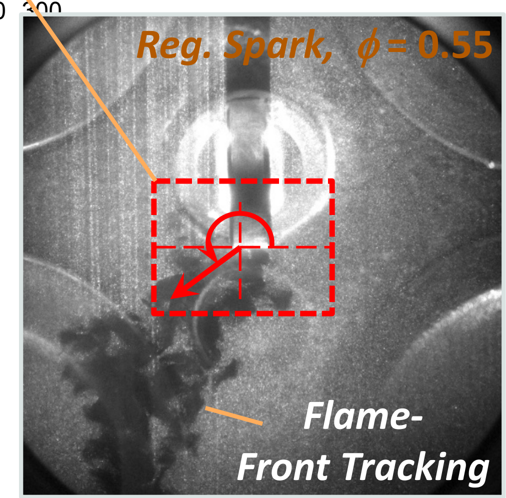
Investigate combined effects of ignition system, gas temperature, fuel chemistry, and flow on robustness of inflammation

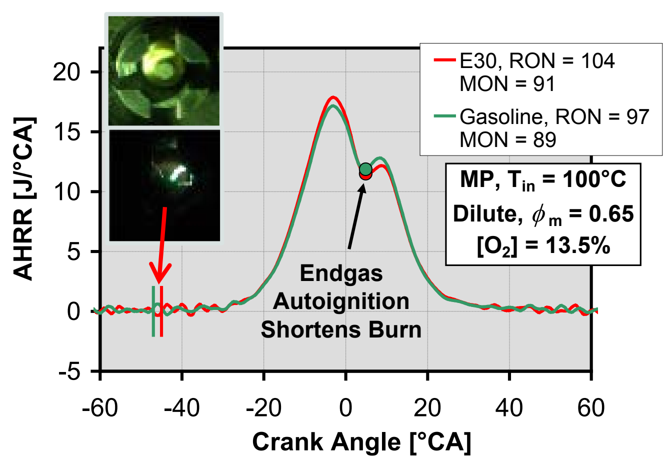
Results

- Combine PIV, flame and plasma imaging to track flow field and flame wrinkling
  - Feed data to CFD effort at ANL
- Intake-air preheating with multi-pulse plasma ignition leads to fast inflammation & mitigates low flame speeds, enabling mixed-mode com-bustion for high-octane fuels
  - This operating point is "beyond MON"









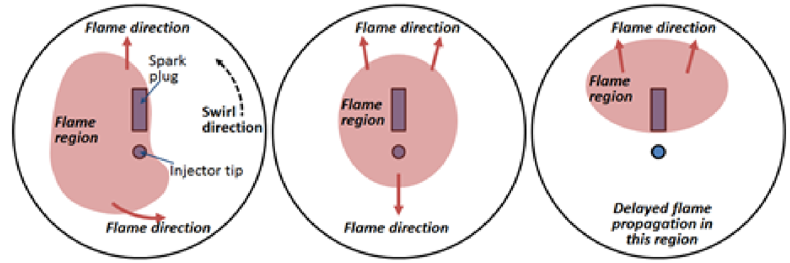
Sjöberg: For stratified-charge operation swirl stabilizes flame spread, but associated tumble causes soot

Motivation

Flow/spray interactions critically impact cycle-to-cycle variability

Results

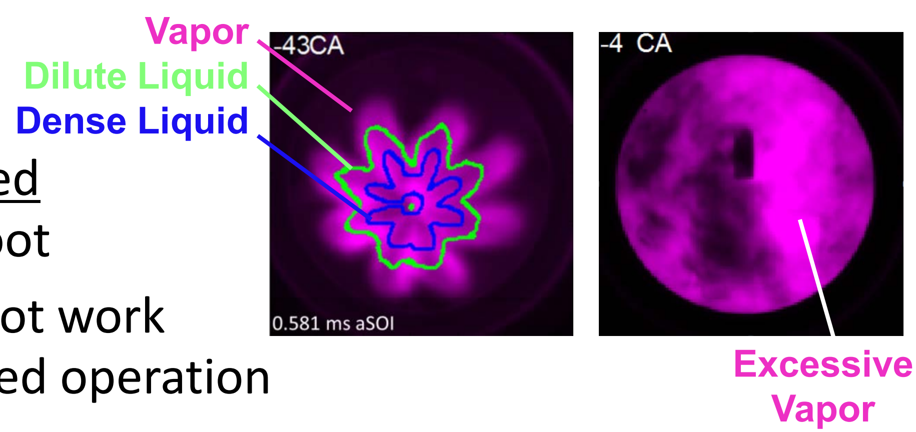
- PIV and flame imaging reveal how flame-spread differences lead to partial burns
  - Swirl helps stability, but increases tumble
- PIV and IR imaging reveal <u>tumble-induced asymmetry</u> of fuel vapor ⇒ increases soot
- Double-injection strategies to reduce soot work equally well for E0 and E30 under boosted operation
- <u>E30 has larger soot challenges</u> for naturally aspirated operation. More wall wetting?
- Collaborative CFD work at ANL matches well both swirl and tumble flow for motored conditions (R. Scarcelli).

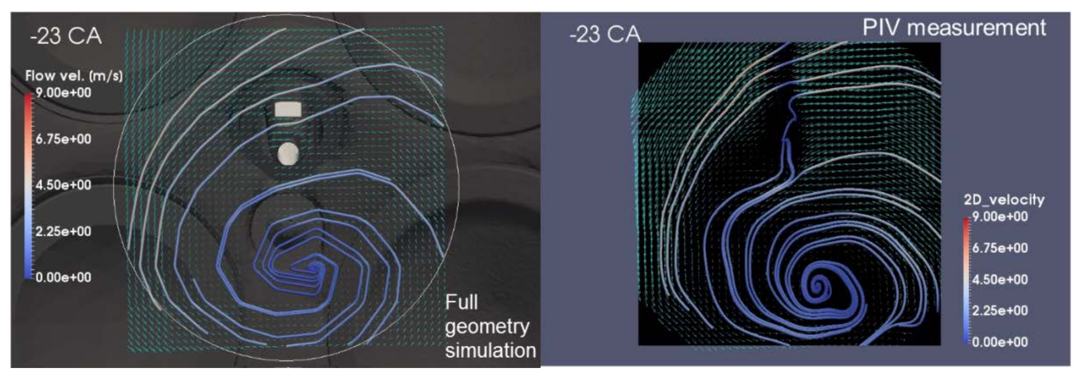


Type A: swirl, always good

Types B & E: no swirl, good burn cycles

Types C & D: no swirl, poor burn cycles

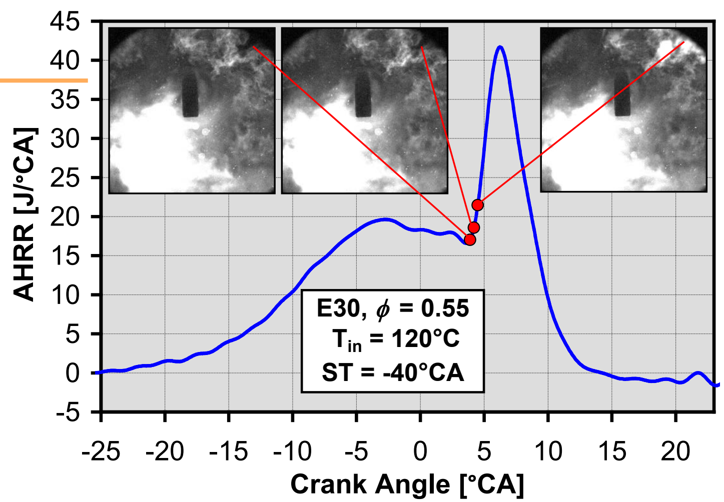




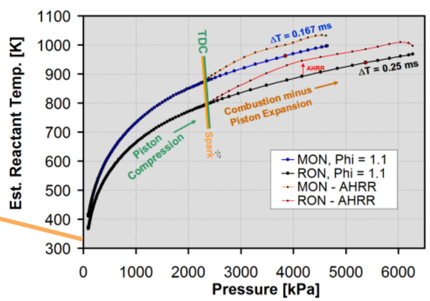
Sjöberg future work: Map out knock limits and extend stratified operation to new biofuels

Well-mixed operation

- Map out knock-limited CA50 (KL-CA50) over ranges of speed and intake pressure for stoichiometric operation. Provide validation data to the Co-Optima Toolkit team
- Compare KL-CA50 maps for Co-Optima core fuels and selected new biofuel blends
- Quantify efficiency gain for ultra-lean or dilute operation at selected operating points
- Assess adequacy of RON and MON, both for stoichiometric and lean operation
- For lean mixed-mode combustion, peak AHRR needs to be controlled $\Rightarrow$ motivates optical work to probe transition from deflagration to autoignition
  - Preliminary E30 results demonstrate feasibility



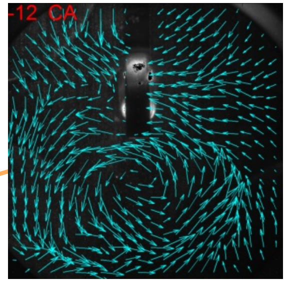
- Continue collaborations on CFD and kinetics modeling with Westbrook/Pitz on fuel-based origin of octane sensitivity



Stratified-charge operation

Build from E0 - E30 knowledge base to include new biofuel blends

- Extend to higher and lower loads, focus on NO_x / soot / stability trade-offs
- Expand conceptual model of swirl-spray stabilization mechanism for stratified operation to include double injections



SNL (Dec) $175k: Thrust I fuel compatibility with Low Temperature Gasoline Combustion (LTGC)

Objectives

1. Provide a fundamental understanding of the autoignition reactivity of Thrust I fuels for boosted operation

⇒ **Well-premixed LTGC provides detailed information on autoignition, valuable to Thrusts I & II.**

- Data for kinetic model development and validation
- Examines whether RON, MON, & Sensitivity (**Sens** = RON - MON) are adequate metrics for autoignition quality in highly boosted engines

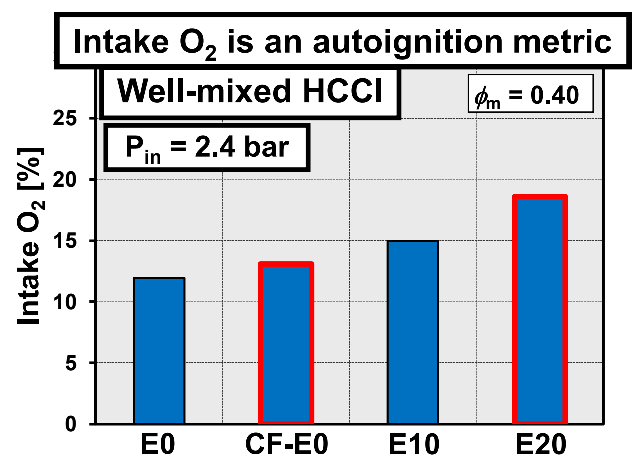
2. Evaluate the potential of Thrust I fuels for ACI, LTGC engines

	RON	MON	AKI
E0	91.0	82.7	86.9
E10	95	86	90.5
E20	98	87.5	92.8
CF-E0	96.6	88.7	92.7

Motivation and Project Plans

Previous work showed that for similar RON and MON, high ethanol fuels suppress autoignition better than straight petroleum-based fuels, for high-boost operation.

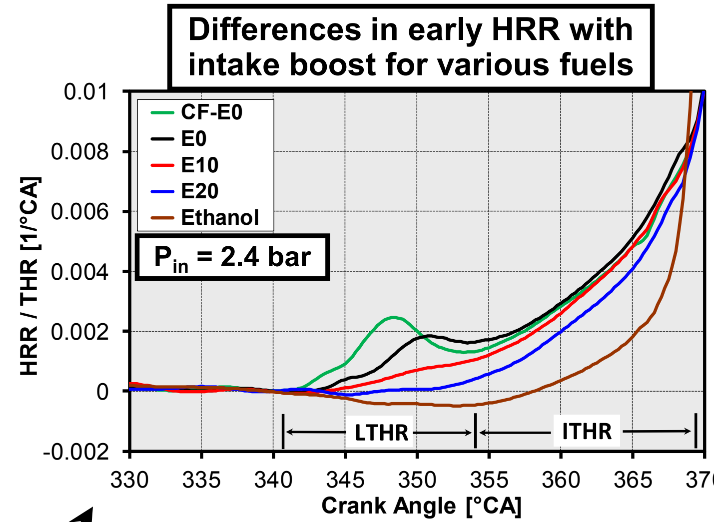
1. Design test matrix to determine the effect of using ethanol (typical biofuel) vs. aromatics (typical petroleum) to obtain high RON & high **Sens** ⇒ test over range of boost pressures
2. Investigate Thrust I gasoline blends with high biofuel content for LTGC (*e.g.* 30% ethanol or other adv. biofuel).



Dec: Thrust I fuel compatibility with Low Temperature Gasoline Combustion (LTGC)

Progress/Accomplishments

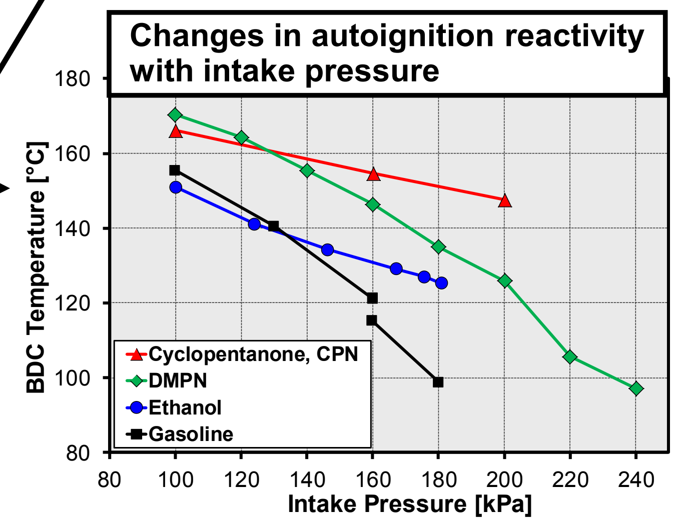
- Collaborated with Scott Sluder of ORNL to develop a test-fuel matrix and fuel specifications to:
  - Determine importance of **Sens** for boosted operation.
  - Determine effect of using 30% ethanol vs. additional aromatics to get high **Sens** for boosted operation.
- The test-fuel matrix will also be used by the FP & AED teams in boosted SI and GCI (Thrust II) studies



Deliverables

- Tests for well-premixed LTGC (HCCI) will provide detailed information on autoignition
  - Detailed HRR data showing changes in LTHR & ITHR with boost Pressure and intake Temperature.
  - Determine sensitivity of autoignition to changes in P & T

  This information is required for kinetic-model validation



- Compare LTGC & knock-limited SI data (from ORNL) for range of boost P ⇒ Recommend fuel-property metrics & specifications for high-boost Thrust I engines
- LTGC performance data for Thrust I fuels (gasoline + new biofuels or high ethanol, ~30%)

ANL (Ciatti/Kolodziej) $175k: Thrust I Fuel Behavior in GCI Combustion Systems

- **Objectives**
  - Assess the impacts of high RON Thrust I near-term fuels on single-fuel GCI operation
  - At fixed RON, identify desirable fuel heat of vaporization (HoV) and sensitivity (RON-MON) qualities for GCI combustion and performance

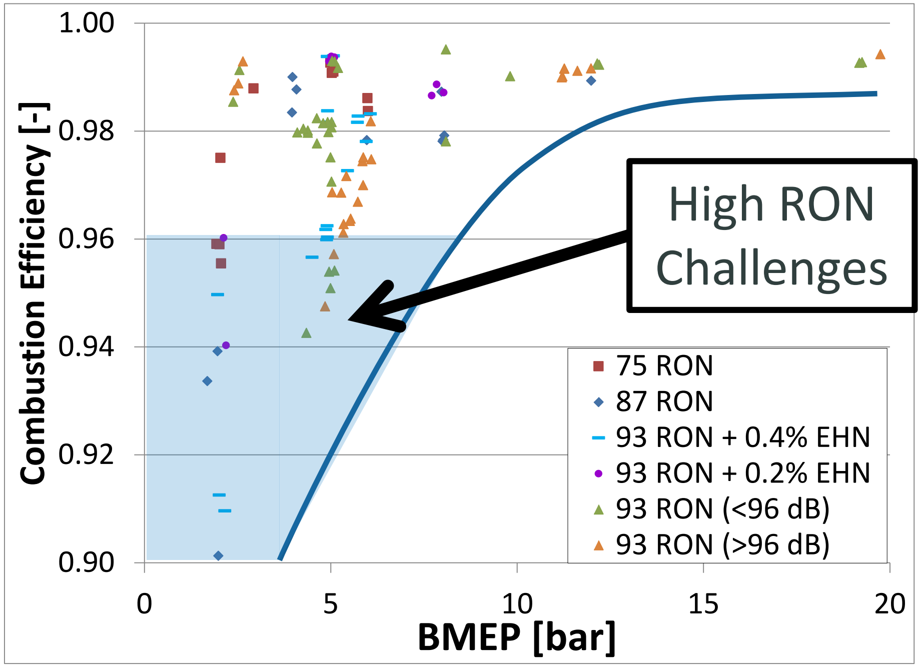
RON 98 Thrust 1 Fuel Properties

Fuel	HoV	Sensitivity
Alkylate Blend	Low	< 1
Ethanol Blend	High	> 10
Aromatic Blend	Low	> 10 (= Eth. Blend)

- **Project Plans**
  - Test the Argonne GCI engine at defined engine speed-load conditions and fixed system level parameters with each Thrust I fuel
    - Fixed intake conditions (temperature, boost, EGR)
  - Identify boost/cylinder pressure requirements to compensate for combustion phasing differences caused by HoV and Sensitivity
  - Analyze the overall effects of fuel HoV and sensitivity on GCI engine combustion, emissions, and performance

Ciatti/Kolodziej: Thrust I Fuel Behavior in GCI Combustion Systems

- **Progress**
  - Previous testing and literature review identified intake pressure as important to achieving combustion stability for high RON fuels
  - Identified engine operating conditions and engine geometry to best manage auto-ignition



- **Deliverables**
  - Completion of initial test matrix by Sep 30, 2016
  - Test Thrust 1 fuels in Argonne GCI engine, operating at low and high load conditions
  - Identify relationships of fuel HoV and sensitivity with GCI combustion, emissions, and performance

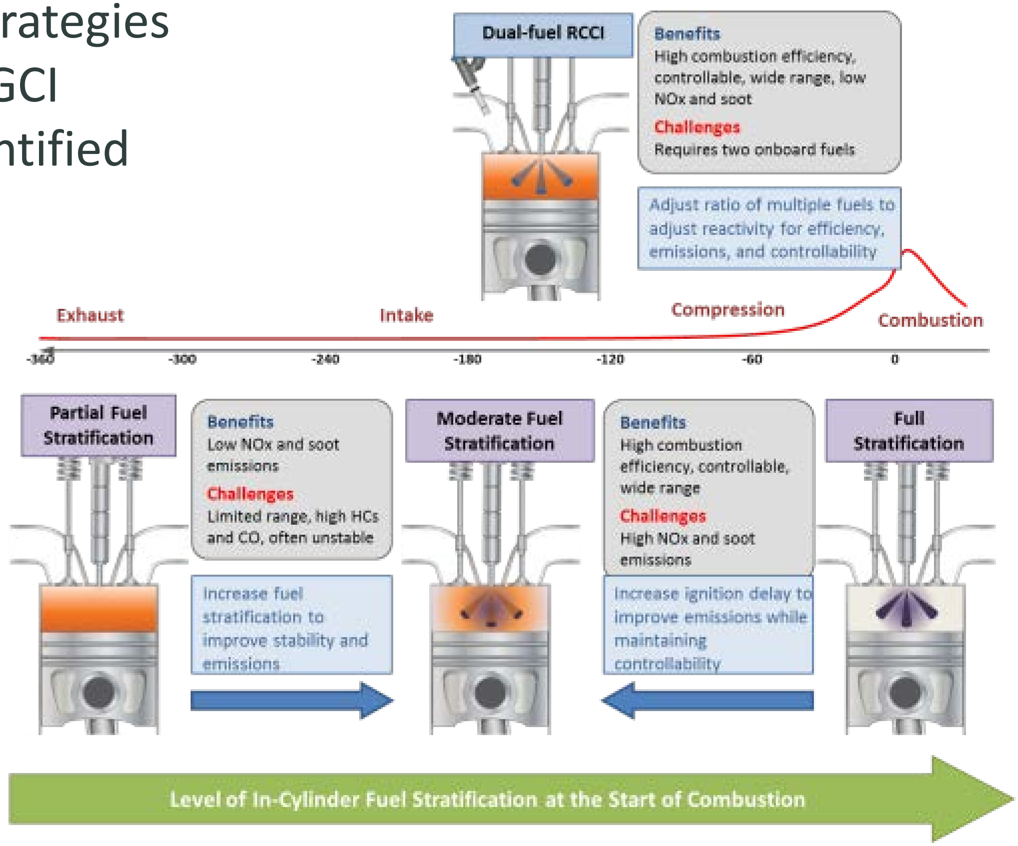
ORNL(Curran) $175k: Continuing ACI/LTC Development in Multi-Cylinder Engines + $175k new Co-Optima fuels

Objectives:

- Gain a greater understanding of fuel effects on single fuel (GCI) and dual-fuel (RCCI) ACI concepts to take advantage of fuel properties for attaining higher efficiency in ACI engines
- Identify performance trends in ACI strategies spanning RCCI + broad landscape of GCI with the targeted fuel properties identified

Operating-Condition Approach:

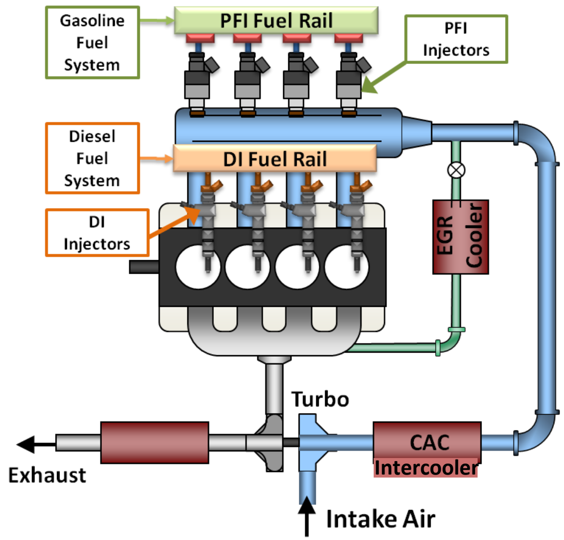
- RCCI: Vary reactivity differential between premixed and DI fuels
  - Supported by optical-engine RCCI E.2.2 task work at SNL
- GCI: Focus on further understanding role of fuel properties on partial- and heavy-stratified GCI modes
- Effect on RCCI and GCI operability with thrust 1 fuels



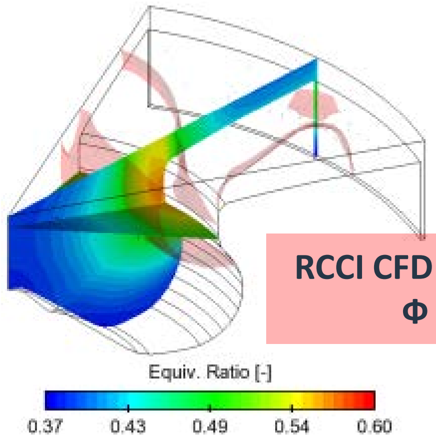
Curran: Accelerate ACI/LTC Development – Multi-Cylinder Engines

Approach:

- 1.9L GM diesel platform modified for both single- and dual-fuel LTC operation
  - Stock-GM re-entrant piston, high-pressure EGR
  - Bosch DI Injectors: 7 holes, 140 µm holes, 148° included angle + added PFI fuel injection system
- Coordinated with optical work at SNL to provide insight into in-cylinder reactivity stratification
  - CFD modeling to gain further insights into fuel specific effects on ACI



ORNL RCCI Multi-Cylinder 1.9L GM



RCCI CFD Isosurface at Φ = 0.49

SNL Optical Work:
Provides in-cylinder diagnostic for measuring reactivity stratification
– adds new insights for CFD as well

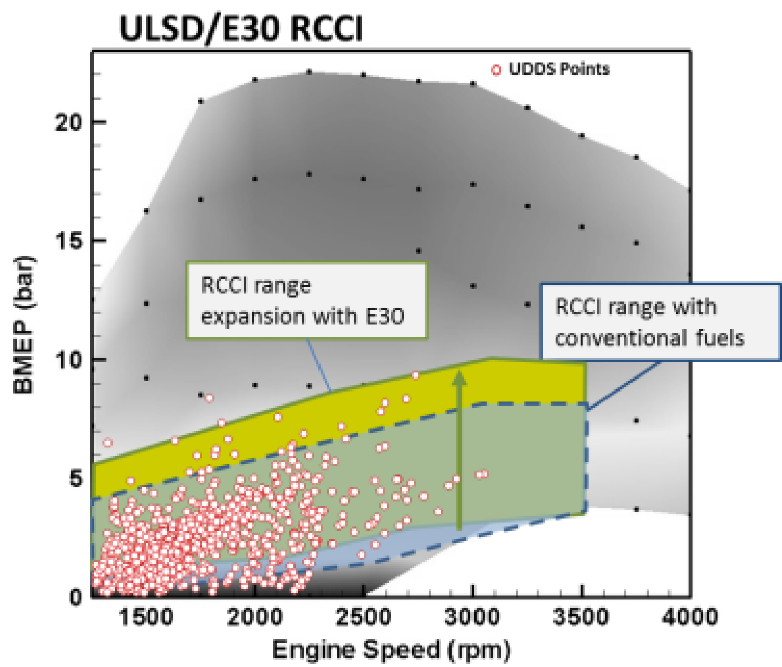
Base Multi-Cylinder 1.9L GM CIDI

Number of Cylinders	4
Bore, mm	82.0
Stroke, mm	90.4
Compression Ratio	17.5
Rated Power, kW	110
Rated Torque, Nm	315

Curran: Accelerate ACI/LTC Development – Multi-Cylinder Engines

RCCI Results

- Continuing ORNL research into fuel effects on RCCI has been focused on ACI load expansion with the goal of increasing potential fuel economy benefits
  - By covering more of the US light-duty drive cycle range, the higher the potential of increasing fuel economy benefits over conventional combustion baselines
  - Past efforts have used vehicle systems simulations to show fuel economy improvements
- Strong fuel properties effect shown for maximum brake thermal efficiency
- Results to date have focused on high reactivity delta between the two fuels
  - Also exploring low delta reactivity options



Fuel properties are a potential path to enabling low temperature combustion

Curran: Accelerate ACI/LTC Development – Multi-Cylinder Engines

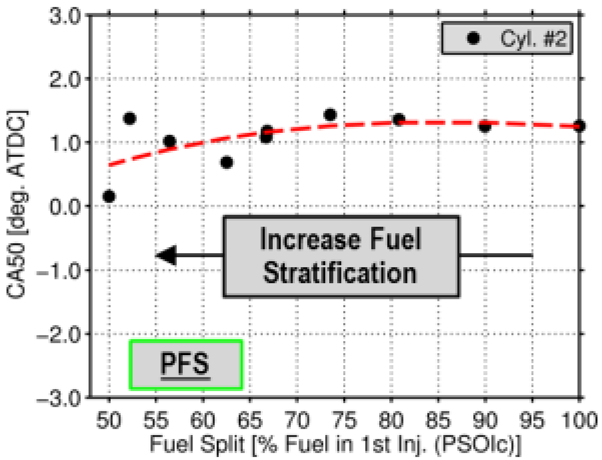
GCI Results:

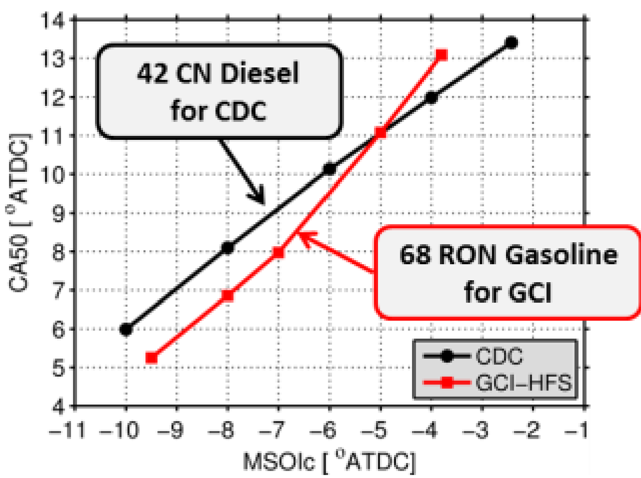
Fuel effects on partial fuel stratification (PFS) and heavy fuel stratification (HFS) GCI modes via MCE experiments and CFD

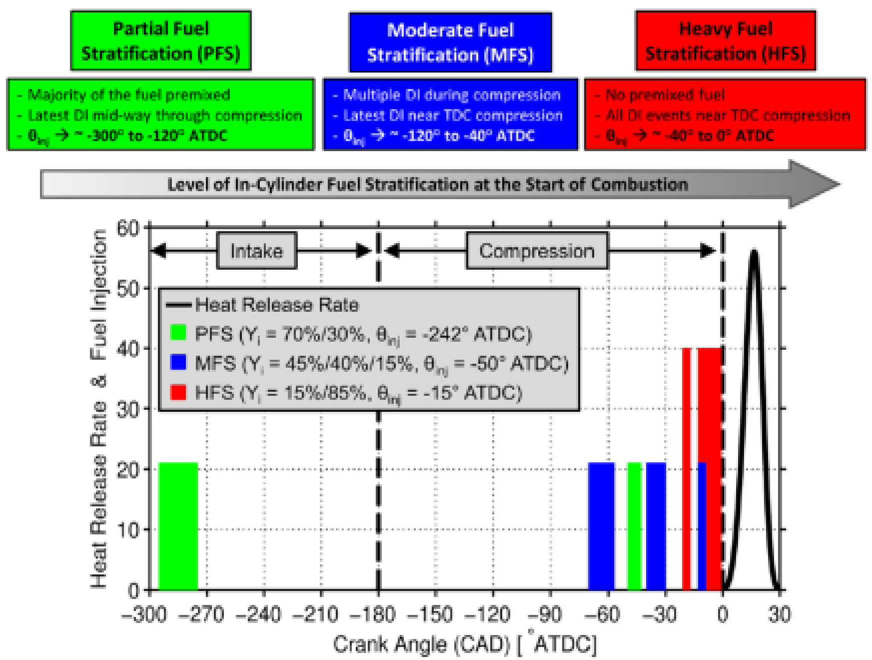
- Experimental results focusing on operability and controllability of wide range of RON (figs. on right)
- CFD results showing fuel effect potential over GCI landscape of (leading to review paper – fig. below)

Experiments with PFS and HFS with 68 RON gasoline controllability

- Use of BOB range RON for ACI







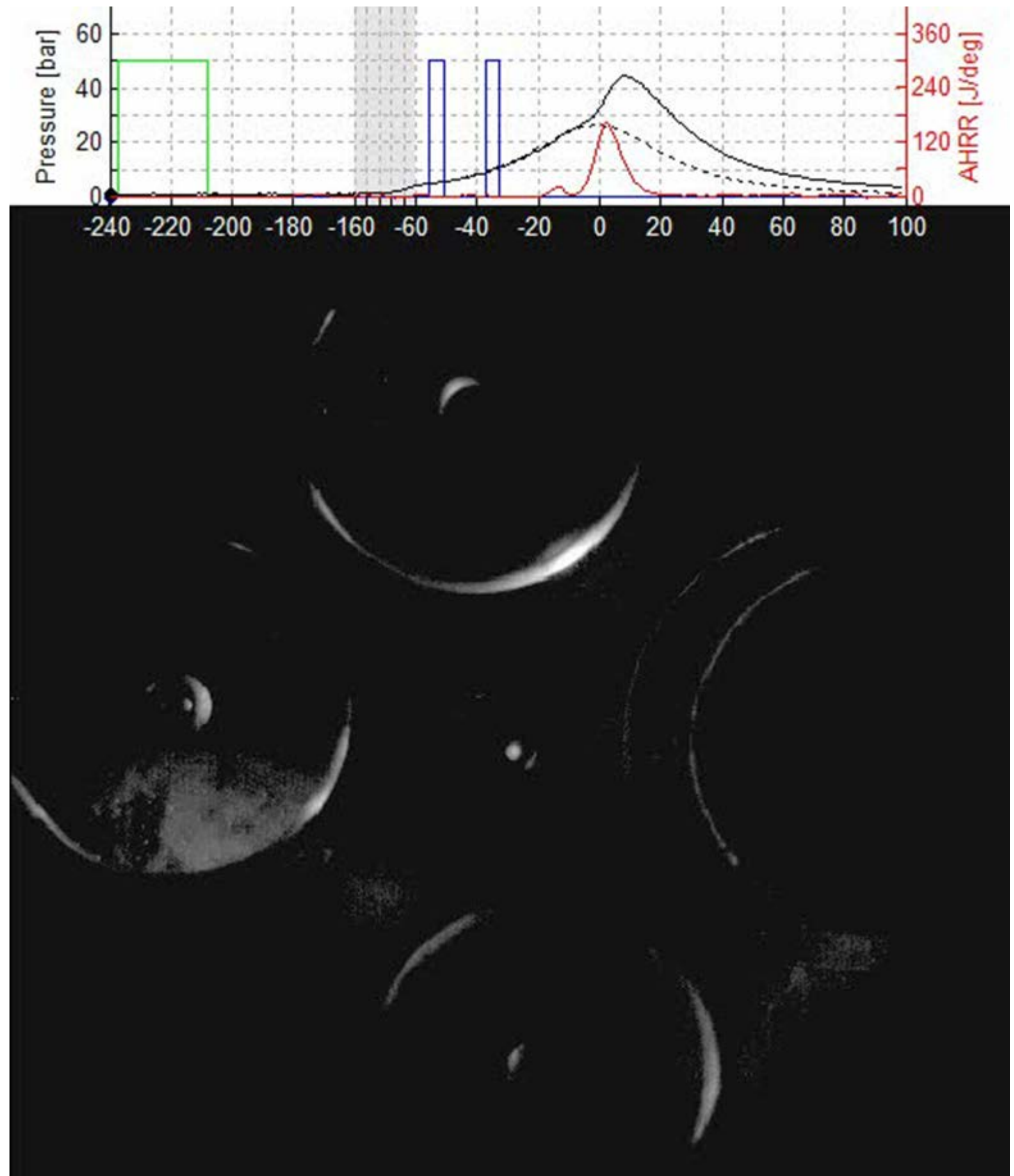
SNL (Musculus) $175k: Accelerate ACI/LTC Development – Optical Diagnostics of RCCI

Objectives:

- Measure in-cylinder mixing/ kinetics to optimize dual-fuel heat-release for noise, efficiency, and load range
- Understand mixing/ignition interaction for different fuel reactivity combinations
- Supports metal-engine RCCI E.2.2 task work at ORNL

Operating-Condition Approach:

- Vary reactivity differential between premixed and DI fuels using various gasoline reference fuel blends

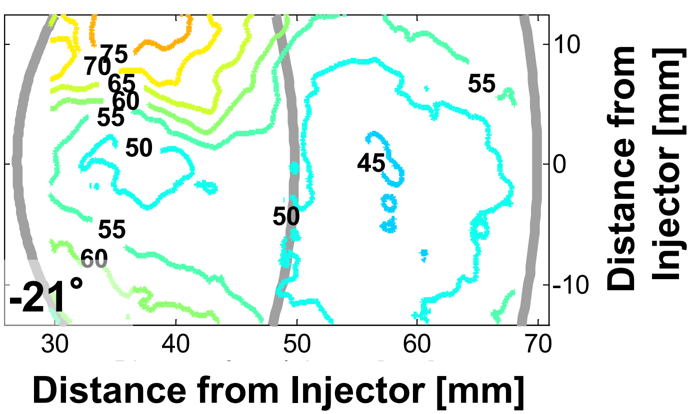


Musculus: Accelerate ACI/LTC Development – Optical Diagnostics of RCCI

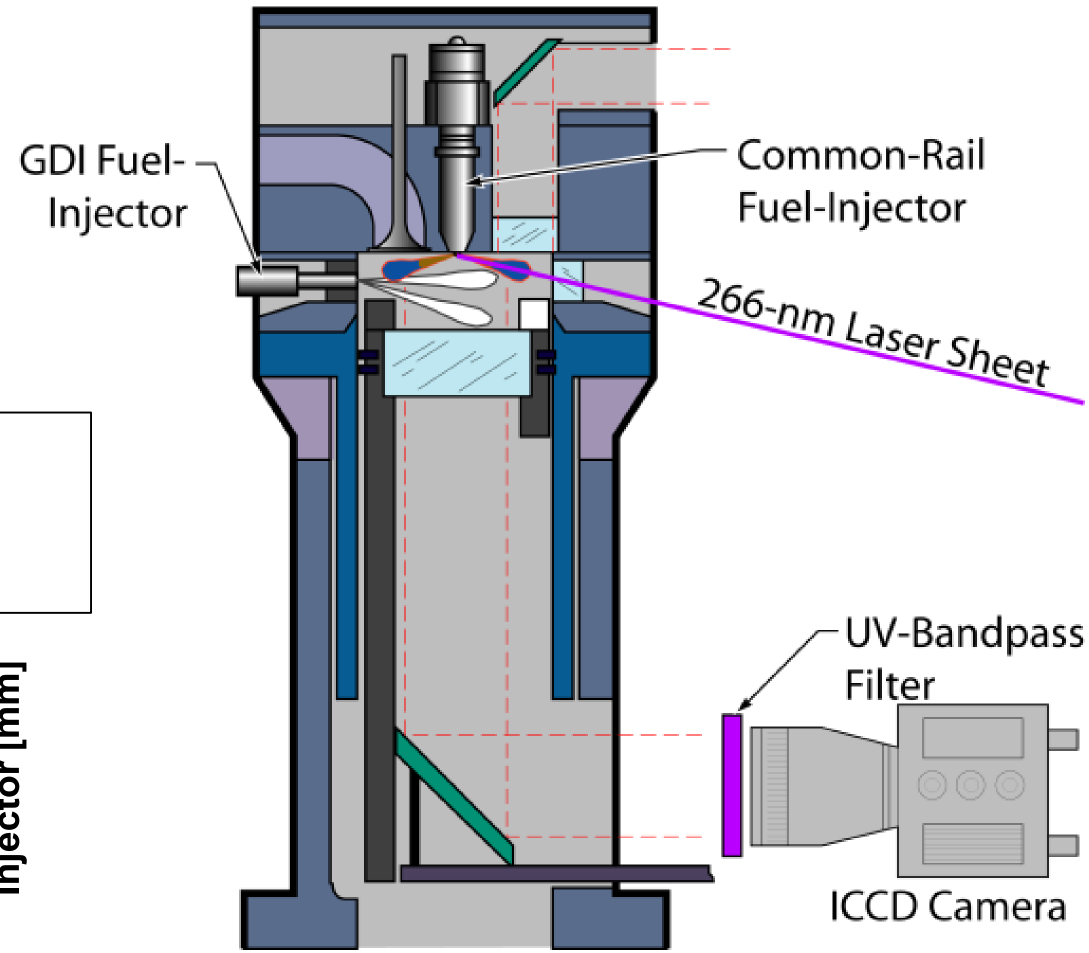
Optical Diagnostic Approach:

- Image ignition w/ high-speed Chemiluminescence
- Generate mixing maps using fuel-tracer laser – induced fluorescence at select operating conditions

Previous RCCI Fuel-Tracer PLIF:
Shows lowest PRF in squish
for wide reactivity differential

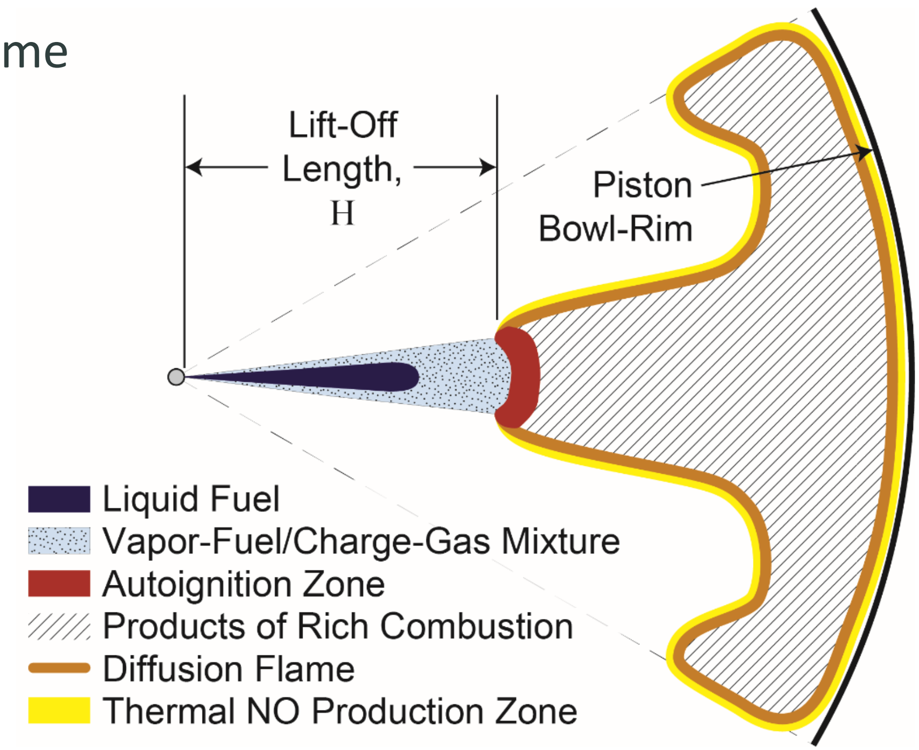


Fuel-Tracer PLIF Diagnostic in Heavy-Duty Optical Engine



SNL (Mueller) $788k: Continuing ACI/LTC Develop. – Leaner Lifted-Flame Combustion (LLFC)

- LLFC is <u>mixing-controlled combustion</u> that <u>does not form soot</u> because it occurs at equivalence ratios ≤ 2
  - Near lift-off length & at diffusion flame

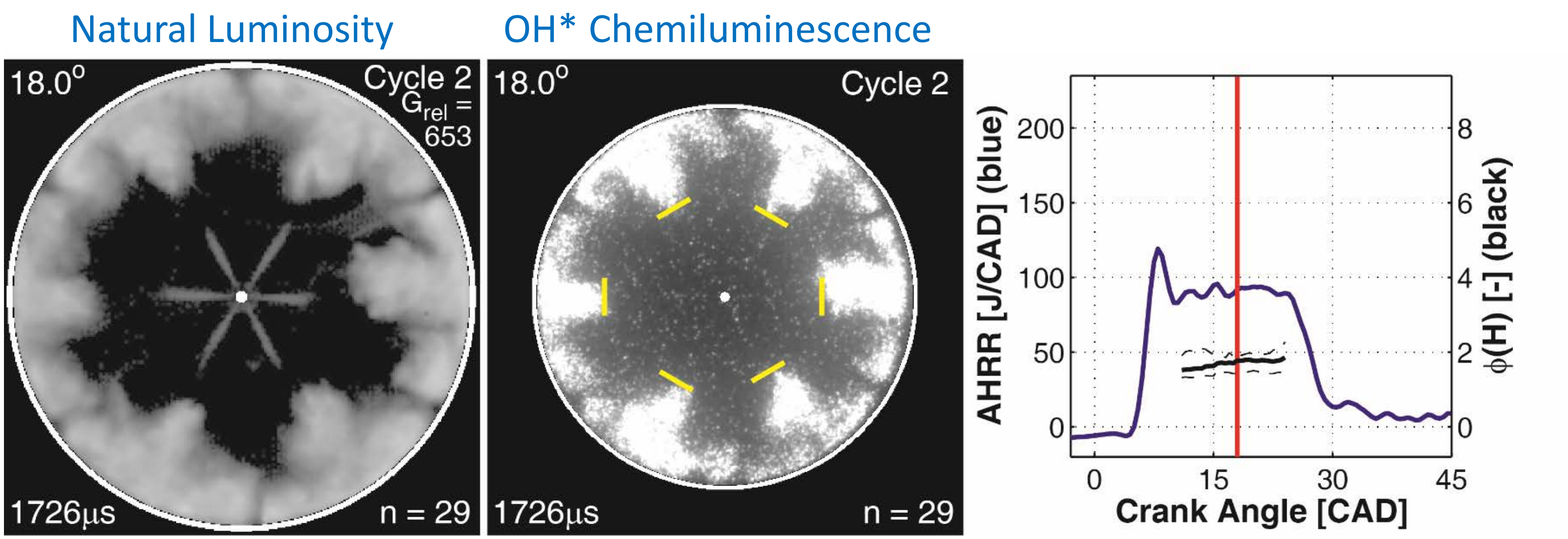


- LLFC has many advantages
  - High efficiency (compression ign.)
  - Fuel-flexible (specs. similar to D2)
  - Low emissions
    - No soot (#2 climate forcer)
    - Tolerant of EGR for NO_x control
    - Less-expensive aftertreatment
  - Easy control (by inject'n timing)
  - Low noise (steady heat release)

- <u>Research challenge</u>: LLFC had not been sustained in an engine at moderate loads using a "practical" injector-tip configuration and fuel

Mueller: Accomplishment #1: 1st Engine Demo of LLFC Using Realistic Operating Parameters

- Sustained LLFC at ~6 bar gross IMEP/ 1500 rpm using 6-hole injector tip
  - Fuel = 50/50 vol% blend of #2 diesel certification fuel + oxygenate

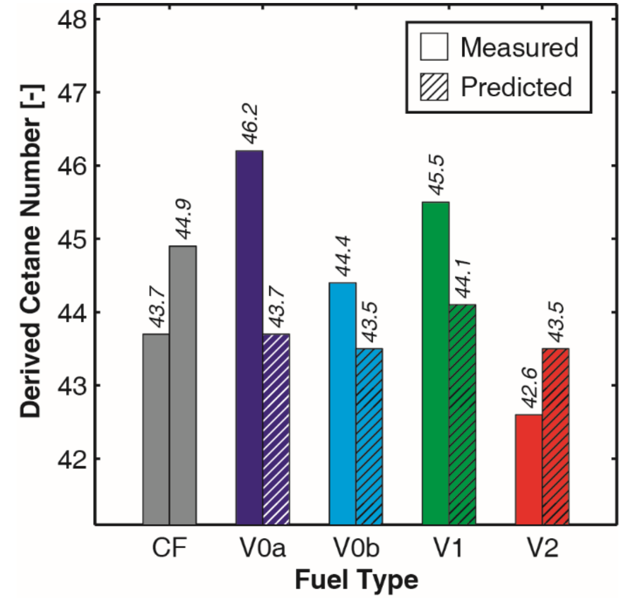


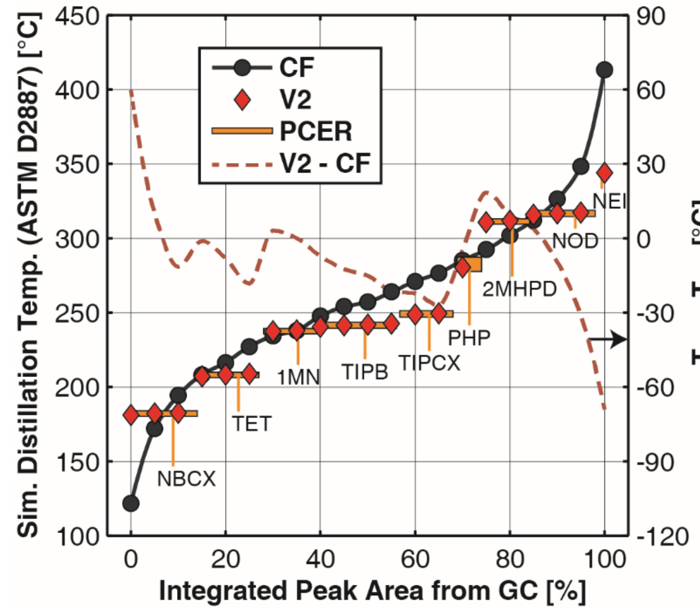
- Explored approaches to extend the high-load limit of LLFC
  - Ducted fuel injection (DFI): inject fuel down a tube coaxial with the fuel jet
  - DFI collaborations
    - Drafted CRADA with Caterpillar and Ford to develop the DFI technology
    - LLNL (simulations), ANL (x-ray mixing meas'ts), Georgia Tech (optical exp'ts)
  - Down-selecting next test fuel from Co-Optima LGGF Team fuel candidates

Mueller Accomplishment #2: Summarized Diesel Surrogate Fuels Research Results to Date

Led the synthesis and documentation of 5 years' worth of surrogate-fuel research results from CRC Project AVFL-18a

- Primarily emulate target-fuel composition (secondarily: ign. quality, volatility, density)
- Created a set of 4 surrogate fuels with increasing compositional accuracy relative to the target fuel
- Surrogates meet or exceed key specs from ASTM D975: sulfur, cetane, lubricity, flash point, viscosity, and corrosivity
- Measures may be required to prevent fuel solidification at high pressures
- Results corroborate hypothesis:
  - The more closely a surrogate fuel emulates its target-fuel <u>composition</u>, the more closely it will also match the target-fuel <u>properties</u>





Mueller: Proposed Future Work (through FY17)

- Leaner lifted-flame combustion (LLFC) / ducted fuel injection (DFI)
  - Experiments in constant-volume and constant-pressure combustion vessels to better establish the potential benefits and challenges of DFI
  - Further analysis to develop a fundamental understanding of how DFI works
- Diesel surrogate-fuel research
  - Overcome problems with surrogate-fuel solidification at high pressures
    - Collaborate with PNNL, Chevron, NREL, and others (CRC) on cold-flow improvers
  - Test diesel surrogate fuels in optical engine to
    - Determine minimum compositional accuracy required to emulate target fuel combustion performance
    - Better understand how fuel composition affects properties and engine performance (e.g., sooting propensity)
    - Collaborate with modelers at LLNL and ANL to identify and overcome barriers to truly predictive, cost-effective, and fast simulation
- In-cylinder soot measurement
  - Continue developing vertical laser-induced incandescence to measure average in-cylinder soot distribution for the assessment of soot models

Advanced Engine Development Team Summary: Thrust II engines

Relevance

- Understanding fuel effects on Advanced SI and CI combustion regimes is central to the rapid development and deployment of highly efficient Thrust II engines

Approach

- Individual projects are coordinated to a high degree and seek to build on the strengths of the individual laboratories

Accomplishments

- Continuing projects have shown strong technical progress in the areas of:
  - Fuel spray/flow interactions, LTC operation with high-octane/low flame speeds
  - Fuel effects on RCCI load extension and controllability
  - Load extension of LLFC and diesel surrogate fuel development
- Technical work on new projects is commencing with many projects focusing on a common fuel matrix

Collaborations

- “Co-Optima” has 9 National Labs, stakeholder engagement, and external advisory board
- Projects presented at AEC semi-annual program review, engaged with ACEC TT
- Numerous other project-level collaborations between labs and with industry

Future Work

- A portfolio of ongoing and future work has been described

Co-Optimization of Fuels and Engines
Advanced Engine Development Team

Sprays & emission control research

June 9th, 2016

Paul Miles,[4] Matt Ratcliff,[2] Lyle Pickett,[4] Chris Powell,[1] Bob McCormick,[2] John Storey,[3] Melanie DeBusk,[3] Todd Toops,[3] Josh Pihl[3]

1. Argonne National Laboratory
2. National Renewable Energy Laboratory
3. Oak Ridge National Laboratory
4. Sandia National Laboratories

Co-Optima DOE VTO Management Team: Kevin Stork, Gurpreet Singh, & Leo Breton

Overview: Sprays & emission control research

Fuels can have a pronounced impact on spray structure and mixture formation, as well as on integration with aftertreatment systems, for all Thrust I and Thrust II engine technologies

- **Examine fuel impacts on spray structure**
  - High-throughput spray chamber (SNL Pickett)
  - X-ray imaging of GDI sprays with alcohol blends (ANL Powell)
- **Examine fuel effects on particulates and gaseous emissions control**
  - Particulate Matter Index (PMI) refinement (**NREL McCormick/ Ratcliff**)
  - PM formation and oxidation fundamentals (**ORNL Storey/DeBusk**)
  - Fuel effects on gaseous emission control (**ORNL Toops/Pihl**)

Bold text designates legacy projects with significant results to present; others are new-starts under Co-Optima

Optima Milestones:
Sprays & emission control research

Tracked Co-Optima Milestones

- **Sprays**

Milestone	Date
SNL: Design and place contracts for high-throughput chamber components	9/30/2016

- **Particulates and Gaseous Emissions Control**

Milestone	Date
NREL: Complete GDI (SCE) PM emissions test matrix with objective of improving predictions of PMI	9/30/2016
ORNL: Evaluate dual SCR system with ethanol-based fuels to determine parameters that enable the emissions targets	9/30/2016

Spray Projects

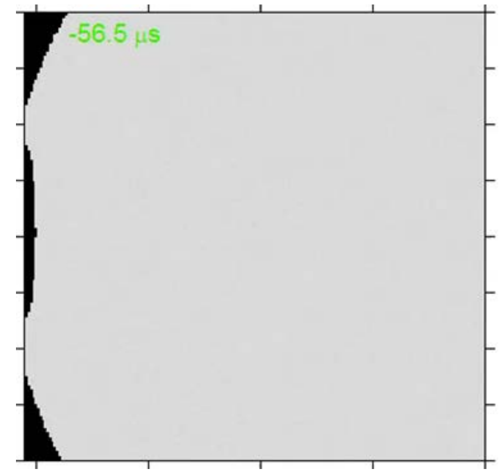
SNL (Pickett) $1115k:
High-throughput spray chamber

Motivation: Fuels affect sprays, and sprays affect efficiency

Fuel properties such as density, viscosity, surface tension, boiling point, heat of vaporization, & oxygen content change the way that fuel mixes with air in an engine

- Fuel distribution affects ignition, burn-rate, COV, particulate matter, temperature field, knock sites — all key parameters that directly impact efficiency
- Predicting/controlling spray distribution is a key enabler for efficiency

8-hole GDI spray



Charge gas: 6 bar, 300° C
Fuel: 200 bar, 90° C, iso-octane

Objective

Develop a continuous flow spray chamber that reproduces engine T & P and enables a 300X data throughput improvement

- Large-volume, uniform-temperature (unlike engines or IQT-like chambers)
- Permits variation of a large number of fuel and/or ambient properties
- Enable acquisition of a statistically-significant number of repetitions in transient sprays
- Support CFD model development, validation, and improvement (toolkit)
- Uses the same injector hardware and operating conditions as engine experiments (SNL Sjoberg) and x-ray imaging experiments (ANL Powell)

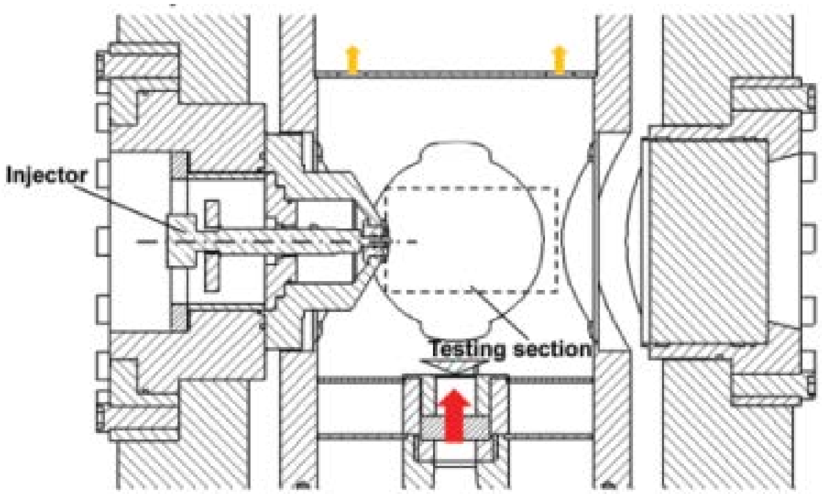
Pickett: Unique spray chamber design provides world-leading capabilities

Status of chamber design:

- Commercial devices do not have capabilities required
- New design includes:
  - Windows with smaller working distance but the same clear aperture
  - Laser access ports
  - Efficient thermal isolation with maximum charge-gas temperature of 1100 K
  - safety features for window ports
  - Improved transient control
- Design established, manufacturing expected to begin by August 2016
- Compressed air, nitrogen, and heater sections currently being procured/installed

Previous concept

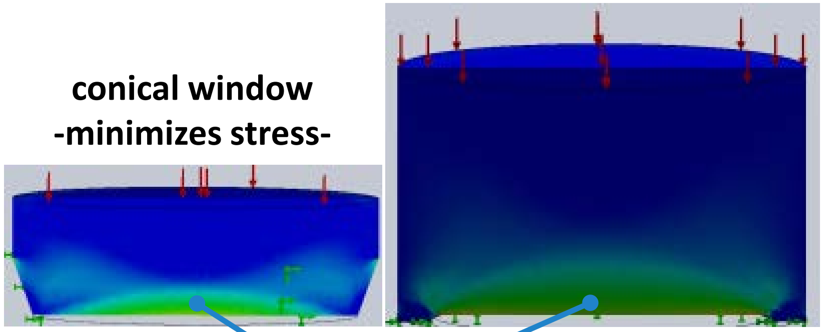
heated, optical chamber



Improved design

conical window
-minimizes stress-

cylindrical window
-twice as thick-



tensile stress concentration

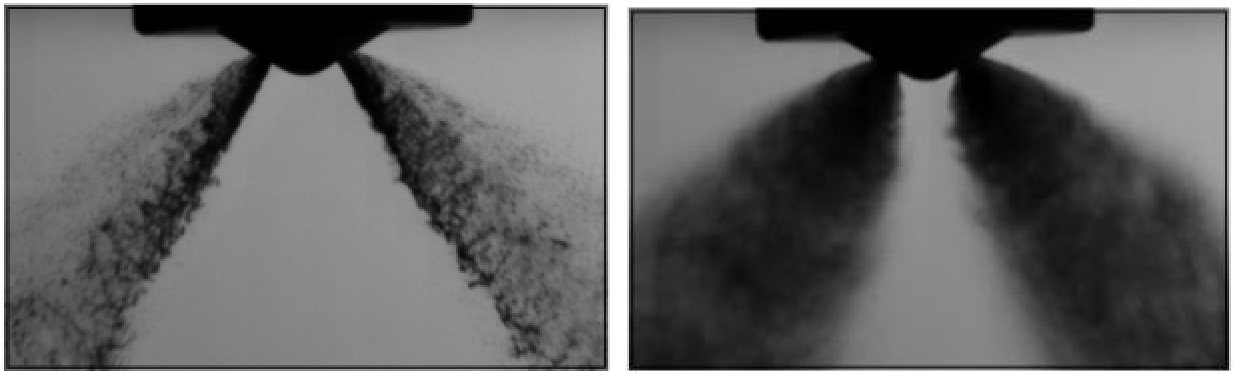
ANL (Powell) $200k: X-ray Imaging of GDI Sprays with Alcohol Blends

Project Plans

- Make quantitative measurements of the fuel distribution from GDI Injectors
- E20 baseline, blends of other alcohols
- Measurements of flash-boiling conditions

Objectives

- Improved understanding of the relation between fuel properties and fuel distribution
- Provide novel, quantitative measurements of flash-boiling sprays
- Deliver data to toolkit group for validation of spray simulations



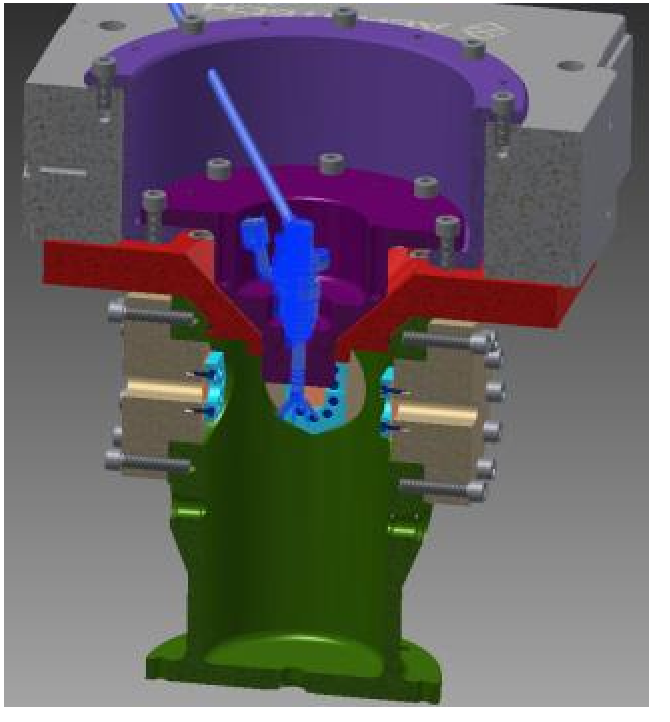
GDI sprays at 323 and 393 K, showing the effect of flash boiling at the higher fuel temperature.

Weber and Leick, ILASS Europe 2014. Used with permission.

Powell: X-ray Imaging of GDI Sprays with Alcohol Blends

Progress

- Modification of spray chamber for flash boiling conditions is complete
- Design of fuel heating system is complete, fabrication is underway
- Procurement of fuel system for high pressure alcohol fuels is in process
- Selection of fuel matrix is underway



New flange to mount ECN Spray G injector in existing spray chamber

Deliverables

- September 31, 2016: Complete measurements of alcohol blend GDI sprays under flash boiling conditions.
- Deliver results to toolkit group for validation and development of spray breakup simulations

Particulates and
Gaseous Emission Control Projects

NREL (Ratcliff/McCormick) $250k: Particulate Matter Index (PMI)

Project Objective

Does PMI breakdown for oxygenates? Studies of oxygenate sooting tendency suggest that it will-

McEnally, C.S., Pfefferle, L.D. Sooting Tendencies of Oxygenated Hydrocarbons in Laboratory Scale Flames. *Environ. Sci. Technol.*, 2011, 45 (6), pp 2498–2503.

PMI is based on detailed hydrocarbon analysis of the base fuel. We also include factors based on oxygenate analysis

$$PMI = \sum_{i=1}^{n}\left[\frac{(DBE_i + 1)}{VP(443K)_i} \times Wt_i\right]$$

Where-

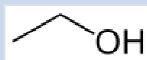
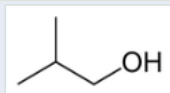
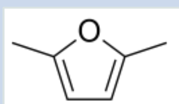
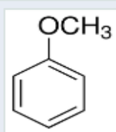
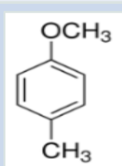
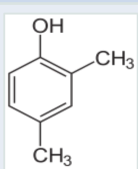
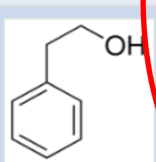
$DBE = \frac{2C+2-H}{2}$ = Double Bond Equivalent – **rough measure of tendency to form particles**

VP = *Vapor pressure at 443K (170°C)* – **rough measure of tendency to evaporate**

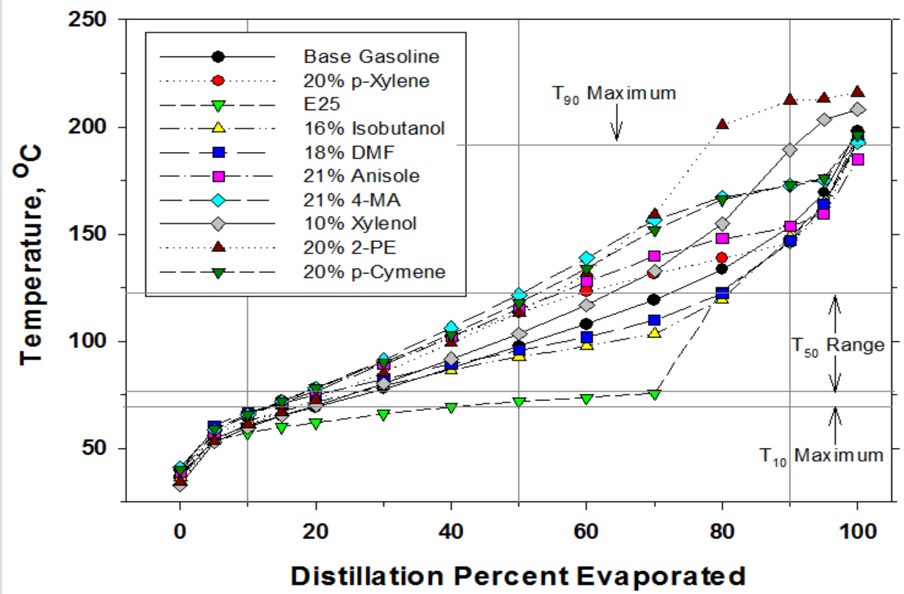
Wt_i = *Weight fraction of compound*

Aikawa, K., Sakurai, T. and Jetter, J. J. Development of a Predictive Model for Gasoline Vehicle Particulate Matter Emissions. SAE International 2010-01-2115.

Ratcliff/McCormick: Oxygenates Used in PM/PN Study

		Boiling Point (°C)	Vapor Pressure, 443K (kPa)	DBE
Ethanol		78	1545	0
Isobutanol		108	596	0
2,5-Dimethyl-furan		94	538	3
Anisole		154	153	4
4-Methyl-anisole		174	87.7	4
2,4-Xylenol		211	30.3	4
2-Phenyl-ethanol		220	21.5	4

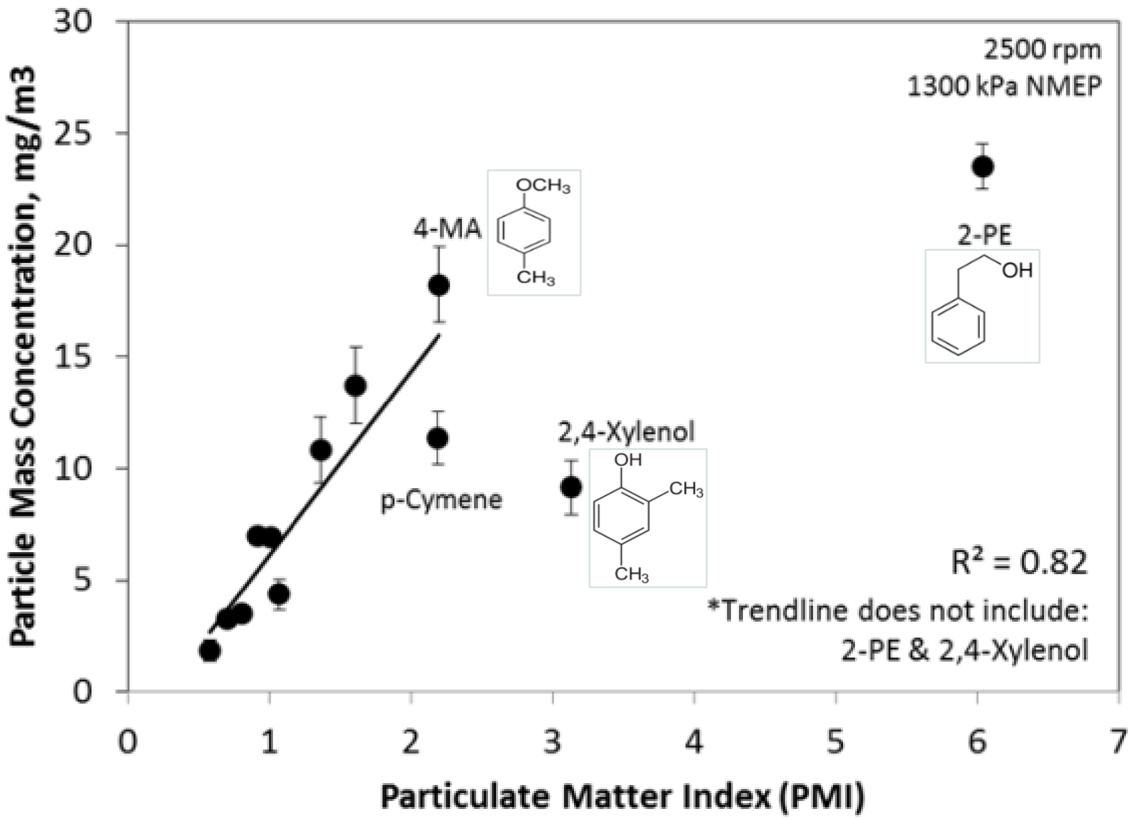
Oxygenates blended with 88 RON summertime BOB at 10 to 25 vol%. Some have large effects on D86 distillation



- **SCE**- 0.5L GDI, side-mounted injector
- **PN**- TSI Fast Mobility Particle Sizer (FMPS) w/ Dekati diluter & thermodenuder
- **PM**- AVL Micro-soot sensor and dilution system

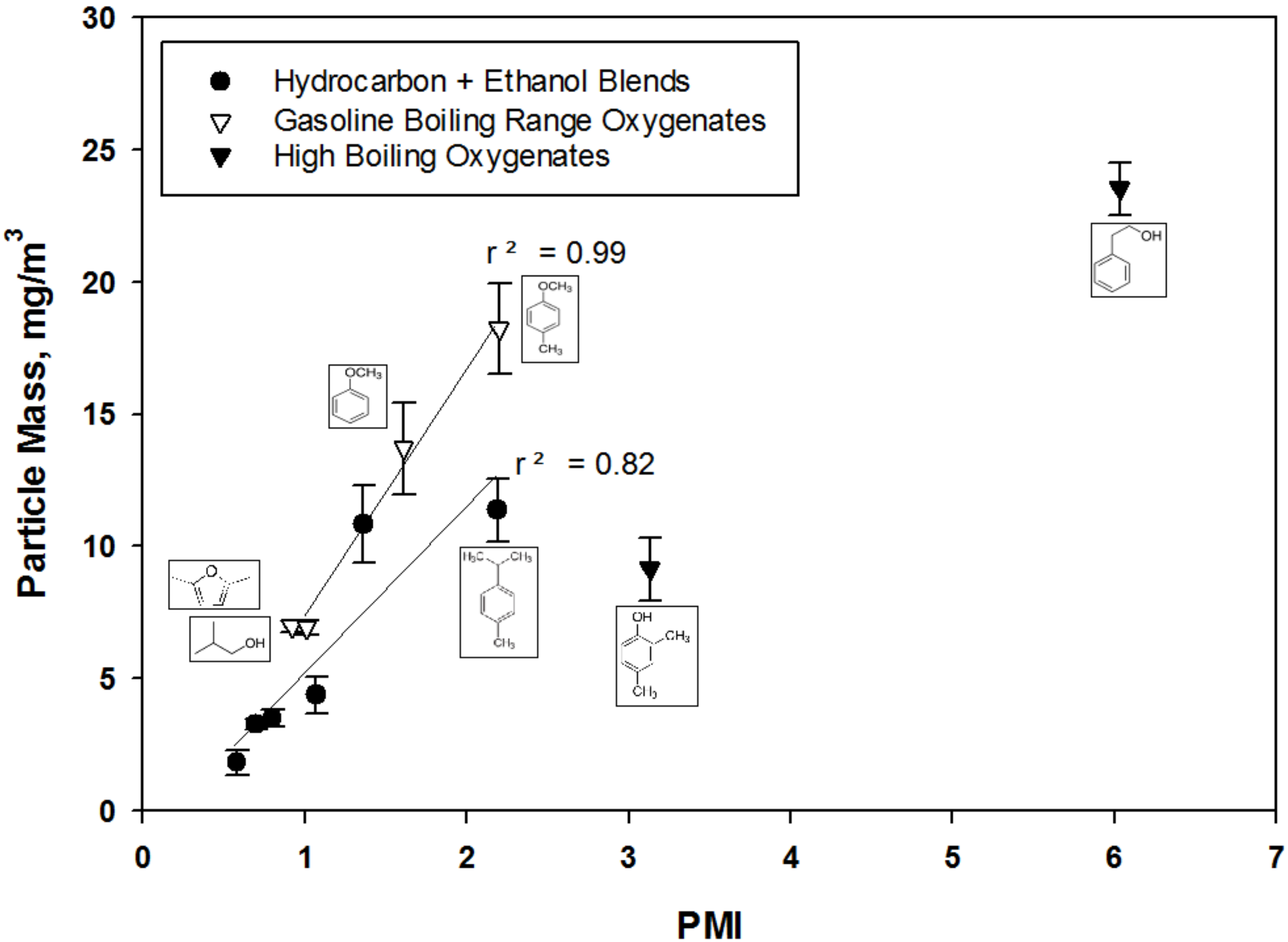
Ratcliff/McCormick:
Oxygenate Effects on GDI PM Emissions

- 2,4-Xylenol and 2-phenylethanol (2-PE) produced much lower PM than predicted – likely not evaporating and burning, instead swept into lube oil
- PMI predicts 4-methylanisole (4-MA) and p-cymene blends should produce same PM, but the results are statistically different, why?



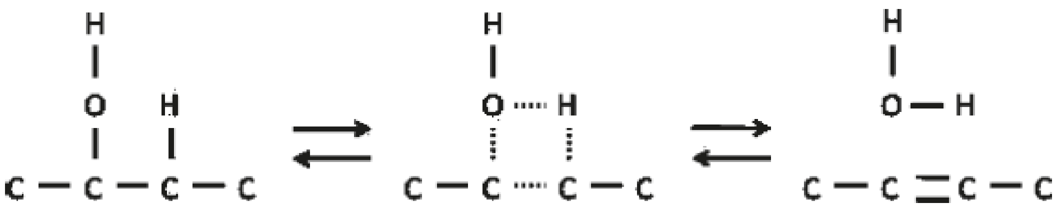
Ratcliff/McCormick: Oxygenate Effects on GDI PM Emissions 2- Alternate Data Analysis

- Separate PM vs. PMI trends for hydrocarbons + ethanol blends, from other oxygenate blends
  - Suggests oxygenate sooting chemistry not captured by PMI

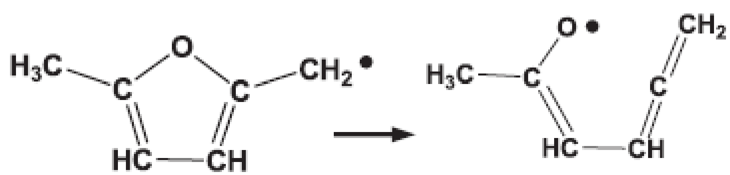


Ratcliff/McCormick: PMI does not Adequately Capture Routes from Oxygenates to Soot Formers

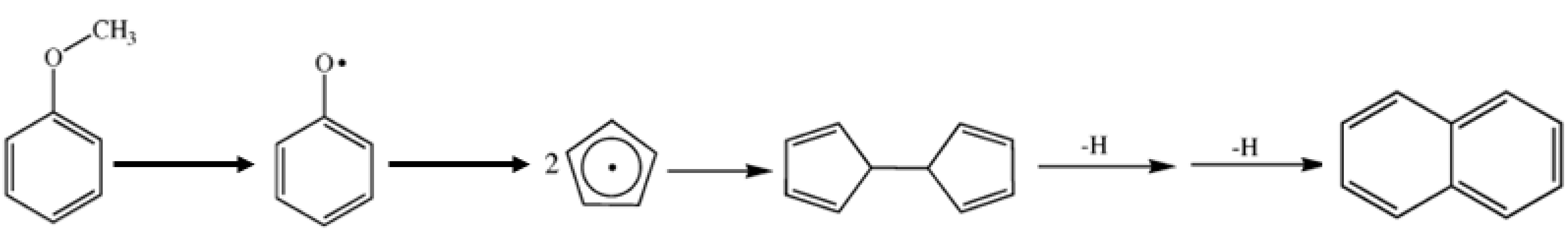
- Alcohol dehydration to alkene (McEnally and Pfefferle, *Environ Sci Technol*, 2011, 45 (6), pp 2498–2503):



- 2,5-DMF decomposition to olefinic carbonyls and radicals (Djokic, M., et al, *Proc Comb Inst,* 2013, 34 251–258):



- Anisole forms cyclopentadienyl radical which couples to naphthalene (Scheer, A., et al., *J. Phys. Chem. A* 2010, 114, 9043–9056):



Ratcliff/McCormick: Future Work

At the planning stage-

- Developing partial and full factorial experimental design fuel matrices to study the interactive effects of ethanol and other oxygenates on PM/PN emissions

- Investigating modifications to PMI, such as replacing DBE with Yield Sooting Index or Oxygen Extended Sooting Index, as well as applying a heat of vaporization factor on VP(443K)

ORNL (Storey/DeBusk) $75k: Continuing GDI PM Formation and Properties + $200k new Co-Optima fuels

Objective: Examine fuel impact on GDI particulate matter (PM) properties

Approach: Study oxidation kinetics of GDI PM loaded on particulate filter (GPF) mini-cores

– GPF PM loading: Exhaust from 2.0 L GDI engine using gasoline-alcohol blends

– GPF PM kinetics: Automated bench flow reactor equipped with a Fourier transform infrared (FTIR) spectroscopy

Major Accomplishments:

– Showed that fuel blend *and* level of GPF regeneration impact GDI PM reactivity

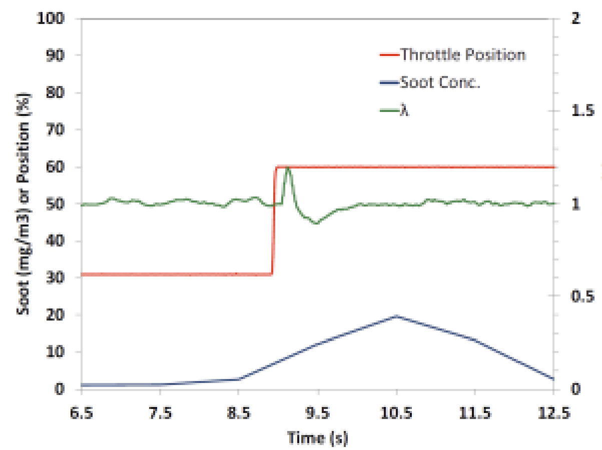
– GDI PM is different than Diesel PM

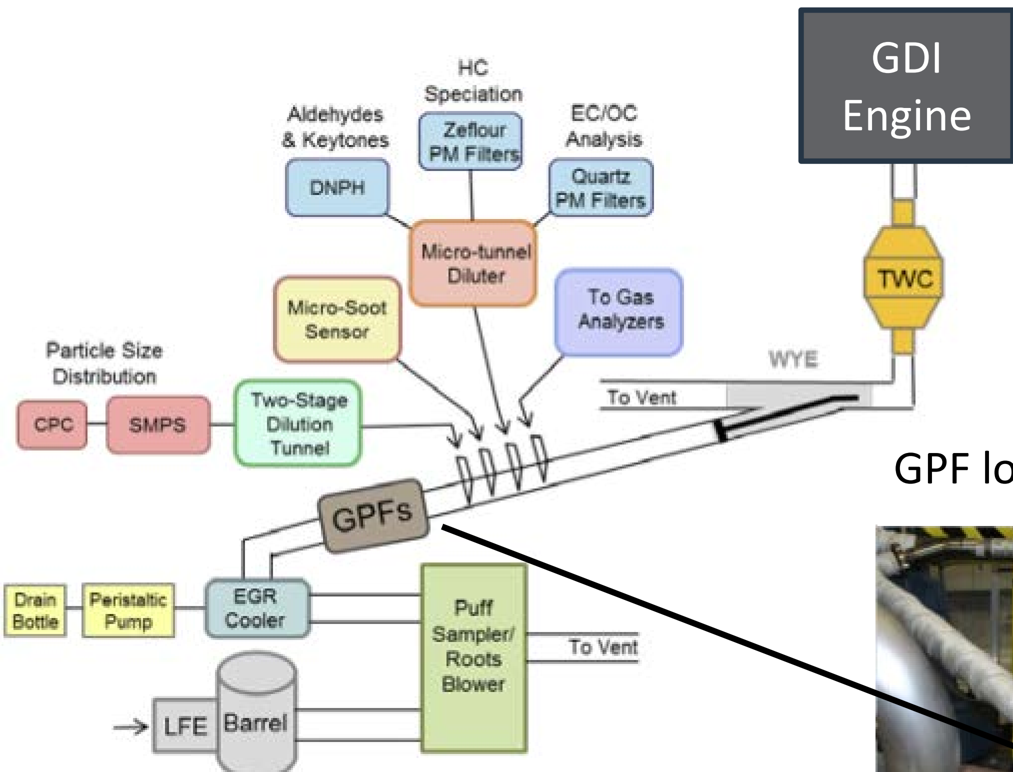
Future Directions:

1. Evaluate the impact of different PMI properties on PM emissions
   – Use a fuel matrix including Thrust 1 fuels and bio-blended fuels
   – Identify biofuel blend-stock contribution to PM formation
2. Assess the impact of Co-Optima fuel blends on PM control by Particulate Filter
   – Impact of PF loading and engine condition

Storey/DeBusk: GDI PM-Soot Cake Layer on Mini-GPFs Collected on Engine Dyno

Loaded Mini-GPFs on 2.0 L GDI engine under fuel-rich conditions
- Mimicking throttle "tip-in" point for acceleration (λ = 0.91)
- Acceleration major source of GDI PM





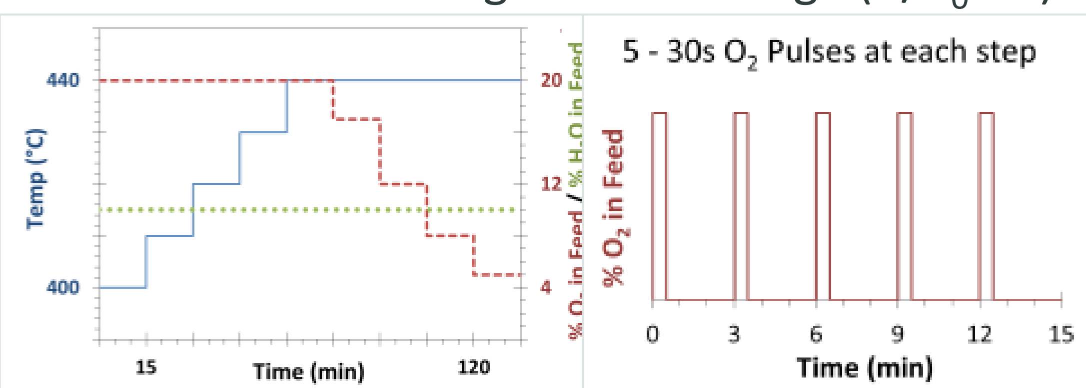
GPF location in Exhaust

Mini-GPF Holder (cores: 1" x 3")

Storey/DeBusk: Bench Flow Reactor Testing of mini-GPFs Captures Kinetics of PM-Soot cake Layer

PM-Soot Ox on mini-GPFs on Bench Flow Reactor: Control of feed gas composition & FTIR analyzer reaction product analysis

- Pulsed Ox: controlled O_2 pulses allows us to capture kinetic (reactivity) information about PM oxidation process
- Temperature Programed Desorption (TPD): Captures active surface area (SA) of PM at 200°C by chemisorption process
- Burn Out (BO) Ox: Oxidizes PM-soot cake layer down to next fractional regeneration stage (C/C_0 Ox)

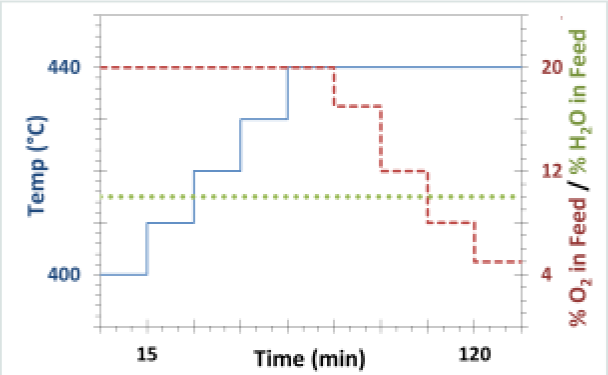


E_A Pulses (10k h^{-1})

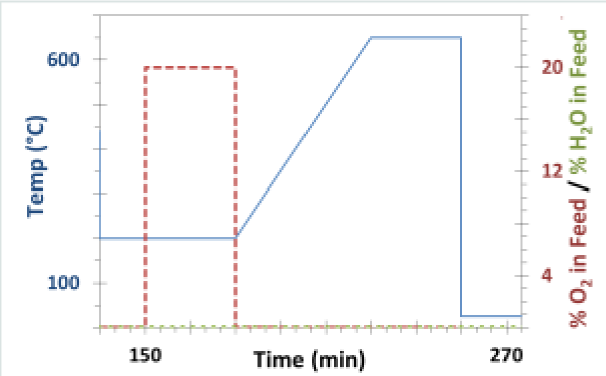
Storey/DeBusk: Bench Flow Reactor Testing of mini-GPFs Captures Kinetics of PM-Soot cake Layer

PM-Soot Ox on mini-GPFs on Bench Flow Reactor:
Control of feed gas composition & FTIR analyzer reaction product analysis

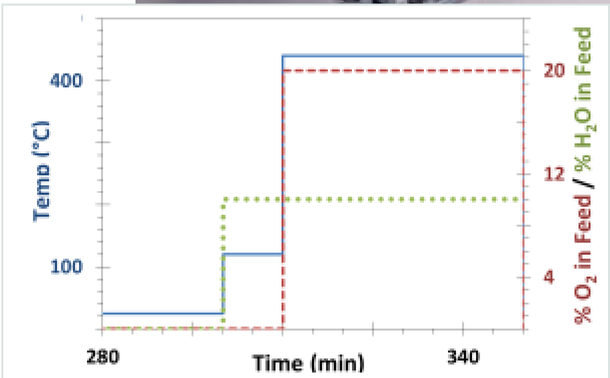
- Pulsed Ox: controlled O_2 pulses allows us to capture kinetic (reactivity) information about PM oxidation process
- Temperature Programed Desorption (TPD): Captures active surface area (SA) of PM at 200°C by chemisorption process
- Burn Out (BO) Ox: Oxidizes PM-soot cake layer down to next fractional regeneration stage (C/C_0 Ox)



E_A Pulses (10k h^{-1})



TPD Ox (4k h^{-1})



Burn Out Ox (10k h^{-1})

Storey/DeBusk: Fuel Blend Impact on GDI PM Implies Differences in Particulate Filter Regeneration

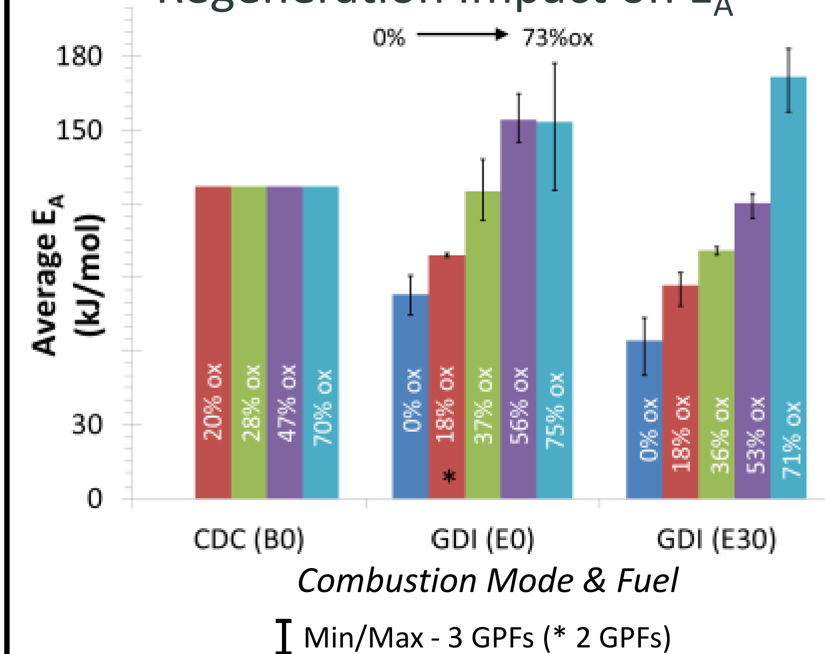
GDI PM vs. Conventional Diesel[1] (CDC) PM

Note: PM = soot + absorbed HC

Reactivity of the PM from a GDI engine changes the Activation Energy (E_A) during fractional regeneration (C/C_0 oxidation) of the soot cake layer

- E_A for E0 PM increases but plateaus near 60% oxidation (ox)
- E_A for E30 PM increases throughout with a significant increase from 60% to 80% ox
- GDI PM is easier to oxidize than CDC initially but after ~55-73% ox GDI PM is harder to oxidize than CDC

Regeneration Impact on E_A



Average Energy required for PM-Soot cake layer Ox

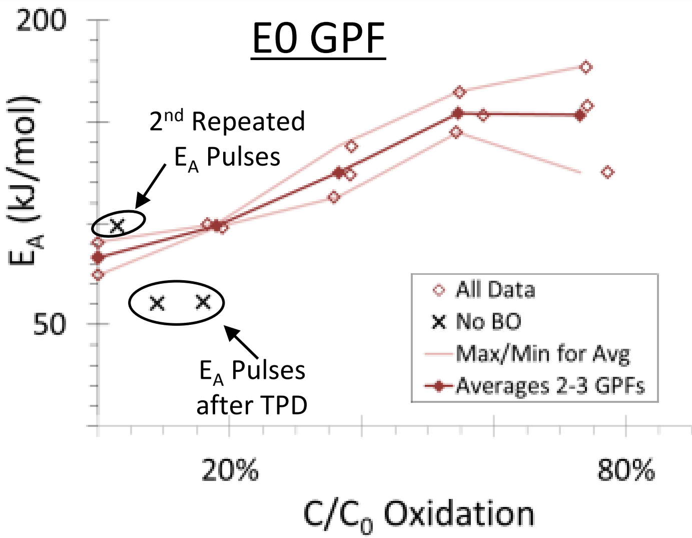
E_A @ 0% ox: CDC > E0 > E30

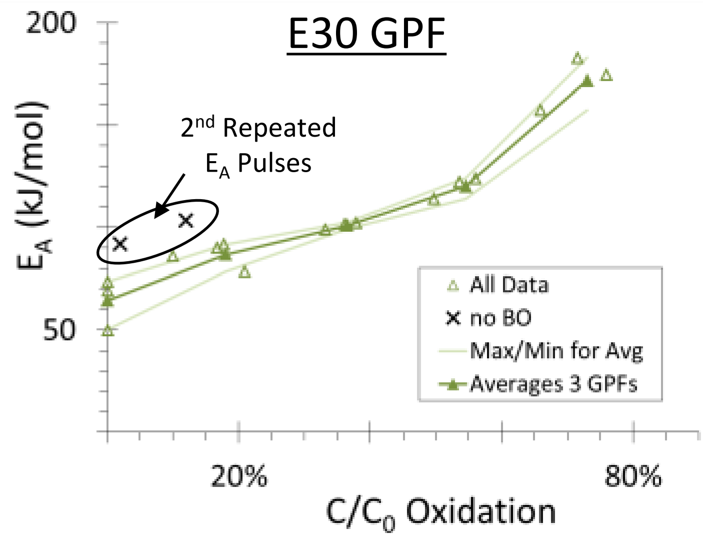
E_A @ 55% ox: E0 > E30 > CDC

E_A @ 73% ox: E30 > E0 > CDC

[1] Pihl, J.; et.al. (2013) *Top. Catal. 56:499*

Storey/DeBusk: GDI PM Environmental History Changes Reactivity of the PM-Soot Cake Layer





Typical protocol at each regeneration/oxidation stage (C/C_0 Ox)

E_A – Pulses → TPD Ox → BO Ox → E_A – Pulses → TPD Ox → BO Ox

0% ox | 20% ox

Deviation from this repetitive protocol changes the reactivity of the PM layer

E_A – Pulses → TPD Ox → E_A – Pulses

INCREASE E_A – harder to regenerate next C/C_0

E_A – Pulses → E_A – Pulses

DECREASES E_A – easier to regenerate next C/C_0

ORNL (Toops/Pihl) $425k: Continuing research on gaseous emissions control

Motivation:

- Develop an understanding of how new fuels can impact the operation of modern emissions control devices

Project focal areas:

- Characterize the impact of trace impurities in fuels
- Evaluate light-off temperature reactivity for new Co-Optima fuels and the impact on THC emissions
- Identify opportunities to co-optimize fuel, engines and emissions control via low cost emissions control

Toops/Pihl: Fuel compatibility with emissions control systems is an important consideration

- Biodiesel compatibility study has shown how a 1 ppm impurity can impact catalysts
  - Na and K displace Cu in zeolite framework
  - Results in Cu-oxide on surface of washcoat
  - Increased ash content also noted
- Emissions standards can still be met, but understanding the impact on catalyst size requirements is important
- As Co-Optima fuels are downselected, it is important understand how they will be processed and which impurities are likely
  - Na + K come from biodiesel synthesis process and are regulated by producers

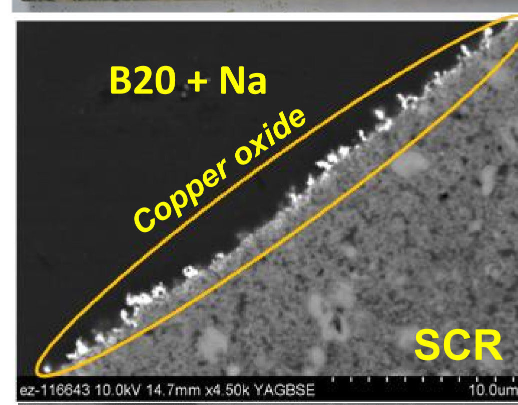
ULSD-Front

flow

Ca-Front

Na-Front

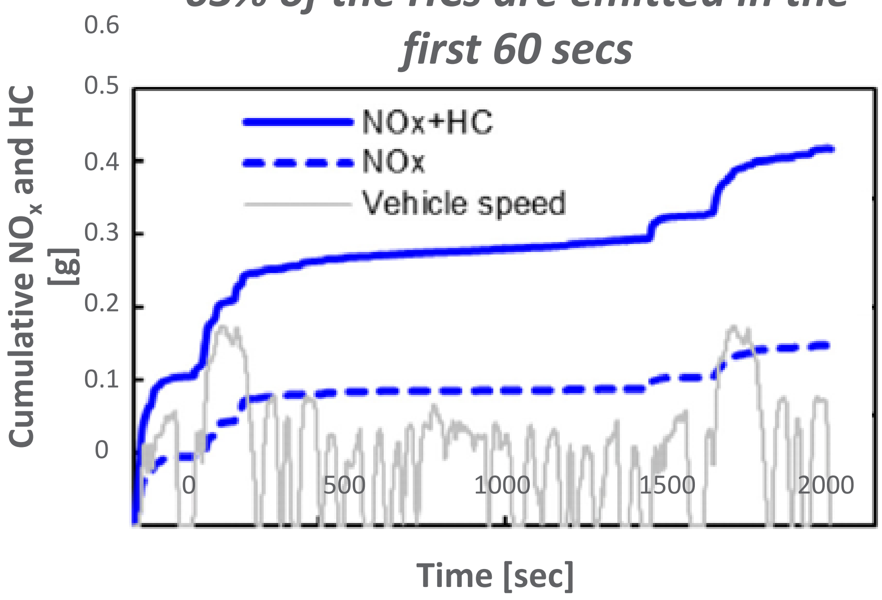
K-Front



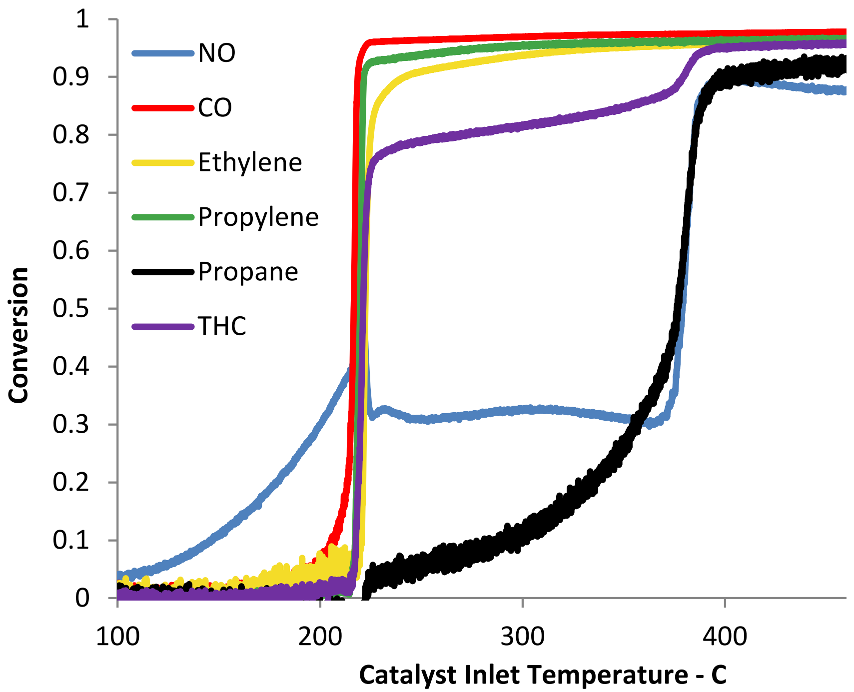
Toops/Pihl: Merit-based term for HC emissions penalty based on light-off temperature

- Current vehicles generate a large fraction of their tailpipe emissions during the first 60s of the cold start test
- Propose to develop threshold-type term to flag un-reactive fuels (e.g. T_{90}<300°C)
- Need to avoid fuels that lead to a high light-off temperature and risk not meeting HC emissions standards
- Evaluate fuels and develop a predictive tool based on functional groups and blends

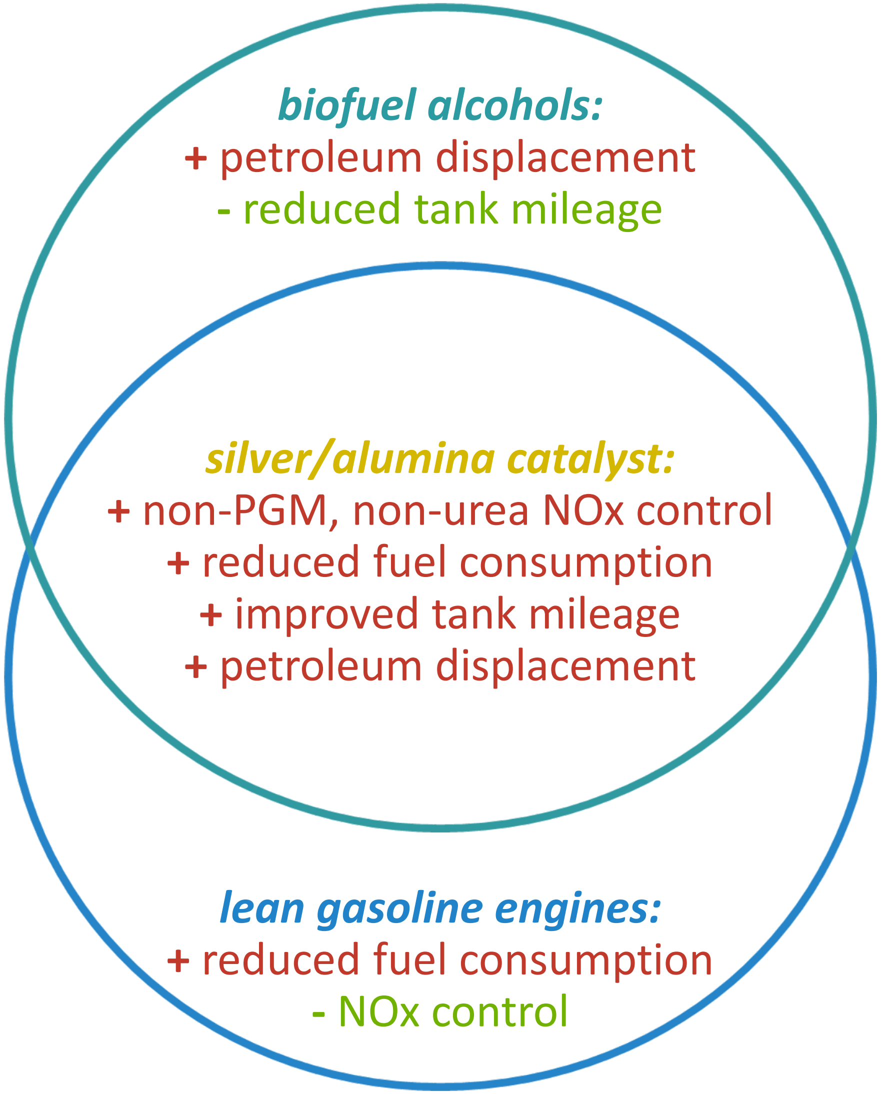
63% of the HCs are emitted in the first 60 secs



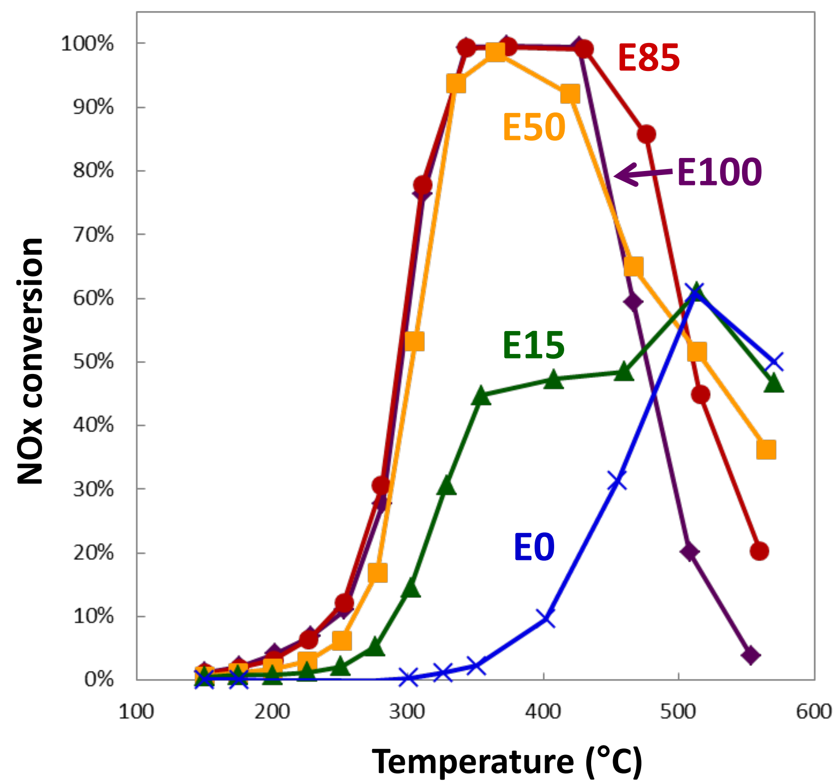
Murata, Y., Morita, T., Wada, K., Ohno, H., SAE Int. J. Fuels Lubr. 8 (2015) 454.



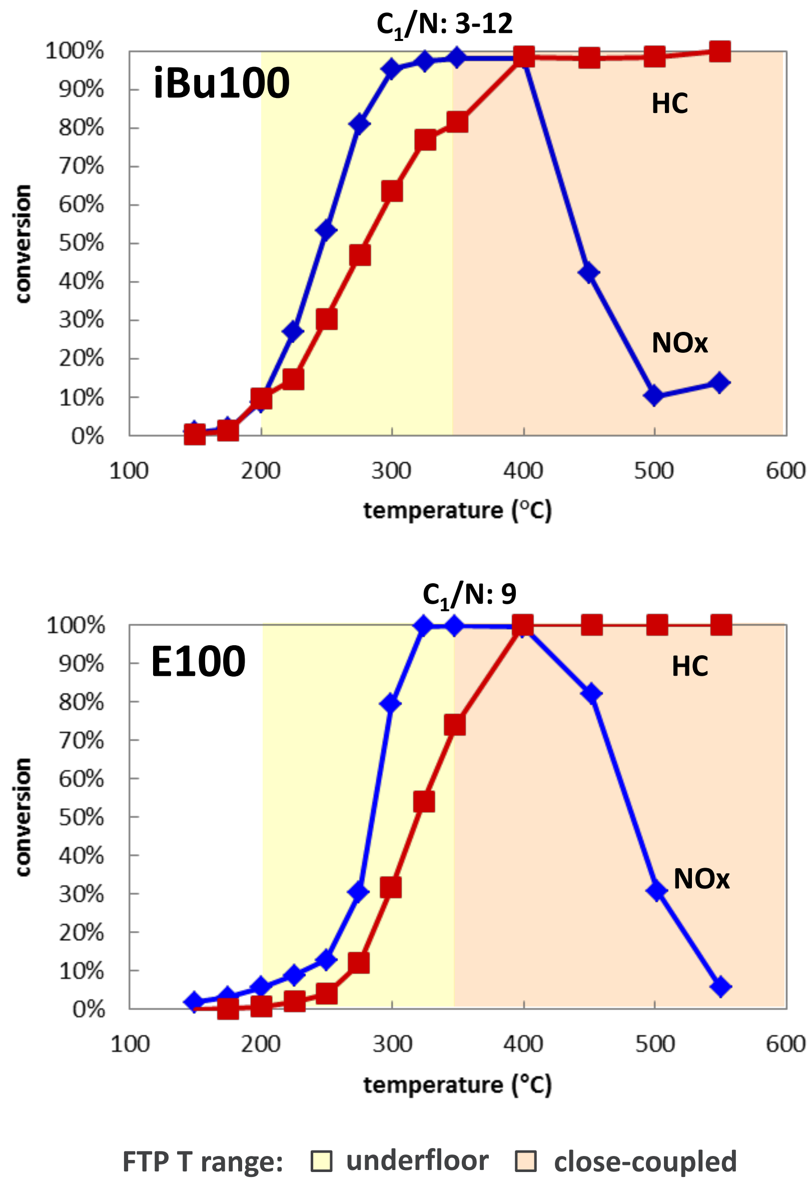
Toops/Pihl: Highlights synergy between biofuels and lean gasoline emissions control



- Ethanol/gasoline blends are active for NOx reduction over 2 wt% Ag/Al_2O_3
  - E85 better than E100
  - E50 still achieves >90% conversion
- Aldehydes may also show similar reactivity



Toops/Pihl: Isobutanol (iBu) shows similar NOx reduction performance to ethanol over Ag catalyst



- iBu100 NOx conversion similar to E100 over silver catalyst
  - > 95% conversion over ~ 100° C window
  - iBu100 performs slightly better at low temperature
  - similar HC doses required to achieve high NOx conversion
- Illustrates potential of fuels and emissions control systems working in synergy to:
  - Increase energy independence
  - Increase combustion efficiency
  - Meet stringent emissions regulations

Advanced Engine Development Team Summary: Sprays & emission control research

Relevance

- Understanding fuel effects on spray structure and on aftertreatment devices is central to the co-optimization of fuels and engines

Approach

- Individual projects are coordinated to a high degree and seek to build on the strengths of the individual laboratories

Accomplishments

- Continuing projects have shown strong technical progress in the areas of:
  - Evaluation of PMI for oxygenated fuels
  - Examining fuel and history effects on GDI PM reactivity
  - Assessing impact of fuels and impurities on performance of aftertreatment systems
- Technical work on new spray projects is progressing with new hardware design and procurement in progress or complete

Collaborations

- "Co-Optima" has 9 National Labs, stakeholder engagement, and external advisory board
- Projects presented at AEC semi-annual program review, engaged with ACEC TT
- Numerous other project-level collaborations

Future Work

- A portfolio of ongoing and future work has been described